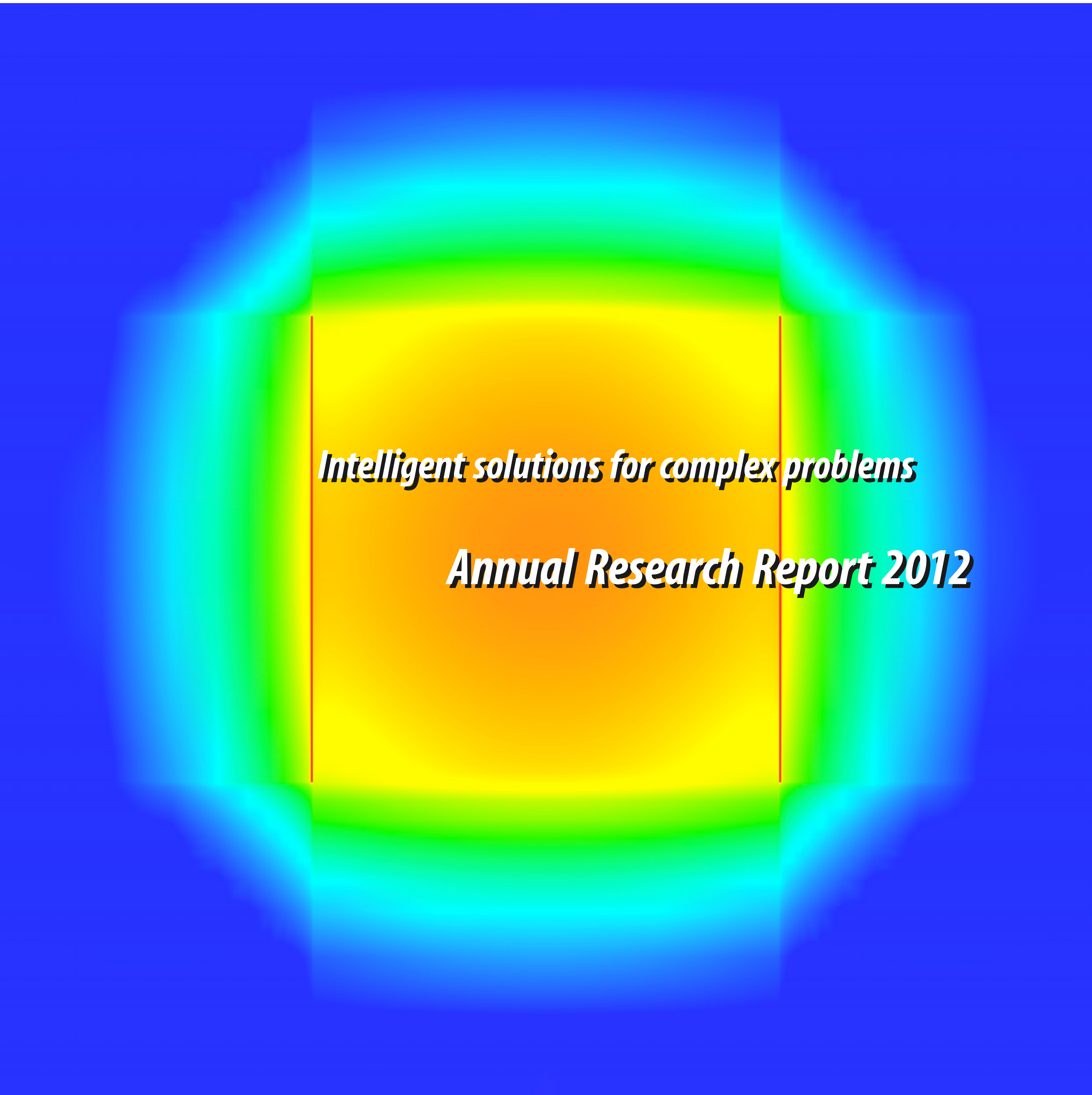
Leibniz Association

Weierstrass Institute for
Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2012

Cover figure: Simulated temperature distribution for an organic semiconductor device.
A strong temperature rise is observed along the edges.

Edited by Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
D – 10117 Berlin
Germany

ISSN 1437-7489
Berlin 2012

Fax: + 49 30 20372 303
E-Mail: contact@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

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 2012. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2012. 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

Special attention was again devoted to the proper functioning of the IMU Secretariat. The eager staff of the IMU Secretariat, headed by the WIAS Deputy Director and IMU Treasurer Prof. Dr. Alexander Mielke, continued their work, serving mathematics and mathematicians all over the world. Meanwhile, only two years after its official opening in February 2011, the IMU Secretariat at WIAS has become a well-known and well-accepted meeting point of the worldwide mathematical community, which has increased the international visibility of WIAS tremendously. In November 2012, the IMU Office Committee, whose responsibility is to monitor the performance of the IMU Secretariat and to report to the IMU Executive Committee, made its first visit to the secretariat. In a two-day workshop, the staff of the secretariat informed the Office Committee in detail about the IMU Secretariat "business".

All this is only possible through the generous financial support provided by the Federal Ministry of Education and Research (BMBF) and the Berlin Senate Department for Economy, Technology and Research; WIAS is very grateful that these two governmental institutions agreed to support the IMU Secretariat financially at equal parts.

The main scientific highlight of the year 2011, the "mega-grant" (approximately 3.4 million Euros) of the Russian government for Prof. Dr. Vladimir Spokoiny, Head of the Research Group "Stochastic Algorithms and Nonparametric Statistics", became fully operative in 2012. Prof. Spokoiny established a research team with focus on "Predictive Modelling" in the field of information technologies at the renowned Moscow Institute of Physics and Technology, which closely cooperates with his research group at WIAS.

Another highlight of 2012 was the foundation of the Leibniz Group "Mathematical Models for Lithium-ion Batteries", which resulted from the success of the Head of the Research Group "Thermodynamic Modeling and Analysis of Phase Transitions", Prof. Dr. Wolfgang Dreyer, in the competition of the Leibniz Association in the framework of the "Joint Initiative for Research and Innovation". This group will strongly influence the institute's future efforts in the field of renewable energies.

A further temporary structural change in the institute became effective in the beginning of 2012 when the Young Scientists' Group "Modeling of Damage Processes" under the leadership of Dr. Dorothee Knees and Dr. Christiane Kraus, which was founded following a recommendation of the institute's Scientific Advisory Board, took up its work.

The above group was founded as a measure of WIAS to promote women in leadership positions. The institute is committed to the implementation of the legally binding German policies and standards to achieve the goal of gender equality. A "Plan of action on gender equality for the years 2012–2015" was developed, and a contract was signed to apply for the "audit berufundfamilie" (audit job and family) seal of quality in 2013. WIAS also committed itself to implement the cascade model of the Leibniz Association and of the Joint Science Conference (GWK).

Besides these important events of the year 2012, 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
- Conversion, storage, and distribution of energy
- 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, 42 additional co-workers (+ 9 outside WIAS; Dec. 31, 2012) could be financed from grants.

Thirteen international workshops organized by WIAS evidenced the institute's reputation and its role as an attractive meeting place for international scientific exchange and cooperation. In addition, WIAS members (co-)organized numerous scientific meetings throughout the world.

In addition to these "global" activities, on the "local" scale WIAS has intensified its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. A cornerstone of this cooperation is the fact that in 2012, 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 2012 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 be 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, and Dr. Dorothee Knees are members 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 16 of its subprojects. In turn, on Dec. 31, 2012, 15 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

In the acquisition of large-scale funds, Berlin's mathematical community has scored another big success. The joint proposal of the three Berlin universities for an "Einstein Center for Mathematics (ECMath)" was positively evaluated. As a result, the ECMath will start operations in the beginning of 2013, funded by the Einstein Foundation Berlin. WIAS will be strongly involved, both scientifically and financially.

Another continuing success story for the mathematical community of Berlin is the "Berlin Mathematical School" (BMS), which was extended until 2017 in the framework of the German "Exzellenzinitiative 2012" (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. Presently, the BMS hosts about two hundred 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 2013

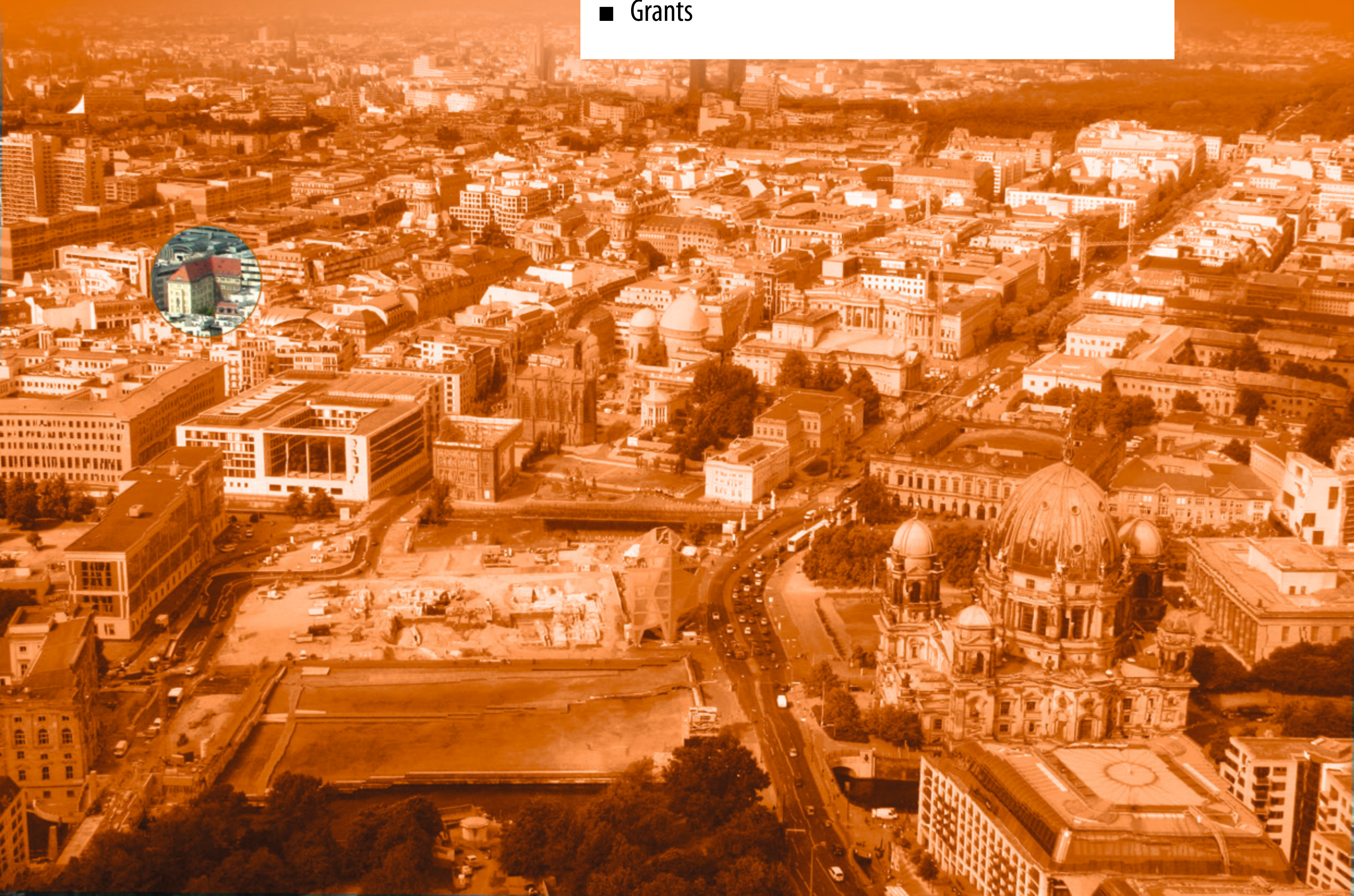
J. Sprekels

Scientific Advisory Board

Chairperson:	
Prof. Dr. B. Wohlmuth	Technische Universität München, Faculty of Mathematics Chair of Numerical Mathematics – M2 Boltzmannstrasse 3, 85748 Garching
Vice-Chairperson:	
Prof. DI. Dr. K. Kunisch	University of Graz, Institute for Mathematics and Scientific Computing Heinrichstrasse 36, 8010 Graz, Austria
Dr. St. Eichler	Freiberger Compound Materials GmbH Technical Director Am Junger-Löwe-Schacht 5, 09599 Freiberg
Prof. Dr. S. van de Geer	ETH Zurich, Seminar for Statistics, HG G 24.1 Rämistrasse 101, 8092 Zurich, Switzerland
Prof. Dr. W. Th. F. den Hollander	Leiden University, Mathematical Institute P.O. Box 9512, 2300 RA Leiden, The Netherlands
Prof. Dr.-Ing. M. Niemeyer	KHS GmbH, CEO Juchostrasse 20, 44143 Dortmund
Prof. Dr. B. Niethammer	University of Bonn, Institute for Applied Mathematics Endenicher Allee 60, 53115 Bonn
Prof. Dr. F. Otto	Max Planck Institute for Mathematics in the Sciences, Director Inselstrasse 22, 04103 Leipzig
Prof. Dr. Ch. Schwab	ETH Zurich, Seminar for Applied Mathematics ETH Zentrum, HG G58.1 Rämistrasse 101, 8092 Zurich, Switzerland

1 WIAS in 2012

- 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 2012 organized into the departments for technical services, the Secretariat of the International Mathematical Union (IMU, see pages 50, 54), the seven scientific research groups, the Young Scientists' Group, and one Leibniz group[1]:

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

The organization chart on the following page gives an overview of the organizational structure of WIAS in 2012.

1.2.2 Main Application Areas

The research at WIAS focused in 2012 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 multi-functional materials**
- **Flow and transport processes in continua**
- **Conversion, storage and distribution of energy**
- **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 promising modern technologies, for instance,

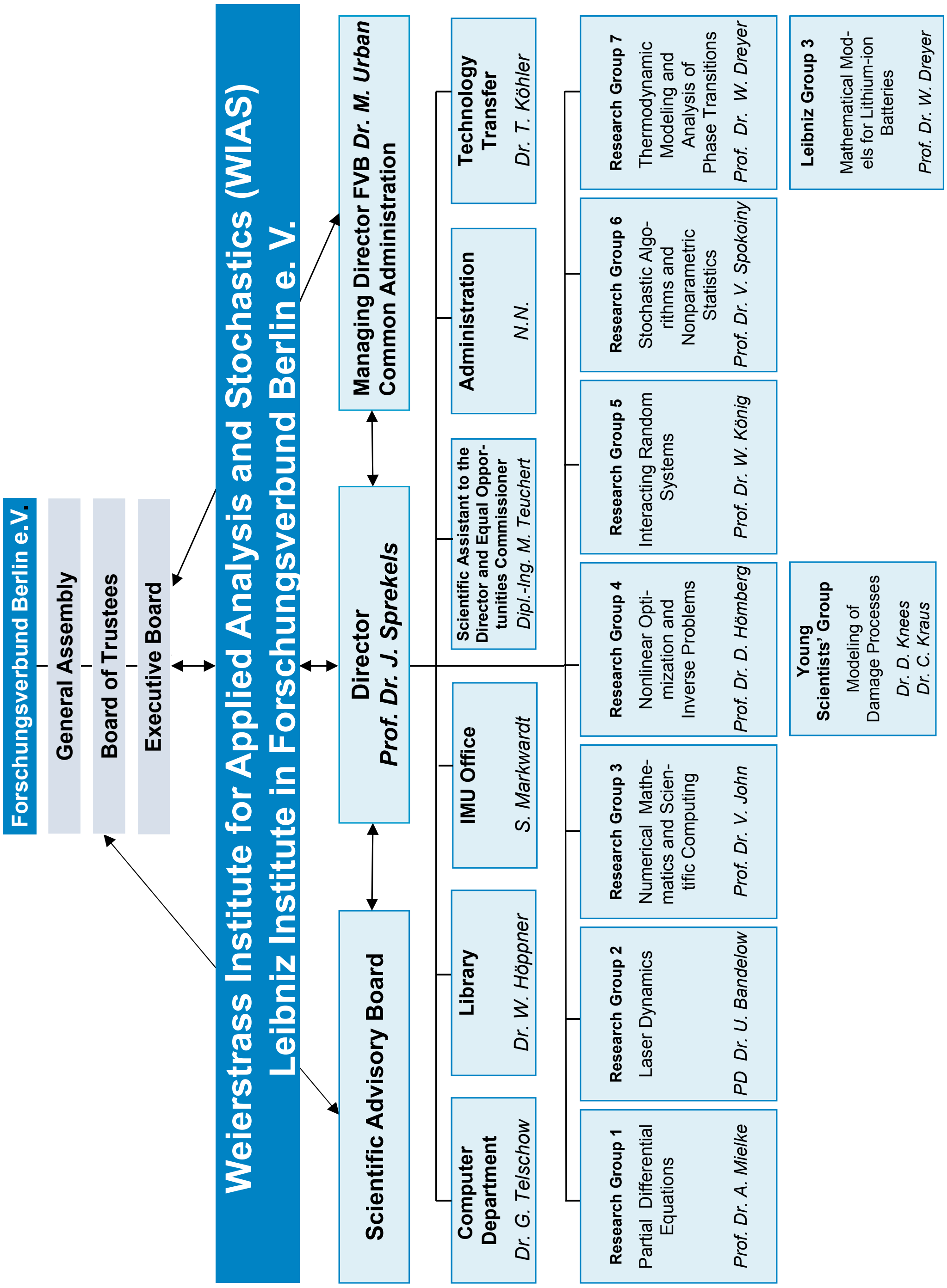
- **Optical technologies** (in particular, diffractive and laser structures, semiconductor devices, and optical fibers)
- **Energy technology** (in particular, direct methanol fuell cells, lithium batteries, hydrogen storage, photovoltaics)

1.2.3 Contributions of the Research, Young Scientists', and Leibniz Groups

The seven research groups, the Young Scientist's group, 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

[1] In the following, the terms "research group" will often be abbreviated by "RG", Young Scientists' Group by "YSG", and "Leibniz group" by "LG".

competence as prerequisite to enter new fields of applications, which necessitates a well-directed long-term *basic research in mathematics*.



The following table gives an overview of the main application areas to which the groups contributed in 2012 in the interdisciplinary solution process described above.

Main application areas	RG 1	RG 2	RG 3	RG 4	RG 5	RG 6	RG 7	YSG	LG 3
Nano- and optoelectronics	*	*	*	*	–	–	–	–	–
Optimization and control of technological processes	*	–	*	*	–	*	*	–	–
Phase transitions and multi-functional materials	*	–	–	*	*	–	*	*	*
Flow and transport processes in continua	*	–	*	–	*	–	*	*	*
Conversion, storage and distribution of energy	*	–	*	*	–	–	*	–	*
Random phenomena in nature and economy	*	–	–	*	*	*	*	–	*

In the following, special research topics are listed that were addressed in 2012 within the general framework of the main application areas. The 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)
- Mathematical 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 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 multi-functional materials

- Modeling of nonlinear phenomena and phase transitions in multi-functional materials (in RG 1, RG 7, and YSG)
- Stochastic modeling of phase transitions (in RG 5)
- Hysteresis effects (elastoplasticity, shape memory alloys, lithium batteries, hydrogen storage; 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 YSG, 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 YSG; and many-body systems, in RG 5)
- Growth of semiconductor bulk single crystals, growth of quantum dots (in RG 7)

4. Flow and transport processes in continua

- Treatment of Navier–Stokes equations (in RG 3, RG 7, LG 3, and YSG)
- Flow and mass exchange in porous media (in RG 3)
- Numerical methods for coupled electrochemical processes (fuel cells, lithium batteries, hydrogen storage, soot; in RG 1, RG 3, RG 5, RG 7, and LG 3)
- 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. Conversion, storage and distribution of energy

- Photovoltaics (in RG 1 and RG 3)
- Light-emitting diodes based on organic semiconductors (OLEDs; in RG 1 and RG 3)
- Modeling of experimental electrochemical cells for the investigation of catalytic reaction kinetics (in RG 3)

- Lithium-ion batteries (in RG 7 and LG 3)
- Modeling and analysis of coupled electrochemical processes (fuel cells, lithium batteries, hydrogen storage, soot; in RG 1, RG 3, RG 5, RG 7, and LG 3)

6. 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)
- Connectivity problems in large telecommunication networks (in RG 5)
- Material models with stochastic coefficients (in RG 4, RG 5, and RG 7)

1.3 Grants

The raising of grants under scientific competition is one of the main indicators of scientific excellence and thus plays an important role in the efforts of WIAS. In this task, WIAS has been very successful in 2012, having raised a total of 2.6 million euros, from which 42 additional researchers (+ 9 outside WIAS; Dec. 31, 2012) have been financed. In total in 2012, 22.9 per cent of the total budget of WIAS and 31.6 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].

BMBF Program *Mathematics for innovations in industry and services*

The aim of this program is to implement mathematics to make an effective contribution to face some of the societal challenges identified in the High-Tech Strategy of the Federal Government. Coordinated by WIAS in the subproject „Modeling, simulation and optimization of multifrequency induction hardening“, four scientific and two industrial partners investigate topics such as control of time-dependent Maxwell’s equations, model reduction, and the influence of uncertain data to further the development of a promising new heat treatment technology.

MeFreSim

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

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 2012, WIAS dedicated considerable financial and personal resources to the Center: Its deputy director, Prof. A. Mielke (RG 1), and Dr. D. Knees (YSG) were members 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 16 of its subprojects. In turn, on Dec. 31, 2012, 15 scientists and several student assistants at WIAS were funded by MATHEON.

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.

Research Training Group 1845 *Stochastic Analysis with Applications in Biology, Finance and Physics* of the DFG

Another big success of Berlin/Potsdam’s probabilists was the approval of a new DFG graduate college, which is located at Humboldt-Universität zu Berlin and took up its activities in October 2012. RG 5 contributes to this college, which is a certified unit of the Berlin Mathematical School.

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 subprojects: “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 subprojects “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).

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 subproject 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 subproject „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 subproject “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 subproject “Dynamics of viscous multi-layer systems with free boundaries” (RG 7).

DFG Priority Program SPP 1590 *Probabilistic Structures in Evolution*

This interdisciplinary nationwide priority program aims at the development of new mathematical methods for the study and understanding of an innovative evolution biology. WIAS participates for the first funding period (2012–2015, principal investigator: Prof. Dr. W. König) with the subproject "Branching random walks in random environment" (in RG 5).

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, supported international workshops in Warwick and Berlin in 2012. 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 subproject "Regularizations and relaxations of time-continuous problems in plasticity" (RG 1; second funding period: until August 2013).

DFG Research Unit 1735 *Structural Inference in Statistics: Adaptation and Efficiency*

Complex data is often modeled using some structural assumptions. Structure adaptive methods attempt to recover this structure from the data and to use for estimation. The research group at WIAS is studying the convergence and efficiency of such algorithms (RG 6; first funding period: April 1, 2012 – March 31, 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 YSG 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 optoelectronics. The methods include variational techniques, gradient structures, Gamma convergence, and nonlinear PDE tools.

2 Scientific Highlights

- Recent Progress in Elastic Wave Scattering
- Optimization of Terahertz Radiation from Gaseous Plasmas Created by Ultra-intense Optical Fields
- Probabilistic Methods for Mobile Ad-hoc Networks
- Representation of Hysteresis Operators Acting on Vector-valued Monotaffine Functions
- Self-heating, Hysteresis, and Thermal Switching of Organic Semiconductors

2.1 Recent Progress in Elastic Wave Scattering

Johannes Elschner and Guanghui Hu

Elastic waves possess some remarkable properties that explain their important role in the processing of electronic signals and the sensing of physical quantities. For example, they can be generated by localized or distributed sources, they can propagate in the core or on the surface of optically transparent or opaque solids, they have velocities one hundred thousand times smaller than those of electromagnetic waves, and they can modify the characteristics of a light beam. Elastic wave phenomena become ever more important in telecommunications (signal processing), medicine (echography), metallurgy (nondestructive testing), and other fields. For example, millions of wave filters are currently produced each month for mobile phones.

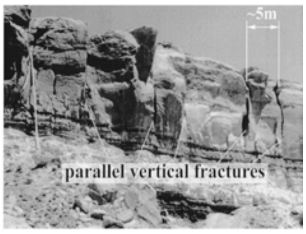


Fig. 1: *Vertical fractures in sandstone (taken from [6])*

Many applications in geophysics, nondestructive testing, and seismology can be efficiently modeled by the propagation of time-harmonic elastic waves in periodic structures (diffraction gratings). In the simplest case, a *diffraction grating* consists of a periodic interface separating two regions filled with different materials. For instance, identifying fractures in sedimentary rocks can have significant impact on the production of underground gas and liquids by employing controlled explosions. The rock under consideration can be regarded as a homogeneous transversely isotropic elastic medium with periodic vertical fractures that can be extended to infinity in one of the horizontal directions (see Figure 1). Using an elastic plane wave as an incoming source, we thus get an *inverse problem of shape identification* from the knowledge of near-field data measured above the periodic structure (see Figure 2).

Analogous inverse problems arise from using transient elastic waves to measure the elastic properties or to detect flaws and cracks in concrete structures. As an example, we mention the nondestructive elastic wave test of foundation slabs in office buildings put under the ground water level. Moreover, the problem of elastic pulse transmission and reflection through the earth is fundamental to both the investigation of earthquakes and the utility of seismic waves in search for oil and ore bodies.

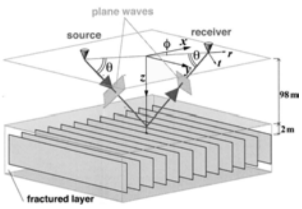


Fig. 2: *Identifying periodic fractures using incident sources and receivers (taken from [6])*

The mathematical investigation of the scattering of time-harmonic elastic waves by unbounded surfaces and interfaces in the case of periodic structures as well as in the nonperiodic case (*rough surfaces*) leads to direct and inverse boundary value problems for the Navier equation in unbounded domains, the analytical and numerical treatment of which is challenging. Compared to acoustic and electromagnetic scattering, elastic scattering problems are more complicated because of the coexistence of *compressional waves* (sometimes called *longitudinal* or *dilatational*) and *shear waves* (sometimes called *transverse* or *distortional*) that propagate at different speeds. These waves are coupled at interfaces where boundary or transmission conditions depending on the elastic medium are imposed.

The research at WIAS on this topic was performed in the framework of a project funded by the German Research Foundation that aimed at a thorough theoretical understanding of these elastic scattering problems. One objective of the project was to develop a new solvability theory (existence and uniqueness of solutions) for the direct scattering problems based on variational formulations. In this respect, diffractive structures with nonsmooth interfaces and several elastic materials are of particular interest. A second aim of the project was concerned with uniqueness results and reconstruction methods for the inverse problem of determining the scattering objects by near- and far-field measurements of the scattered elastic fields. To keep this presentation short, we will give a summary of our results in the case of two-dimensional elastic diffraction gratings.

Elastic scattering by diffraction gratings

Consider a periodic surface that is invariant in x_3 direction, and its cross-section in the (x_1, x_2) plane is given by a curve Λ, which is 2π-periodic in x_1. We suppose further that all elastic waves propagate perpendicular to the x_3 axis so that the problem can be treated as a problem of plane elasticity. The unbounded region Ω_Λ above the grating profile Λ is filled with a homogeneous and isotropic elastic material with the Lamé constants λ, μ and the mass density ρ. Assume that a time-harmonic plane elastic wave with the incident angle $\theta \in (-\pi/2, \pi/2)$ is incident on Λ from the top. The incident wave is either an incident pressure wave or shear wave,

$$u^{in}(x) = \hat{\theta} \exp(ik_p x \cdot \hat{\theta}), \quad u^{in}(x) = \hat{\theta}^\perp \exp(ik_s x \cdot \hat{\theta}), \quad x = (x_1, x_2),$$

where $\hat{\theta} := (\sin\theta, -\cos\theta)$, $\hat{\theta}^\perp := (\cos\theta, \sin\theta)$, $k_p := \omega\sqrt{\rho/(2\mu+\lambda)}$ and $k_s := \omega\sqrt{\rho/\mu}$ are the compressional and shear wavenumbers, respectively, and $\omega > 0$ denotes the angular frequency of the harmonic motion. Then the total displacement u, which can be decomposed as the sum of the incident field u^{in} and the scattered field u^{sc}, satisfies the Navier equation (or system)

$$(\Delta^* + \omega^2)u = 0 \quad \text{in} \quad \Omega_\Lambda, \quad \Delta^* := \mu\Delta + (\lambda+\mu)\,\text{grad div}\,. \tag{1}$$

In the case of a rigid boundary Λ, (1) has to be combined with the *first-kind* (or Dirichlet) boundary condition $u = 0$ on Λ, whereas for a stress-free boundary the stress vector Tu has to vanish on Λ (the *second-kind* or Neumann condition). If both the normal displacement and the tangential stress (respectively, the tangential displacement and normal stress) are zero on Λ, we speak of the *third-* and *fourth-kind* boundary conditions. The periodicity of Λ together with the form of u^{in} implies that the total field u is α-quasi-periodic, i.e., $u(x_1 + 2\pi, x_2) = \exp(2i\alpha\pi)u(x_1, x_2)$, where α corresponds to the quasi-periodicity of the incoming wave. For physical reasons, the field must be bounded in x_2 direction. Therefore, above the grating region, the scattered field can be represented as a series of outgoing plane pressure and shear waves:

$$u^{sc}(x) = \sum_{n\in\mathbb{Z}} \left\{A_{p,n}(\alpha_n, \beta_n)\exp(i\alpha_n x_1 + i\beta_n x_2) + A_{s,n}(\gamma_n, -\alpha_n)\exp(i\alpha_n x_1 + i\gamma_n x_2)\right\}, \tag{2}$$

where $\alpha_n := \alpha + n$, $\beta_n := \sqrt{k_p^2 - \alpha_n^2}$, and the square root is chosen such that its imaginary part is positive. The numbers γ_n are defined analogously with k_p replaced by k_s. The constants $A_{p,n}$, $A_{s,n}$ are called the *Rayleigh coefficients*, and they are needed to compute the energy and the phase shift of the outgoing plane waves. Note that only a finite number of plane waves in (2) propagate into the far field, with the remaining *evanescent waves* (or surface waves) decaying exponentially as $x_2 \to +\infty$. Now our direct diffraction problem can be formulated as the following boundary value problem.

(DP): Given a grating profile curve $\Lambda \subset \mathbb{R}^2$ (which is 2π-periodic in x_1) and an incident field u^{in} with the incidence angle θ, find an α-quasi-periodic vector function $u = u(x;\theta) = u^{in} + u^{sc}$ that satisfies the Navier equation (1) in Ω_Λ, one of the above-mentioned boundary conditions, and the Rayleigh expansion (2).

Let $u(x;\theta_j)$ denote solutions to (DP) corresponding to N incident pressure or shear waves u^{in} with distinct incident angles $\theta_j \in (-\frac{\pi}{2}, \frac{\pi}{2})$ $(j = 1, 2, \cdots, N)$. The inverse problem, which involves near-field measurements $u(x_1, b)$ on some line $x_2 = b$ above the grating structure, can be formulated as follows.

(IP): Given N incident angles θ_j, determine the grating profile Λ from the knowledge of the near-field data $u(x_1, b; \theta_j)$ for all $x_1 \in (0, 2\pi)$, $j = 1, 2, \cdots, N$.

Solvability results for direct scattering problems

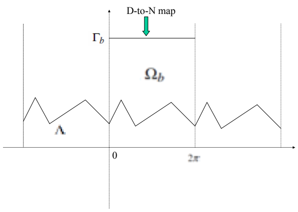


Fig. 3: *Variational formulation posed in a periodic cell*

To prove existence and uniqueness results for rather general periodic diffractive structures, we developed a variational formulation of the boundary value problem (DP), which is posed in a bounded periodic cell in $\mathbb{R}^2$ and is enforcing the radiation condition (2). Introduce an artificial boundary $\Gamma_b := \{(x_1, b) : 0 \le x_1 \le 2\pi\}$ and the bounded domain Ω_b, lying between the segment Γ_b and one period of the grating profile Λ; see Figure 3. Let V_α denote the energy space of α-quasi-periodic functions on Ω_b that corresponds to the boundary condition used. By the first Betti formula, the problem (DP) is then equivalent to the variational problem of finding $u \in V_\alpha$ such that

$$\int_{\Omega_b} \left(a(u,\overline{\varphi}) - \omega^2 u\cdot\overline{\varphi}\right) dx - \int_{\Gamma_b} \overline{\varphi}\cdot \mathcal{T}u\, ds = \int_{\Gamma_b} (\mathcal{T}u^{in} - \mathcal{T}u^{in})\cdot\overline{\varphi}\, ds\,, \quad \forall\, \varphi\in V_\alpha\,, \qquad (3)$$

where $\mathcal{T}$ denotes the Dirichlet-to-Neumann (DtN) map on the artificial boundary, and the bilinear form a corresponds to the usual elastic energy. Relation (3) extends well-known variational formulations for the quasi-periodic Helmholtz equation, but in contrast to acoustic scattering, the DtN map in (3) is not coercive. Nevertheless, it is possible to prove strong ellipticity of the variational problem, and combining this with the Fredholm alternative leads to the following solvability results.

Theorem. *If the grating profile Λ is a Lipschitz curve, then there always exists a solution of (DP) under the boundary conditions of the first, second, third, or fourth kind. The solution is unique for small frequencies and for all frequencies excluding a discrete set with the only accumulation point at infinity. Moreover, if Λ is the graph of a Lipschitz function, then for any frequency $\omega > 0$ there exists a unique solution of (DP) under the Dirichlet boundary condition.*

These solvability results have been extended to the practically important cases of biperiodic elastic diffraction gratings and transmission problems in 3D where regions of different elastic materials are separated by periodic interfaces [3]. The uniqueness to (DP) at arbitrary frequency is not true in general under the second-, third-, and fourth-kind boundary conditions, and non-uniqueness examples can even be constructed for a flat interface. On the other hand, uniqueness results for all frequencies can be proved again if mixed Dirichlet and Robin boundary conditions are imposed.

Recently, we developed a novel variational approach for the elastic scattering by unbounded rough surfaces, leading to existence and uniqueness results for the Dirichlet problem at arbitrary frequency [5]. In this case, it is not possible to reduce the problem to a bounded periodic cell, and the proof relies heavily on new a priori estimates for the Navier equation in unbounded domains. The variational formulation is also the basis for the finite element solution of direct elastic scattering problems, which will be a topic of future research. Integral equation methods offer an attractive alternative for solving diffraction grating problems, and we refer to [4] for first results in the case of elastic scattering.

Inverse elastic scattering problems

Inverse wave scattering problems are highly nonlinear, since the measured near- or far-field data do not depend linearly on the shape of the scatterer. They are also severely ill-posed, which is more serious from the viewpoint of numerical computations. Therefore, unless regularization methods are used, small perturbations of the measured data can lead to large errors in the reconstruction of the scatterer. We refer to the monograph [1] for the much-studied case of inverse acoustic and electromagnetic scattering by bounded obstacles. Conventionally, such inverse problems are solved by an iterative approach based on Newton's method, which requires the solution of direct scattering problems for each iteration step. An alternative method that improves the numerical performance is to formulate the problem as a nonlinear optimization problem, which is then discretized and solved by standard iterative schemes for nonlinear least-squares problems, e.g., by the Gauss–Newton or Levenberg–Marquardt methods.

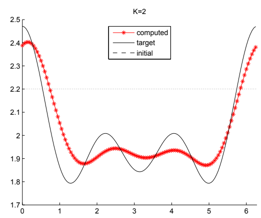


Fig. 4: *Reconstruction from part of far-field data*

To solve our inverse problem (IP) of recovering the profile of a two-dimensional elastic diffraction grating from far- and near-field data, we followed an approach first developed by Kirsch and Kress for acoustic obstacle scattering (see [1]). In this method, we assume the a priori information that the unknown profile Λ is given by the graph of a 2π -periodic function f lying between the horizontal lines $x_2 = 0$ and $x_2 = b$ for some $b > 0$. The first step is to reconstruct the scattered field u^{sc} above Λ from its values on the line $x_2 = b$ above the grating. We represent u^{sc} as an elastic single-layer potential with kernel Π and an unknown density φ (defined on $x_2 = 0$) and then solve the first-kind integral equation

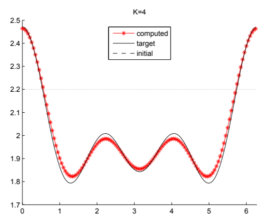


Fig. 5: *Reconstruction from far-field data*

$$\frac{1}{2\pi}\int_0^{2\pi} \Pi(x_1, b; t, 0)\,\varphi(t)\,dt = u^{sc}(x_1, b), \qquad x_1 \in (0, 2\pi).$$

This step is the linear severely ill-posed part and requires Tikhonov regularization involving the singular value decomposition of the integral operator. For simplicity, we only consider the inverse problem (IP) with one incident plane wave ($N = 1$) under the first-kind boundary condition $u = u^{in} + u^{sc} = 0$ on Λ. Then the second step, which is nonlinear, but well posed, is to determine the profile function f by minimizing the defect

$$u^{in}(x_1, f(x_1)) + \frac{1}{2\pi}\int_0^{2\pi} \Pi(x_1, f(x_1); t, 0)\,\varphi(t)\,dt$$

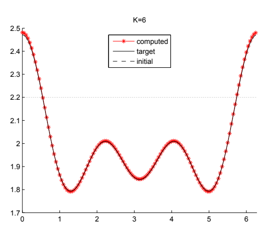


Fig. 6: *Reconstruction from far-field and six evanescent modes*

in the L^2 norm on the interval $(0, 2\pi)$ over an admissible set of profile functions. We discretized the objective functional by the trapezoidal rule and solved the resulting minimization problem in a finite-dimensional space.

The two-step algorithm is easily implemented, and satisfactory reconstructions can be obtained with a low computational effort for suitable initial values of grating parameters. This is mainly because the singular value decomposition of the derived first-kind integral equation can be readily achieved, and only the unknown grating profile function needs to be determined in the second step. Moreover, no direct scattering problems need to be solved in the process of the inversion algorithm. Figures 4–6 illustrate the reconstruction results for a smooth grating, depending on the number of propagating and evanescent modes used for the far- and near-field data. The reconstruction scheme can also be applied to piecewise linear grating profiles with a finite number of corners, and it can be readily adapted to the case of several incident angles and/or a finite number of incident frequencies [4]. However, the convergence of the two-step algorithm is still open.

We finally discuss the uniqueness in our inverse problem (IP), i.e., the question whether the near-field data for a finite number of incident waves completely determine an unknown grating profile without further a priori information. In contrast to the widespread belief in the uniqueness in bounded-obstacle scattering problems with only one incident plane wave, we cannot expect the same global uniqueness in wave diffraction by periodic structures. Moreover, in general it is difficult to characterize the exceptional grating profiles that cannot be identified by one incident plane wave. However, for polygonal grating profiles, this characterization is possible, and global uniqueness by finitely many incident waves has been proved for the inverse scattering of time-harmonic electromagnetic waves. These results are essentially based on reflection principles for the Helmholtz and Maxwell equations.

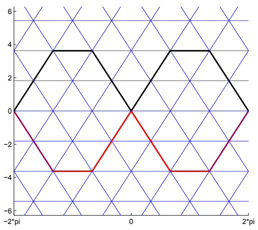


Fig. 7: *Unidentifiable profiles under 3rd-kind boundary conditions*

Using a new reflection principle for the Navier equation, we were able to prove corresponding uniqueness results for polygonal elastic diffraction gratings under third- or fourth-kind boundary conditions [2]. It turns out that the uniqueness with one incident pressure or shear wave holds, except for a few symmetric configurations of piecewise linear profiles that can be completely described; see, e.g., Figures 7 and 8, where all profiles lying on the triangular and rectangular grids, respectively, may generate the same scattered field. The results can be extended to the case of biperiodic gratings in 3D, and all unidentifiable polyhedral grating profiles that correspond to only one given incident elastic field can be classified again. As one would expect, the derivation of the unidentifiable classes in 3D is more complicated than in 2D, since one must take into account biperiodic structures that vary in both x_1 and x_2 and where the incident wave is not perpendicular to the x_3 axis. There seems to be no reflection principle for the Navier equation under the classical Dirichlet or Neumann conditions, and it is a challenging open problem to extend the uniqueness results to these boundary conditions.

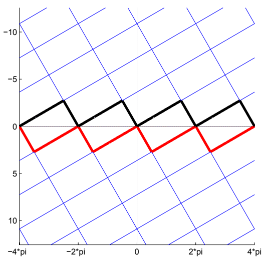


Fig. 8: *Unidentifiable profiles under 4th-kind boundary conditions*

References

[1] D. Colton, R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, 3rd edn., Springer, Berlin, 2012.

[2] J. Elschner, G. Hu, *Inverse scattering of elastic waves by periodic structures: Uniqueness under the third or fourth kind boundary conditions*, Methods Appl. Anal., **18** (2011), pp. 215–244.

[3] ———, *Scattering of plane elastic waves by three-dimensional diffraction gratings*, Math. Models Methods Appl. Sci., **22** (2012), pp. 1150019/1–1150019/34.

[4] ———, *An optimization method in inverse elastic scattering for one-dimensional grating profiles*, Commun. Comput. Phys., **12** (2012), pp. 1434–1460.

[5] ———, *Elastic scattering by unbounded rough surfaces*, SIAM. J. Math. Anal., **44** (2012), pp. 4101–4127.

[6] S. Nakagawa, K.T. Nihei, L.R. Myer, E.L. Majer, *Three-dimensional elastic wave scattering by a layer containing vertical periodic fractures*, J. Acoust. Soc. Am., **113** (2003), pp. 3012–3023.

2.2 Optimization of Terahertz Radiation from Gaseous Plasmas Created by Ultra-intense Optical Fields

Ihar Babushkin

Introduction

Ultrashort pulses in the terahertz (THz) range, that is, in the range from approximately 0.1 to approximately 30 THz, are extremely important for various time-resolved studies in molecular physics, chemistry, materials science, and security applications. However, the production of such pulses is rather difficult because this frequency interval lies beyond the accessibility of usual optical methods of frequency conversion. Recent studies gave rise to methods of frequency generation in the extremely wide frequency range from THz to X-rays, which use nonlinear processes in laser-induced plasma.

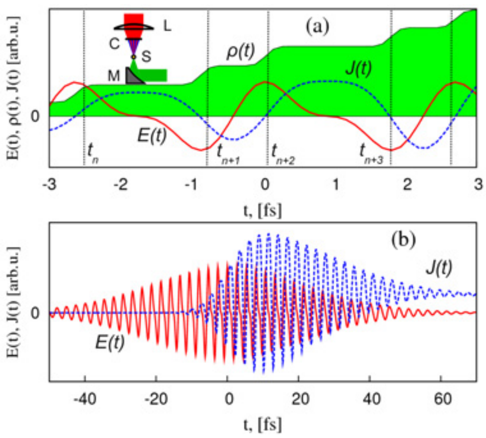


Fig. 1: *The mechanism of THz generation: (Inset) A short optical pump pulse propagates through a nonlinear crystal (C), where its second harmonic is generated, and then both are focused by a lens (L) into a gas chamber (S), where THz radiation is generated. (a) In a gas spot (S), a pump electric field $E(t)$ generates free electrons with a stepwise increase of the electron density $\rho(t)$ via tunneling photoionization. The ionization occurs mostly near the maxima of the electric field at time instances t_n. (b) The stepwise ionization yields a slow component of the plasma current J growing on the time scale of the pulse duration and, in turn, giving rise to the THz emission.*

In particular, it was found [1] that ultrashort broadband THz pulses are generated in two-color optical pulses focused in a gas cell if the pump is so strong that ionization of atoms takes place (see Figure 1). The physical mechanism of this process was attributed to ionization and subsequent dynamics of free electrons in the field. It was also shown [2, 3] that the process is related to interaction on two sufficiently different time scales: the attosecond time scale of the ionization process and the subpicosecond time scale of the pump pulse dynamics (see Figure 1). Namely, free electrons that are ejected from the atoms by the ionization process in sharp attosecond-long steps at times t_n create the net macroscopic current J, which contains low frequency components, in particular, in the THz range. It rises on the time scale of hundreds of femtoseconds and is responsible for the observed THz radiation.

Analyzing the process, we were able to show [2, 3] that the spectral shape of the THz pulses generated by this mechanism is determined by a superposition of contributions from individual ionization events t_n. This finding provides a straightforward analogy with linear diffraction theory, where the ionization events play the role of slits in a diffraction grating. This analogy offered simple explanations for recent experimental observations and opened new avenues for THz pulse shaping based on temporal control of the ionization events. In particular, to obtain a THz source with particular characteristics, we should create a certain "grating", that is, a set of t_n, by engineering the pump pulse waveform. In other words, the *nonlinear optimization problem* that we have to solve is to find the pump pulse which would give the particular set of ionization events t_n and thus the particular THz radiation.

General nonlinear model

In a realistic setup not only the THz field is generated, but also the pump field is modified due to atomic and ionization nonlinearities as it propagates through the plasma spot. We take these processes into account by using a realistic, sophisticated model describing both the light and plasma dynamics. The equation for the light field $E(x,y,z,t)$ can best be written for the partial Fourier transform: $\mathcal{F}_{x,y,t}[E(x,y,z,t)] \to E(k_x,k_y,z,\omega)$

$$\partial_z E(k_x,k_y,z,\omega) = i\sqrt{k^2(\omega) - k_x^2 - k_y^2}\,E(k_x,k_y,z,\omega) + i\frac{\mu_0\omega^2}{2k(\omega)}\mathcal{P}_{\mathrm{NL}}(k_x,k_y,z,\omega). \tag{1}$$

Here, $k = \omega n(\omega)/c$ is the wave number, c is the speed of light, $n(\omega)$ is the linear refractive index of argon, μ_0 is the vacuum permeability. The nonlinear polarization $\mathcal{P}_{\mathrm{NL}}(k_x,k_y,z,\omega) = P_{\mathrm{Kerr}}(k_x,k_y,z,\omega) + iJ(k_x,k_y,z,\omega)/\omega + iJ_{\mathrm{loss}}(k_x,k_y,z,\omega)/\omega$ accounts for third-order nonlinear polarization $P_{\mathrm{Kerr}}(x,y,z,t) \propto E(x,y,z,t)^3$, electron current $J(x,y,z,t)$, and the loss term $J_{\mathrm{loss}}(x,y,z,t) \propto W_{ST}(E(x,y,z,t))(\rho_{at} - \rho(x,y,z,t))/E(x,y,z,t)$ (see (3) for notations) due to photon absorption during ionization. The plasma current J is described by the equation:

$$\partial_t J(x,y,z,t) + \gamma J(x,y,z,t) = \frac{q^2}{m}E(x,y,z,t)\rho(x,y,z,t), \tag{2}$$

where γ is the recombination collision rate and m, q are electron mass and charge. The electron density ρ is described by the equation

$$\partial_t \rho(x,y,z,t) = W_{\mathrm{ST}}(E)[\rho_{at} - \rho(x,y,z,t)], \tag{3}$$

where ρ_{at} denotes the neutral atomic density. We use a quasi-static tunneling ionization rate for hydrogen-like atoms: $W_{\mathrm{ST}}(E) = [\alpha/|E|]\exp[-\beta/3|E|]$, where α and β are some constants. In our three-dimensional numerical code, (1), (2), and (3) are solved using a pseudo-spectral method with the fast Fourier transform to resolve the (x,y,t) dependence and the Runge–Kutta 4 scheme for proceeding in z-direction.

Local field dynamics

It was shown in [2, 3] that on a small spatial scale (which we call *local current (LC) limit*), the complicated dynamics described by (1)–(3) can be significantly simplified and reduced to an expression for the THz field $E^J(t)$ (now the spatial dependence is eliminated because we consider a single spatial point) generated by the plasma in the pre-given pump field $E(t)$, which can be written in the frequency domain as:

$$E^J(\nu) = \sum_n C_n e^{2\pi i \nu t_n} \equiv \sum_n E_n^J. \tag{4}$$

Here, $\nu = \omega/2\pi$, $C_n = q\delta\rho_n v_f(t_n)$, $v_f(t) = \frac{q}{m}\int_{-\infty}^{t} E(\tau)e^{\gamma(\tau-t)}d\tau$ is the free electron velocity, $\delta\rho_n \propto W_0 e^{-1/|E(t_n)|}$ is the electron density created in the n-th ionization event. This simple formula demonstrates that the set of t_n plays a role of "slits" in a "temporal diffraction grating", and the spectral shape of the generated THz field $E^J(\nu)$ is determined by the interference of the secondary sources created by the slits, according to the well-known Huygens–Fresnel principle.

This interference process is illustrated in Figure 2. Every contribution in the sum (4) has its own frequency dependence determined by the value of t_n. For $\nu \gg 0$ the contributions cancel each other resulting in a narrow spectral line near $\nu \approx 0$.

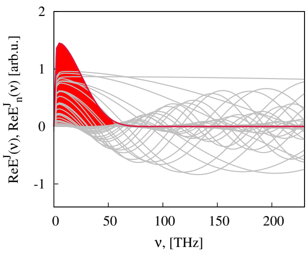


Fig. 2: *The interference of impacts* Re $E_n^J(\nu)$ *of different ionization events (gray curves) in the frequency domain* ν *leading to the resulting THz spectral line* Re $E^J(\nu)$ *(red filled curve)*

Control of THz pulses

The simple interference picture drawn in the introduction tells us that the THz radiation is a zero-order diffraction peak of a grating with slits defined by values of t_n. This fact allows a very interesting and fruitful physical insight, which provides a possibility to control the THz radiation by engineering the ionization event positions in time t_n and their strength C_n in (4). This procedure makes it possible to arbitrarily control the THz shape, frequency, and other parameters, as explained in the following.

Control of the THz pulse duration and spectral width. In particular, it is known from the general theory of diffractive gratings that if the number of slits in a grating grows, the width of a zero-order peak decreases. This view is valid also for our "temporal grating". Increasing the number of ionization events makes the spectral width of THz radiation smaller as illustrated by Figure 3. In the temporal domain, this means increasing the THz pulse duration.

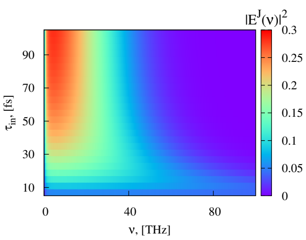


Fig. 3: *The dependence of the spectrum of the THz radiation* $|E^J(\nu)|^2$ *on the input pulse duration* τ_{in}

Control of the THz pulse frequency and shape. Another example of the Huygens–Fresnel principle in application to our problem is a possibility to control the THz pulse frequency and shape. It becomes possible if we modify the phase between the fundamental and second-harmonic frequency of the two-color pump pulse as well as the detuning between the fundamental and second harmonics. That is, the pump field is taken in the form $E(t) = F(t)(\cos 2\pi\nu_0 t + \cos(4\pi(\nu_0 + \delta\nu)t + \theta))$, where $F(t)$ is the pump pulse envelope, ν_0 is the fundamental frequency, θ is the relative phase, and $\delta\nu$ is a small frequency shift. The free parameters to change in this case are θ and $\delta\nu$. By adjusting these parameters, one can modify the interference pattern and thus the central THz frequency as shown in Figure 4.

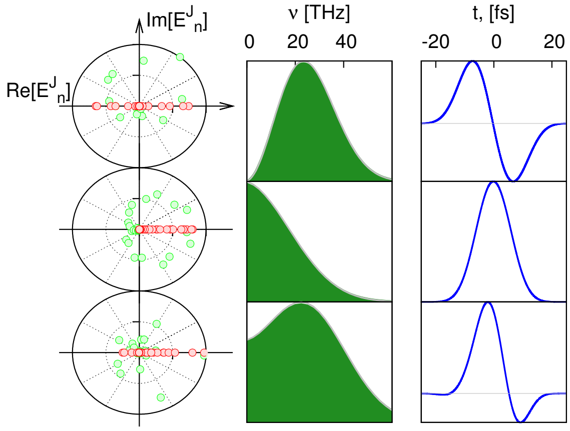


Fig. 4: *Control of THz pulse central frequency and shape by changing the phase and detuning between the fundamental and second harmonics. In (a), the relative impacts $E_n^J(\nu=0)$, in (b), the spectral $|E(\nu)|^2$ and in (c), the temporal $E(t)$ shapes of the resulting THz pulse are shown.*

For instance, if $\theta = \pi/2$ and $\delta\nu = 0$ (Figure 4, second row), the interference is minimal at $\nu \approx 0$ because all C_n in 4 have the same sign. The situation is changed if $\delta\nu > 0$ (third row) or $\theta \neq \pi/2$ (first row). In this case, for $\nu \approx 0$ destructive interference takes place, and thus the maximum of the spectrum is shifted away from the zero frequency.

Control of the THz pulse energy. The control of the pulse energy can be achieved by modifying the pump pulse in such a way that C_n in 4 are maximal. One possibility to do this is to depart from the requirement that the pump pulse has two frequencies that were made before. For instance, one can consider a three-frequency pulse (presented in Figure 5). There, the pump frequencies are $\nu_0 = 375$ THz and $\nu_s = 0.55\nu_0$, $\nu_i = 0.45\nu_0$. One can see that for such pulse C_n are much larger than for a two-color pulse, giving a tenfold gain in THz energy.

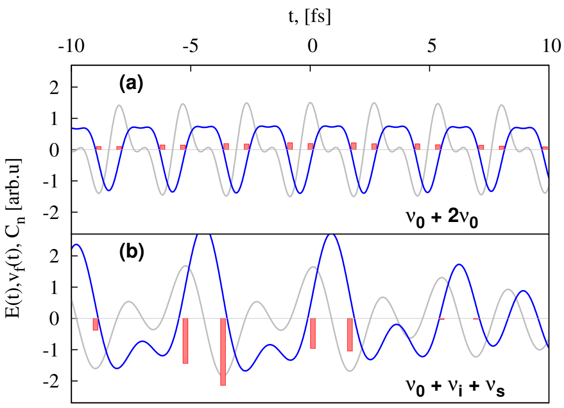


Fig. 5: *Control of THz pulse energy and spectral width with three-color pulses. The local field $E(t)$ is shown by the gray line, the free electron velocity $v_f(t)$ by the blue one, and C_n are shown by the red bars for the three-color pulse (b) as well as, for comparison, for a two-color pump (a).*

Spatial effects in different propagation geometries

Although the optimization schemes described above do not take into account the influence of the pump pulse propagating effects, they give surprisingly good results when applied to complicated real-life situations such as, for example, the one depicted in Figure 6 for the case of self-focused light propagation in a filament or multi-filament regime [4]. In such cases, $E(t)$ changes from point to point in space. This situation requires a direct solution of the full set of equations (1)–(3). The task of full-scale three-dimensional simulations of (1)–(3) is a challenge by itself because of the extremely different time and spatial scales involved in the problem. In particular, we have to resolve the time scales from tens of attoseconds to tens of picoseconds and the spatial scales from micrometers to meters. The power of our simple model (4) is seen from the fact that, despite of the propagation effects, the results of such simulations clearly support its predictions.

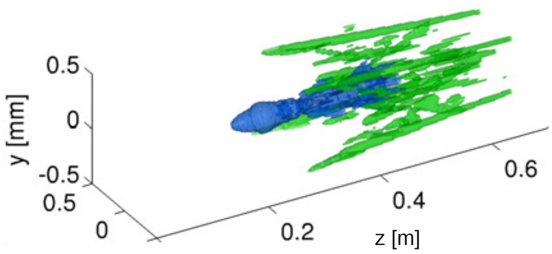


Fig. 6: *Plasma channels created by two-color pulse in a 0.5-meter-long filament in course of THz generation in the case of a single-filament (blue) and multi-filament (green) regimes*

References

[1] K.-Y. Kim, A.J. Taylor, J.H. Glownia, G. Rodriguez, *Coherent control of terahertz supercontinuum generation in ultrafast laser-gas interactions*, Nat. Photon., **2** (2008), pp. 605–609.

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

[3] I. Babushkin, S. Skupin, C. Köhler, L. Bergé, J. Herrmann, *Tailoring terahertz radiation by controlling tunnel photoionization events in gases*, New J. Phys., **13** (2011), pp. 123029/1–123029/16.

[4] L. Bergé, S. Skupin, C. Köhler, I. Babushkin, J. Herrmann, *3D numerical simulations of THz generation by two-color laser filaments*, Phys. Rev. Lett., **110** (2013), pp. 073901/1–073901/5.

2.3 Probabilistic Methods for Mobile Ad-hoc Networks

Gabriel Faraud

We present some mathematical techniques used by the Research Group *Interacting Random Systems* in the study of large mobile ad-hoc networks. Emphasizing the important role of probability for modeling the individual members of the system, we apply techniques from probability theory, in particular, from the theory of statistical mechanics, in order to study global properties of a complex telecommunication network connecting users moving in a given domain. Our main and novel approach is an introduction of random dynamics to well-known models of statistical physics and an utilization of the theory of stochastic processes for deeper studies of the system.

An ad-hoc network is built out of the users themselves, without relying on any pre-existing infrastructure. Indeed, in an ad-hoc network, connected devices can be used as transmitter-receiver, but they can also serve as relays and forward messages from other users. Ad-hoc networks have been introduced in the context of telecommunications to deal with situations where the infrastructure is either inexistent (e.g., in a war or in a natural catastrophe) or unable to perform (e.g., in a case of saturation or a malfunction). More recently, an interest arose also for cases where infrastructure is not wished, in particular, in the context of open software (see, for example, http://opengarden.com). Other advantages of such networks are that they are cheaper to install and to maintain and that they are less vulnerable than wired networks or existing wireless networks entirely based on antennas and base stations. They could also be a solution for dealing with an extremely high amount of information passing through the network, in particular, in situations where a lot of users want to communicate within a small, crowded area. We focus on *Mobile Ad-hoc Networks* (MANETs), where the involved devices move in some domain. For a general reference see [5].

The two main drawbacks of ad-hoc networks are the following. First, concerning the question of *coverage*, the fact whether or not two given users can exchange messages depends on the locations of *all the members* of the system and is therefore a priori an enormously complicated question. The big size of the system makes it necessary to introduce randomness for the description of the locations and movements of all the individuals. Below, we will describe some of our results in that direction.

Second, the absence of wires limits the capacity of such networks, due to interferences. Indeed, the number of frequencies that can be used in a given location is bounded. In future collaboration with the *Leibniz-Institut für innovative Mikroelektronik (IHP)* in Frankfurt/Oder, the group will study also this problem.

The model

The network we consider can be described in mathematical terms as a *random dynamic geometric graph*. Formally, a geometric graph in a given domain is a set of *vertices*, the locations of the users, with *edges* between them. The meaning of “ad-hoc” is that the edges appear in dependence on their spatial locations. More precisely, we fix some radius R and give the simple rule:

There is an edge between two users if and only if their distance is smaller than $2R$.

An important additional feature is the random movement of the users in the domain. As a consequence, the geometric graph is a time-dependent random process.

An interpretation is the following: Users move around, carrying devices that not only can send or receive information, but can in addition relay it from one user to another. Thus the message can be transmitted from one user to a distant one through many hops of distance $\leq 2R$. This type of transmission could be very effective when the delay is not a problem (which, for example, excludes voice communication). More specifically, we assume that the time scale of the transmission of the message is much smaller than the time scale of the movement of the users, in the sense that:

the messages are instantaneously transmitted.

Under this assumption, whenever there is a path of users between two users A and B, where the distance between two subsequent users is always smaller than $2R$, A and B are *connected* and can therefore exchange information.

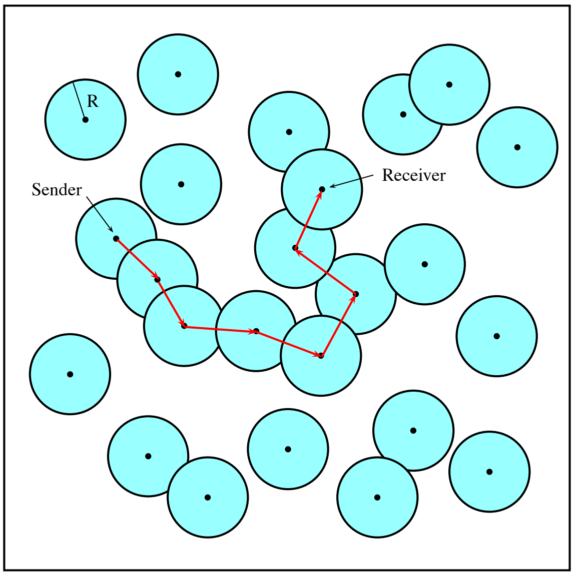


Fig. 1: *Connection rule*

We stress that there are two important features in the model, one is the connectivity structure, and the other is the random movement. In the following section, we introduce some suitable model of statistical physics that describes the instantaneous connectivity structure of the system. Afterwards, we will introduce some mobility component to the model.

Continuum percolation

The connectivity structure of a large geometric graph at a given time is defined by a huge number of random microscopic (local) influences, and we are interested in the macroscopic (global) properties of the system. Hence, we are facing a typical problem of *statistical mechanics*. This theory gives us a number of classical tools to use, like ergodic or thermodynamic limits. In particular, the well-known model of *continuum percolation* turns out to be rather suitable for our topic.

We recall the definition of a *Poisson point process*, which corresponds intuitively to a discrete set of points uniformly distributed over $\mathbb{R}^d$. A Poisson point process with parameter λ is a random discrete infinite set of points in $\mathbb{R}^d$ defined by the two properties:

- If A and B are disjoint subsets of $\mathbb{R}^d$, then the numbers of points falling in A and B are independent.

- The law of the number of points falling in a set A is Poisson with parameter equal to λ times the volume of A.

Now connect these points according to the rule formulated above, which results in a random geometric graph on $\mathbb{R}^d$. We have the following well-known fact:

There exists some threshold $R_c \in (0, \infty)$ (depending on λ) such that

- For $R < R_c$, with probability one, there is no infinite connected component.

- For $R > R_c$, with probability one, there is a unique infinite connected component.

However, the existence of an infinite connected component at R_c is still an open question.

We are, in particular, interested in the set defined as the union of the balls of radius R around all the Poisson points. Then there is an obvious natural one-to-one correspondence between the notion of connectivity of the random geometric graph and the usual topological notion of connectivity of this union. An alternate way of understanding the latter connectivity is via the so-called *percolation function* $\overline{\Theta}(\lambda, R)$, which represents the density of the infinite component. More precisely, $\overline{\Theta}(\lambda, R)$ is the probability that the ball with radius R around zero intersects the infinite component. An easy scaling argument gives

$$\overline{\Theta}(\lambda, R) = \overline{\Theta}(1, R\lambda^{1/d}) = \overline{\Theta}(R^d\lambda, 1).$$

For fixed R, we define $\lambda_c(R) = (R_c/R)^d$ as the critical density above which a unique infinite component exists.

The graph of $\overline{\Theta}(\lambda, \cdot)$ is depicted in Figure 2. However, its continuity at $R = R_c$ is still unknown, although it is widely believed to be true.

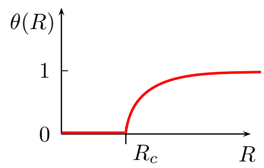


Fig. 2: *Plausible shape for* $\overline{\Theta}(\lambda, \cdot)$

Introducing dynamics

Now we present our assumptions on the random movement of the users. We describe the content of [3], which is joint work with Hanna Döring (Bochum). This article covers a large scope of movement schemes, but we are mainly interested in the *random waypoint model*, where the walker travels subsequently from waypoint to waypoint, linearly with constant speeds. The waypoints, respectively the speeds, are random and independent identically distributed. In information science, this model and its variants are considered as very suitable for the description of the movement of real people [5].

We call f_s the distribution density of the position of the walker at time s. Much work has already been done in order to describe the long-time limiting distribution for the random waypoint model. In particular, explicit formulas exist, and numerical simulations have been conducted for several classical cases [1].

Result

Our main interest is in a regime that is called *thermodynamic limit* in statistical physics: Many users are moving in a large domain such that the location density of the users is fixed, positive, and finite, but may be time- and space-dependent. For practical reasons we rescale the system such that the domain does not depend on the number of users anymore. Indeed, we take a finite domain $D \subset \mathbb{R}^d$ and let N independent walkers $X_1, X_2, \dots, X_N$ move in D according to the previous movement scheme, and we take the above-mentioned connection rule with radius $R_N := R/N^{1/d}$.

We are interested in the total time length during which two walkers (say X_1 and X_2) are connected until some given time T (denoted by $\tau^N_{1,2}(T)$) and, in particular, in its limit for large N.

It turns out that this limit is described in terms of a combination of a global, deterministic effect and a local, probabilistic effect. The first effect is due to the existence of a path from $X_1(s)$ to $X_2(s)$ through an area where the density f_s is supercritical, and the second one comes from the questions wether or not each of them belongs to the local macroscopic component. More precisely, given the trajectories X_1 and X_2,

$$\lim_{N\to\infty} \tau^N_{1,2}(T) = \int_0^T \mathrm{d}s\, \mathbf{1}\{X_1(s) \neq X_2(s), X_1(s) \underset{f_s > \lambda_c(R)}{\longleftrightarrow} X_2(s)\}\overline{\Theta}\big(f_s(X_1(s)), R\big)\overline{\Theta}\big(f_s(X_2(s)), R\big)$$
$$+ |\{s \in [0,T] : X_1(s) = X_2(s)\}|, \tag{1}$$

where $\{X_1(s) \underset{f_s > \lambda_c(R)}{\longleftrightarrow} X_2(s)\}$ is the event that $X_1(s)$ and $X_2(s)$ are in the same connected component of $\{x : f_s(x) > \lambda_c(R)\}$.

Results for large T are also discussed in [3], in particular, large deviations results.

Heuristic explanation

Obviously, it is sufficient to consider times s at which $X_1(s) \neq X_2(s)$. Recall that we consider a large number N of users and small balls of radius $RN^{-1/d}$ around each of them. The two users X_1 and X_2 can exchange a message at time s if both $X_1(s)$ and $X_2(s)$ belong to the same component of the union of these balls, which we want to denote by U_N. For this to happen, it is necessary that there is a corridor between $X_1(s)$ and $X_2(s)$ in which the density f_s is beyond criticality, since through this corridor, with probability tending to one, a neighborhood of $X_1(s)$ is connected with a neighborhood of $X_2(s)$. However, the probabilities that both sites $X_1(s)$ and $X_2(s)$ are locally connected with the macroscopic component of the union of the balls are precisely expressed by the two $\overline{\Theta}$-terms, since the users approximately form locally a homogeneous Poisson point process with the respective densities. Since these locations are disjoint, these two events are asymptotically independent, and the product of these terms describes that probability.

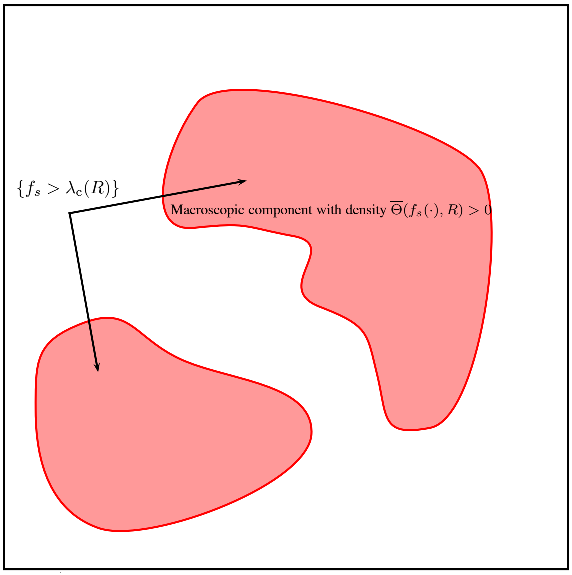


Fig. 3: *Two components of the supercritical area at time* s. *The square is the domain* D, *the white empty area contains only components with vanishing diameters as* $N \to \infty$.

Perspectives

There are already quite a number of mathematical results about connectivity in static random geometric graphs, partially also in view of a possible application to telecommunication systems, as well as computer simulations and experiments for mobile systems. In spite of its importance for the understanding of real-world telecommunication systems, the mathematical study of random geometric graphs in combination with mobility is still in its infancy. Our paper [3] is one of the first studies in that direction, to the best of our knowledge. Many further questions are to be studied, some of which have already been tackled or targeted by our group. For example, in joint work with Andrea Collevecchio (Melbourne), we study the delay in the situation where the sender and the receiver do not belong to the same component, but all users keep a copy of the message to be delivered. Furthermore, we work on relaxing some of the assumptions presented above. The research group is also developing a collaboration with the IHP Frankfurt with the goal to add the advantages of MANETs to the ones of classical wired networks by designing MANETs locally around each of the base stations of the wired system.

References

[1] J.-Y. Le Boudec, *Understanding the simulation of mobility models with palm calculus*, Performance Evaluation, **64** (2007), pp. 126–147.

[2] J. Díaz, D. Mitsche, P. Santi, *Theoretical aspects of graph models for MANETs*, in: Theoretical Aspects of Distributed Computing in Sensor Networks, S. Nikoletseas, J.D.P. Rolim, eds., Springer, Heidelberg et al., 2011, pp. 161–190.

[3] H. Döring, G. Faraud, W. König, *Connection times in large ad hoc mobile networks*, in preparation.

[4] D.B. Johnson, *Routing in ad hoc networks of mobile hosts*, in: Proceedings of the Workshop on Mobile Computing Systems and Applications (WMCSA 1994), IEEE Computer Society, Santa Cruz, CA, Dec. 1994, pp. 158–163.

[5] R.R. Roy, *Handbook of Mobile Ad Hoc Networks for Mobility Models*, Springer, New York et al., 2011.

2.4 Representation of Hysteresis Operators Acting on Vector-valued Monotaffine Functions

Olaf Klein

Processes having a causal and rate-independent input-output behavior

Many time-dependent processes in physics, biology, economics, and engineering exhibit an input-output behavior showing memory effects, i.e., even if the values of the input at two times coincide, the corresponding values of output may be different; see, e.g., [1, 5, 6].

For example, an elasto-plastic body that is deformed by some load may stay deformed if the load is removed. If periodic loading cycles are considered, one may observe so-called *hysteresis loops* as in Figure 1.

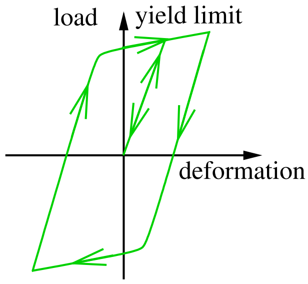


Fig. 1: *Load-deformation diagram for a non-ideal elasto-plastic behavior*

For many processes, the input-output behavior is *causal*, i.e., the value of the output at any time only depends on the current value and on former values of the input. In this study, we only consider *rate-independent* processes, i.e., a rescaling of the input function with respect to time leads to the same rescaling of the output function. Therefore, one is interested to investigate mathematical operators with a corresponding behavior, the so-called *hysteresis operators*, and to derive representation results for them. In the following, a representation result that has been formulated for hysteresis operators acting on scalar input functions is extended to hysteresis operators acting on vector-valued input functions.

Hysteresis operators

Let T be some fixed positive time, and let X, Y be two nonempty sets. Following the monographs [1, 6], an operator $\mathcal{H}$ mapping appropriate functions $u : [0,T] \to X$ into functions $\mathcal{H}[u] : [0,T] \to Y$, i.e., an operator $\mathcal{H} : D(\mathcal{H}) \to \mathrm{Map}\big([0,T], Y\big) := \{v : [0,T] \to Y\}$ with $D(\mathcal{H}) \subseteq \mathrm{Map}\big([0,T], X\big)$, is called a *hysteresis operator* if it is causal and rate-independent according to the following definitions:

- The operator $\mathcal{H}$ is said to be *causal* if for every $v, w \in D(\mathcal{H})$ and every $t \in [0,T]$ the following condition holds: If $v(\tau) = w(\tau)$ is satisfied for all $\tau \in [0,t]$, then it follows that $\mathcal{H}[v](t) = \mathcal{H}[w](t)$.
- The operator $\mathcal{H}$ is called *rate-independent* if $\mathcal{H}[v \circ \alpha](t) = \mathcal{H}[v](\alpha(t))$ for all $t \in [0,T]$ and for every $v \in D(\mathcal{H})$ and every $\alpha : [0,T] \to [0,T]$ with $\alpha(0) = 0$, $\alpha(T) = T$, α being continuous and increasing (not necessarily strictly increasing), and $v \circ \alpha \in D(\mathcal{H})$.

For example, let us consider the relay operator that is defined on the set $C([0,T], \mathbb{R})$ of all functions mapping $[0,T]$ continuously into the real numbers. For $a < b$ and $\eta \in \{0,1\}$ let the relay operator $\mathcal{R}_{a,b,\eta} : C([0,T], \mathbb{R}) \to \mathrm{Map}([0,T], \{-1,1\})$ be the operator mapping $u \in C([0,T], \mathbb{R})$ into $\mathcal{R}_{a,b,\eta}[u] : [0,T] \to \{1,-1\}$ defined by (see [1, 5, 6]):

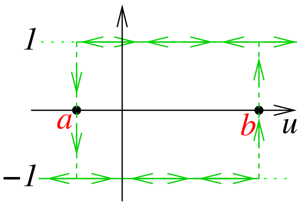


***Fig. 2:** Input-output relation of the relay operator $\mathcal{R}_{a,b,\eta}$*

$$\mathcal{R}_{a,b,\eta}[u](t) := \begin{cases} \eta, & \text{if } \; u(s) \in]a,b[\quad \forall\, s \in [0,t], \\ 1, & \text{if } \; u(t) \geq b, \\ -1, & \text{if } \; u(t) \leq a, \\ \mathcal{R}_{a,b,\eta}[u]\left(\left(\max\{s \in [0,t] : u(s) \notin]a,b[\,\}\right)\right), & \text{otherwise.} \end{cases}$$

The input-output behavior of the relay is shown in Figure 2, and the corresponding behavior for two other important hysteresis operators, the scalar stop and the scalar play, are shown in Figure 3 and Figure 4, respectively.

Representation results for hysteresis operators with scalar-valued inputs

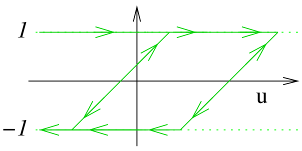


***Fig. 3:** Input-output relation of the stop operator*

In [1], Brokate and Sprekels investigated hysteresis operators for scalar-valued continuous piecewise monotone input functions and proved the following representation result:

Let a function $u : [0,T] \to \mathbb{R}$ be given.

- u is called *piecewise monotone* if there exist $0 = t_0 < t_1 < \cdots < t_n = T$ such that u is monotone on $[t_{i-1}, t_i]$ for all $i = 1, \ldots, n$.
- If u is piecewise monotone, the *standard monotonicity decomposition of* $[0,T]$ *for* u is the uniquely defined decomposition $0 = t_0 < t_1 < \cdots < t_n = T$ of $[0,T]$ so that t_i is the maximal number in $]t_{i-1}, T]$ such that u is monotone on $[t_{i-1}, t_i]$ for all $i = 1, \ldots, n$.

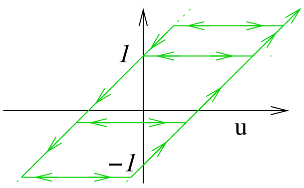


***Fig. 4:** Input-output relation of the play operator*

Let $\mathrm{C_{pm}}[0,T]$ be the set of all continuous, piecewise monotone functions from $[0,T]$ to $\mathbb{R}$.

From [1], one obtains:

1. *Definition:* Let a function $G : S_A \to \mathbb{R}$ be given, with S_A denoting the set of all finite alternating strings of real numbers, i.e.,

$$S_A := \{(v_0, v_1, \ldots, v_n) \in \mathbb{R}^{n+1} \,|\, n \geq 1,\; (v_{i+1} - v_i)(v_i - v_{i-1}) < 0, \quad \forall\, 1 \leq i < n\}. \tag{1}$$

   - For any continuous and piecewise monotone $u : [0,T] \to \mathbb{R}$, let $\mathcal{H}_G[u] : [0,T] \to \mathbb{R}$ be defined by considering the standard monotonicity partition $0 = t_0 < t_1 < \cdots < t_n = T$ of $[0,T]$ for u and requesting that

$$\mathcal{H}_G[u](t) := G\,(u(t_0), u(t)), \quad \forall\, t \in [t_0, t_1], \tag{2}$$

$$\mathcal{H}_G[u](t) := G\left(u(t_0), \ldots, u(t_{i-1}), u(t)\right), \qquad \forall\, t \in]t_{i-1}, t_i],\; i = 2, \ldots, n. \tag{3}$$

   - Using the above definition, one gets the *hysteresis operator* $\mathcal{H}_G : \mathrm{C_{pm}}[0,T] \to \mathrm{Map}([0,T], \mathbb{R})$ *generated by* G.

2. *Representation result:*

   For every hysteresis operator $\mathcal{B} : \mathrm{C_{pm}}[0,T] \to \mathrm{Map}([0,T], \mathbb{R})$ there exists a unique functional $G : S_A \to \mathbb{R}$ such that $\mathcal{B}$ is the hysteresis operator $\mathcal{H}_G$ generated by G.

The representation result yields that for evaluating a hysteresis operator for continuous, piecewise monotone inputs it is sufficient to memorize the local maxima and minima of the input. In particular, one does not need to keep track of the details of the input between these extrema. Moreover, thanks to the representation result, we can investigate hysteresis operators by considering the functional on S_A generating the operator. This approach has big advantages if one wants to study the mechanisms of storage and deletion of memory exhibited by hysteretic nonlinearities. There are a number of conditions that are easier to formulate and to check for the string representation, for example, the forgetting according to some deletion rule; see, e.g., [1].

Monotaffine functions and convexity-triple-free strings

Since the above-mentioned representation results have proved to be a very powerful tool in the analysis of scalar hysteresis, it has been a longstanding open problem to devise a corresponding method in the vector-valued case. We now present such a construction.

To this end, let X be some topological vector Hausdorff space (e.g., $X = \mathbb{R}^n$).

In order to generalize the notion of monotonicity from scalar-valued to vector-valued functions, the composition of a **monot**one with an **affine** function is considered and leads to a **monotaffine** function defined as follows; see [2, 3, 4]:

- Let some $t_1, t_2 \in [0, T]$ with $t_1 < t_2$ and some function $u : [0, T] \to X$ be given. u is called *monotaffine on* $[t_1, t_2]$ if there exists a monotone increasing (not necessarily strictly increasing) function $\beta : [t_1, t_2] \to [0, 1]$ such that $\beta(t_1) = 0$, $\beta(t_2) = 1$, and

$$u(t) = (1 - \beta(t))u(t_1) + \beta(t)u(t_2), \quad \forall\, t \in [t_1, t_2].$$

- Let $C_{\text{p.w.mo.af.}}([0, T], X)$ be the set of all continuous, piecewise monotaffine functions from $[0, T]$ to X. An example is illustrated in Figure 5 for $X = \mathbb{R}^2$.
- For a continuous, piecewise monotaffine function $u : [0, T] \to X$ the *standard monotaffinicity decomposition of* $[0, T]$ *for* u is the uniquely defined decomposition $0 = t_0 < t_1 < \cdots < t_n = T$ of $[0, T]$ such that t_i is the maximal number in $]t_{i-1}, T]$ with the property that u is monotaffine on $[t_{i-1}, t_i]$ for all $i = 1, \ldots, n$.

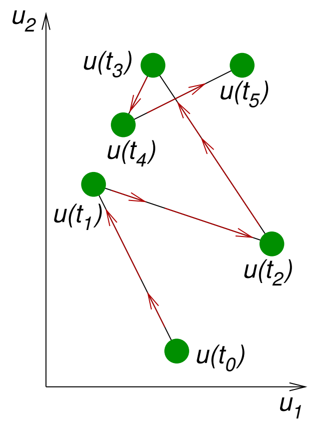


Fig. 5: *An example for a continuous, piecewise monotaffine function* $u = (u_1, u_2) : [0, T] \to \mathbb{R}^2$*; the points marked by* $u(t_i)$ *are the corresponding values for* u *at the times* $0 = t_0 < t_1 < \cdots < t_5 = T$*, being the standard monotaffinicity decomposition of* $[0, T]$ *for* u

The observation that an element of $V \in \mathbb{R}^{n+1}$, with n being a natural number, is an alternating string if and only if no component in V can be written as a convex combination of its predecessor and its successor, is the reason for the following definition:

1. A *convexity-triple-free string of elements of* X is any $(v_0, \ldots, v_n) \in X^{n+1}$, where $n \in \mathbb{N}$, such that for all $i = 1, \ldots, n-1$ it holds that $v_i \notin \operatorname{conv}(v_{i-1}, v_{i+1}) := \{(1-\lambda)v_{i-1} + \lambda v_{i+1} \,|\, \lambda \in [0, 1]\}$.
2. Let $S_F(X)$ denote the set of all convexity-triple-free strings of elements of X.

Representation result for hysteresis operators dealing with continuous, piecewise monotaffine input functions

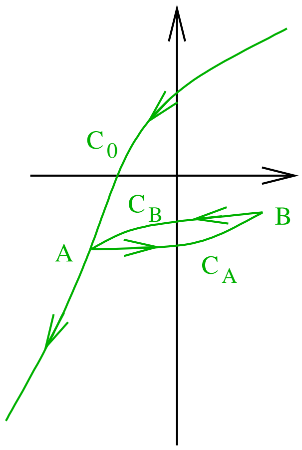


Fig. 6: *Madelung's rules*

The following definition and extension of the above representation result can be found in [2, 3, 4]:

- Let some function $G : S_F(X) \to Y$ be given.
  1. Let $u : [0, T] \to X$ be some continuous, piecewise monotaffine function, and let $0 = t_0 < t_1 < \cdots < t_n = T$ be the standard monotaffinicity decomposition of $[0, T]$ for u. Now, $\mathcal{H}_G[u] : [0, T] \to Y$ is defined by requesting that the equations (2) and (3) are satisfied.
  2. The mapping $\mathcal{H}_G : \mathrm{C}_{\mathrm{p.w.mo.af.}}([0, T], X) \to \mathrm{Map}\left([0, T], Y\right)$ defined by 1. is called the *hysteresis operator* $\mathcal{H}_G$ *generated by* G.
- For every hysteresis operator $\mathcal{B}$ from $\mathrm{C}_{\mathrm{p.w.mo.af.}}([0, T], X)$ to $\mathrm{Map}\left([0, T], Y\right)$ there exists a unique string function $G : S_F(X) \to Y$ such that $\mathcal{B}$ is the hysteresis operator generated by G.

If one needs to evaluate a hysteresis operator acting on all continuous, piecewise monotaffine functions, then it is sufficient to keep track of the positions of the direction changes of the input function. Then these values may be used as input for the string function $G : S_F(X) \to Y$ generating the hysteresis operator.

Madelung's rules and forgetting according to Madelung deletion

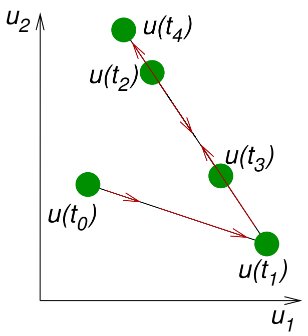


Fig. 7: *An example for a continuous, piecewise monotaffine function* $u = (u_1, u_2) : [0, T] \to \mathbb{R}^2$ *such that for the standard monotaffinicity decomposition* $0 = t_0 < t_1 < \cdots < t_4 = T$ *of* $[0, T]$ *for* u *it follows that* $\left(u(t_0), u(t_1), u(t_4)\right)$ *is the result of a Madelung deletion in* $\left(u(t_0),\right.$ $\left.u(t_1), u(t_2), u(t_3), u(t_4)\right)$

Madelung formulated some rules to describe the relations between an applied magnetic field and the generated magnetization. Recalling the reformulation and translations of these rules in [1, p. 27], we have

1. Any curve C_A emanating from a turning point A of the input-output graph (see Figure 6) is uniquely determined by the coordinates of A.
2. If any point B on the curve C_A becomes a new turning point, then the curve C_B originating at B leads back to the point A.
3. If the curve C_B is continued beyond the point A, then it coincides with the continuation of the curve C_0 that led to the point A before the $C_A - C_B$ cycle was traversed.

Madelung's second rule is also called the *return-point memory* property. For hysteresis operators with scalar, piecewise monotone inputs the second and the third Madelung rules are satisfied if the string function $G : S_A \to \mathbb{R}$ generating the operator is invariant to the so-called *Madelung deletion rule*; see [1, Def. 2.6.1, Def. 2.6.2, and Def. 2.7.1]. The following definitions generalize this consideration to the case of strings with elements of X.

- Let $V = (v_0, \ldots, v_n) \in X^{n+1}$, with some natural number $n > 2$, be given. W is called *the result of a Madelung deletion in* V if there is some $j \in \{1, \ldots, n-2\}$ such that

$$W = (v_0, \ldots, v_{j-1}, v_{j+2}, \ldots, v_n), \quad \mathrm{conv}\left(v_j, v_{j+1}\right) \subseteq \mathrm{conv}\left(v_{j-1}, v_{j+2}\right),$$
$$v_j \notin \mathrm{conv}\left(v_{j-1}, v_{j+1}\right), \quad v_{j+1} \notin \mathrm{conv}\left(v_j, v_{j+2}\right).$$

- Let a hysteresis operator $\mathcal{G} : \mathrm{C}_{\text{p.w.mo.af.}}([0,T],X) \to \mathrm{Map}\big([0,T],V\big)$ be given. The *operator $\mathcal{G}$ forgets according to the Madelung deletion*, if the function $G : S_F(X) \to Y$, generating $\mathcal{G}$, satisfies the following condition:
  For all $V, W \in S_F(X)$ such that W is the result of a Madelung deletion in V we have $G(V) = G(W)$.

Some of the vectorial relay operators considered in the literature, for example, Visintin's formulation in [6, IV (5.1)] of Mayergoyz's vectorial relay, can be rewritten in the following form: Let a nonempty, open subset O of X, a nonempty set Y, a function $\zeta : X \setminus O \to Y$, and some η on the boundary of O be given. We consider the following *generalized vectorial relay operator*:

$$\mathcal{R}_{X,O,Y,\zeta,\eta} : C([0,T];X) \to \mathrm{Map}\big([0,T],Y\big),$$

$$\mathcal{R}_{X,O,Y,\zeta,\eta}[\eta,u](t) := \begin{cases} \zeta(u(t)), & \text{if} \quad u(t) \notin O, \\ \zeta(\eta), & \text{if} \quad u([0,t]) \subseteq O, \\ \zeta\big(u\big(\max\big\{s \in [0,t] \,\big|\, u(s) \notin O\big\}\big)\big), & \text{otherwise.} \end{cases}$$

It turns out that the generalized vectorial relay operator is a hysteresis operator and forgets according to the Madelung deletion.

Further consequences of the new representation result

Further consequences of the new representation result and further representation results for more general input functions and more general operators can be found in the forthcoming thesis [4].

References

[1] M. Brokate, J. Sprekels, *Hysteresis and Phase Transitions*, Springer, New York, 1996.

[2] O. Klein, *Representation of hysteresis operators for vector-valued continuous monotaffine input functions by functions on strings*, to appear in: Adv. Math. Sci. Appl.

[3] O. Klein, *Representation of hysteresis operators for vector-valued inputs by functions on strings*, Phys. B, **407(9)** (2012), pp. 1399–1400.

[4] O. Klein, *Darstellung von Hysterese-Operatoren mit stückweise monotaffinen Input-Funktionen durch Funktionen auf Strings*, Habilitation Thesis, Humboldt-Universität zu Berlin, submitted on March 27, 2013.

[5] M.A. Krasnosel'skiĭ, A.V. Pokrovskiĭ, *Systems with Hysteresis*, Springer, Berlin, 1989.

[6] A. Visintin, *Differential Models of Hysteresis*, vol. 111 of Applied Mathematical Sciences, Springer, New York, 1994.

2.5 Self-heating, Hysteresis, and Thermal Switching of Organic Semiconductors

Klaus Gärtner, Annegret Glitzky, and Thomas Koprucki

Fig. 1: *OLEDs for lighting developed at IAPP*

Over the last years, electronic devices based on organic semiconductors have received increasing attention. Especially organic light-emitting diodes (OLEDs) occur in displays of mobile phones and are an emerging technology for TV screens and large-area lighting panels. Organic solar cells have reached a mature stage, allowing for commercialization. Moreover, organic field-effect transistors (OFETs) are already used in first products such as e-readers or radio frequency identification tags.

We started in 2011 the investigation and numerical treatment of models for organic semiconductor devices. The presented results were obtained in an intensive cooperation with the Institut für Angewandte Photophysik (IAPP) of Technische Universität Dresden.

Electronic transport in organic semiconductor devices

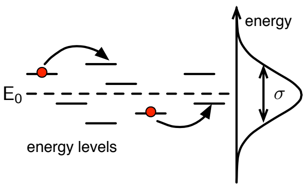


Fig. 2: *Hopping transport between Gaussian-distributed energy states*

Organic semiconductors consist of amorphous thin films of conductive polymers or of small organic molecules. The charge transport occurs by hopping of electrons between discrete energy levels of nearby molecular sites. The disordered nature of these organic semiconductor materials induces a random variation of the relative position of the conducting molecular energy states. The distribution of these disordered energy levels can be approximated by a Gaussian density of states centered around an energy E_0 and having a variance σ; see Figure 2.

Presently, Monte Carlo simulations of hopping transport are used to describe the electronic transport properties of organic semiconductors. The typical mean free path of the order of one nanometer is sufficiently small compared to the device dimensions to justify a drift-diffusion approximation [1]. The carrier mobility obtained by Monte Carlo simulations can be approximated by analytic expressions describing the dependence of the mobility on the temperature T, the carrier density n, and the electric field strength; see [1]. These mobilities can be successfully used for a macroscopic description of organic semiconductor devices by drift-diffusion models of the so-called *van Roosbroeck type*.

Due to the hopping transport mechanism, organic semiconductors are characterized by a positive feedback of the mobility with respect to temperature, density, and the electric field strength. In the low-density and low-field regime, the temperature dependence of the mobility [2] has the form

$$\mu(T) = \mu_0 \exp\Big[-C\Big(\frac{\sigma}{k_B T}\Big)^2\Big], \qquad (1)$$

where $C \approx 0.4$, and k_B denotes Boltzmann's constant. In this article, we focus on one of the novel features of organic semiconducting materials, namely the strong increase of the carrier mobility μ with temperature. This behavior leads to self-amplification of the current and to strong self-heating effects at large currents.

Three-dimensional heat flow simulations

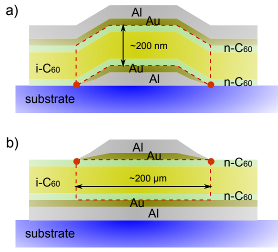


***Fig. 3:** Schematic of a device and cross sections along top (a) and bottom contact (b). Vertical size enlarged by three orders of magnitude.*

The investigated test structures are thin n-doped/intrinsic/n-doped (nin) devices based on the fullerene C_{60}; see Figure 3. At first, the lower metal contact is deposited on a glass substrate, followed by the highly n-doped C_{60} layer, the intrinsic C_{60} layer, a second highly n-doped C_{60} layer, and a second metal contact strip, orthogonal to the first one. The device is closed from above by an encapsulation glass. These crossbar contacts are widely used to contact organic devices. The temperature distribution around the crossbar structure is approximated by solving a stationary three-dimensional heat equation on the relevant huge spatial domain $\Omega \subset \mathbb{R}^3$,

$$-\nabla \cdot (\lambda(x)\nabla T(x)) = f(x) \quad \text{in } \Omega, \tag{2}$$

with boundary conditions $\nu \cdot (\lambda(x)\nabla T(x) = \kappa(x)(T(x) - T_a)$ on the boundary $\partial\Omega$ (ν – outward unit normal vector, λ – material-dependent heat conductivity, κ – heat transfer coefficient, T_a – ambient temperature). The heat source f is defined by the dissipative processes in the organic semiconductor nin structure.

In order to study heating effects in these “cross-contacted” thin organic layers, comprehensive three-dimensional simulations were carried out using the WIAS software package `pdelib`. The spatial discretization is based on a Voronoi finite volume scheme, which features global and local heat conservation and guarantees that the numerical solution respects the a priori bounds of the solution to the continuous problem. 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.

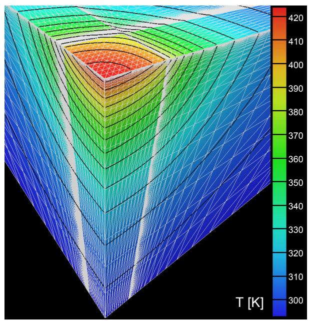


***Fig. 4:** 3D temperature distribution for homogeneous heat supply in the active area*

Our simulations for a homogeneously distributed heat source in the active area, indicated by the red dashed region in Figure 3, provide a detailed insight into the heat transport through the substrate away from the electrical circuit; see Figure 4. In particular, the effects of edge heat sources caused by electrical cross currents producing Joule heat were studied. In accordance with the dissipation rate density, the heat source f is decomposed into edge and volume contributions. In Figure 5, the edge-related contribution is clearly visible along the edges of the contacts, where a large fraction of the current is entering the metal contact. Due to the influences of the edge sources, a more homogenous temperature distribution within the active area results, see Figure 5, as it would be the case for a pure volume heat source alone. The temperature distributions obtained by thermal imaging and by simulation are in accordance with each other. For details, see [4].

To study the self-amplification qualitatively, one is interested in the characteristic temperature distribution and in the global thermal resistance Θ_{th} of the device. This quantity describes the heat losses of the complete device, which consists of the contacts, the organic circuit, the substrate, and the encapsulation glass, characterizing the temperature rise at specific points of the electrically active region with respect to the ambient temperature. The thermal resistance Θ_{th} is an important parameter in our investigations of self-heating, thermal switching, and hysteresis of organic semiconductors. For our C_{60} nin device, the simulated thermal resistance in the center of the active area turned out to be approximately $1000\,\mathrm{K/W}$.

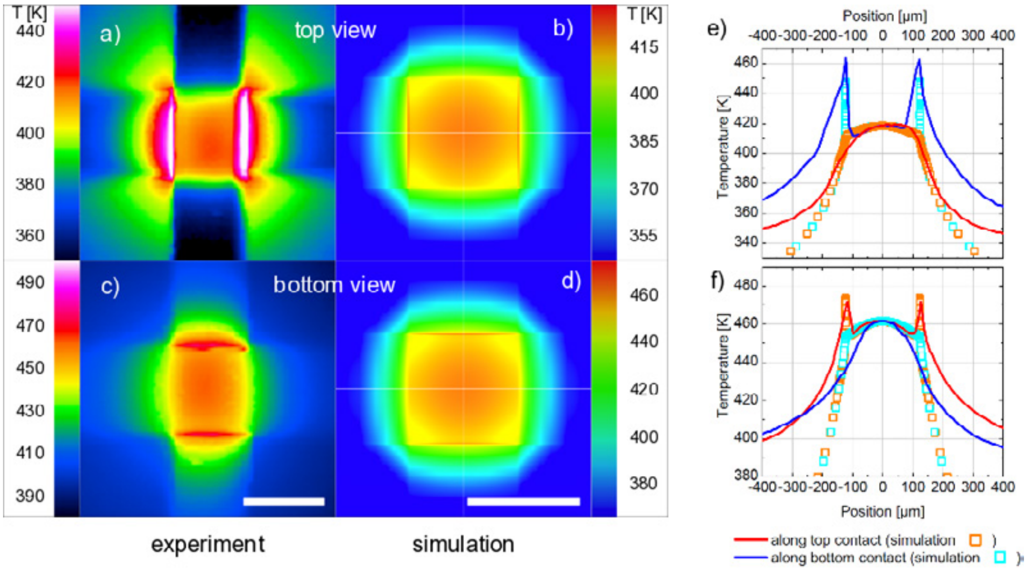


Fig. 5: *Temperature distribution by thermal imaging and simulation. Top view means thermal imaging through the encapsulation glass and bottom view, through the substrate glass. A strong temperature rise is observed along the edges. Line heat sources in the simulation are necessary to approximate the experimental results. Temperature differences in the active area between top and bottom view are mainly due to calibration (possible for top contact only). Line scans are shown for top view (e) and bottom view (f).*

Thermal switching in organic semiconductors

For materials with Arrhenius-like conductivity laws $\mu(T) \propto \exp(-E_{act}/k_B T)$, thermal switching phenomena induced by self-heating occur for activation energies $E_{act} > 4k_B T_a$, where T_a denotes the ambient temperature. Typically, the temperature dependence of the mobility (1) can be approximated by an Arrhenius law with an activation energy $E_{act} = 2C\sigma^2/(k_B T_a)$; see [2]. For usual values of the disorder parameter σ between $2\,k_B T_a$ and $6\,k_B T_a$, activation energies between $3\,k_B T_a$ to $30\,k_B T_a$ are large enough to allow for thermal switching.

We discuss the classical theory of self-heating for a thermally activated conductivity [3] and suppose that the isothermal current-voltage relation for the nin structure is given by a power law

$$I_{iso}(U,T) = I_{ref}\Big(\frac{U}{U_{ref}}\Big)^{\alpha} F(T) \tag{3}$$

with a positive exponent α and a temperature-dependent conductivity factor F(T) resulting from an Arrhenius law

$$F(T) = \exp\Big[-\frac{E_a}{k_B}\Big(\frac{1}{T} - \frac{1}{T_a}\Big)\Big]. \tag{4}$$

The quantities U_{ref}, I_{ref}, and $P_{ref} = U_{ref} I_{ref}$ denote reference values for voltage, current, and power, respectively. The homogeneous steady states of the device are given by equilibria of the global heat balance equation expressing that the dissipated Joule power IU equals the heat loss $\frac{1}{\Theta_{th}}(T - T_a)$ to the surroundings described by the thermal resistance Θ_{th}

$$\frac{1}{\Theta_{th}}(T - T_a) = P_{ref}\Big(\frac{U}{U_{ref}}\Big)^{\alpha+1} F(T). \tag{5}$$

The self-consistent current-voltage characteristics $(U(T), I(T))$ including self-heating parametrized by the temperature $T \geq T_a$ is obtained by combining (3) and (5),

$$U(T) = U_{\mathrm{ref}}\Big(\frac{T - T_a}{\Theta_{\mathrm{th}} P_{\mathrm{ref}}}\Big)^{\frac{1}{\alpha+1}} F(T)^{-\frac{1}{\alpha+1}}, \quad I(T) = I_{\mathrm{ref}}\Big(\frac{T - T_a}{\Theta_{\mathrm{th}} P_{\mathrm{ref}}}\Big)^{\frac{\alpha}{\alpha+1}} F(T)^{\frac{1}{\alpha+1}}. \qquad (6)$$

Different points on the self-consistent current-voltage characteristics, see Figure 7 (left), correspond to different values of the temperature rise $T - T_a$. The red curves show the calculated self-consistent current-voltage curves resulting from a linear isothermal current-voltage characteristics ($\alpha = 1$) for different values of the activation energy E_{act}. For activation energies $E_{\mathrm{act}} > 4k_{\mathrm{B}}T_a$, a region of negative differential resistance $\frac{\mathrm{d}U}{\mathrm{d}I} < 0$ appears. The turning points of the S-shaped current-voltage curve are characterized by the condition $\frac{\mathrm{d}U}{\mathrm{d}I} = 0$.

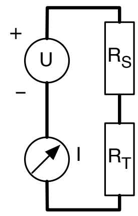


Fig. 6: *Schematic measurement setup. The organic layer is represented by the temperature-dependent resistor R_T, R_S is the additional series resistance, I is the measured current, and U the applied voltage.*

Along the S-shaped current-voltage characteristics, two stable branches exist: an 'ON' state with high conductivity and an 'OFF' state with low conductivity, whereas the intermediate region of negative differential resistance is unstable; see the dashed red lines in Figure 7 (left). This bistable behavior of the current-voltage characteristics is related to thermal switching at the turning points, involving a hysteresis loop, where the switching between the OFF and the ON branches occurs. In detail, a device will behave as follows: If the device is switched on by increasing the applied voltage, the current will follow the lower branch in the right diagram in Figure 7. With rising voltage, current and dissipated power increase, resulting in a higher temperature in the device. Reaching the turning point, the temperature is large enough, and the current in the organic semiconductor jumps to the upper, highly conducting branch, because the connecting branch between the turning points with negative differential resistance (NDR) is unstable. Reducing the voltage, the current now follows the upper branch to the left turning point and jumps down to the lower, less conducting branch. This behavior results in a closed hysteresis loop.

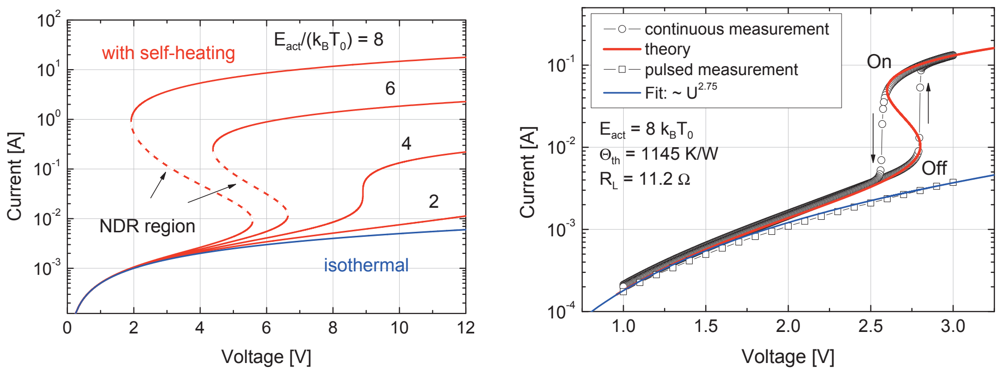


Fig. 7: *Left: Current-voltage curves including self-heating (red) for an organic device with a linear isothermal current-voltage behavior (blue). Right: Thermal switching measured by first increasing and then decreasing the voltage. Isothermal current-voltage curve obtained by short voltage pulses (blue).*

Setting up the experiment, one has to take into account all conductors outside the organic layer as an additional constant series resistance R_S; see Figure 6. This information together with the homogeneous self-heating theory allows to predict the ranges of voltage, current, and temperature where, for given activation energy and thermal resistance, a pronounced hysteresis loop can be expected; see [5]. The measured activation energies of the C_{60} nin crossbar test structures are about $8 k_{\mathrm{B}} T_0$, $T_0 = 293\,\mathrm{K}$. This is large enough to observe thermal switching ($E_{\mathrm{act}} > 4k_{\mathrm{B}}T_0$). Thermal switching was directly measured by our colleagues at IAPP [5] by cooling the device to an ambient temperature of $T_a = -52^{\circ}C$; see right diagram in Figure 7. The experimental results are in very good agreement with theory. For higher voltages the destruction of the device as a consequence of strong self-heating is starting at the contact edge as predicted by the calculated temperature distribution; compare Figure 8.

Summary and outlook

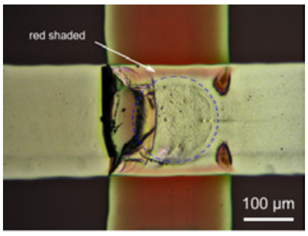


Fig. 8: *Delaminated top contact due to strong self-heating*

We demonstrated thermal switching and a pronounced hysteresis loop as a natural consequence of the hopping transport in amorphous organic semiconductors, provided that the activation energy (or disorder) is large enough. Hence, this finding is a step forward in the understanding of electro-thermal effects in organic semiconductors. Since almost all organic semiconductors show Arrhenius-like thermally activated conductivity laws, the results have a significant impact on various types of organic devices, including OLEDs, OFETs, and high-power rectifying diodes. Even in cases where the thermal switching is inhibited by a large series resistance, self-heating can lead to a negative differential resistance such that all organic devices with sufficiently large activation energies have to be understood as thermistors. This fact implies that the positive feedback between temperature and conductivity has to be taken into account in device simulations together with an analysis of the heat conduction away from the organic device. The group at IAPP Dresden observed S-shaped current-voltage characteristics with a region of negative differential resistance in OLED devices, too. Consequently, a spatial inhomogeneity of power dissipation and light emission in OLED lighting panels appears. Moreover, self-heating can promote current filaments or other spatial inhomogeneities. Hence, three-dimensional simulations of charge and heat transport through organic materials with negative differential resistance are required for a deeper understanding of devices operating far from thermodynamic equilibrium.

References

[1] W.F. Pasveer, J. Cottaar, C. Tanase, R. Coehoorn, P.A. Bobbert, P.W. Blom, D.M. Leeuw, M.A.J. Michels, *Unified description of charge-carrier mobilities in disordered semiconducting polymers*, Phys. Rev. Lett., **94** (2005), pp. 206601/1–206601/4.

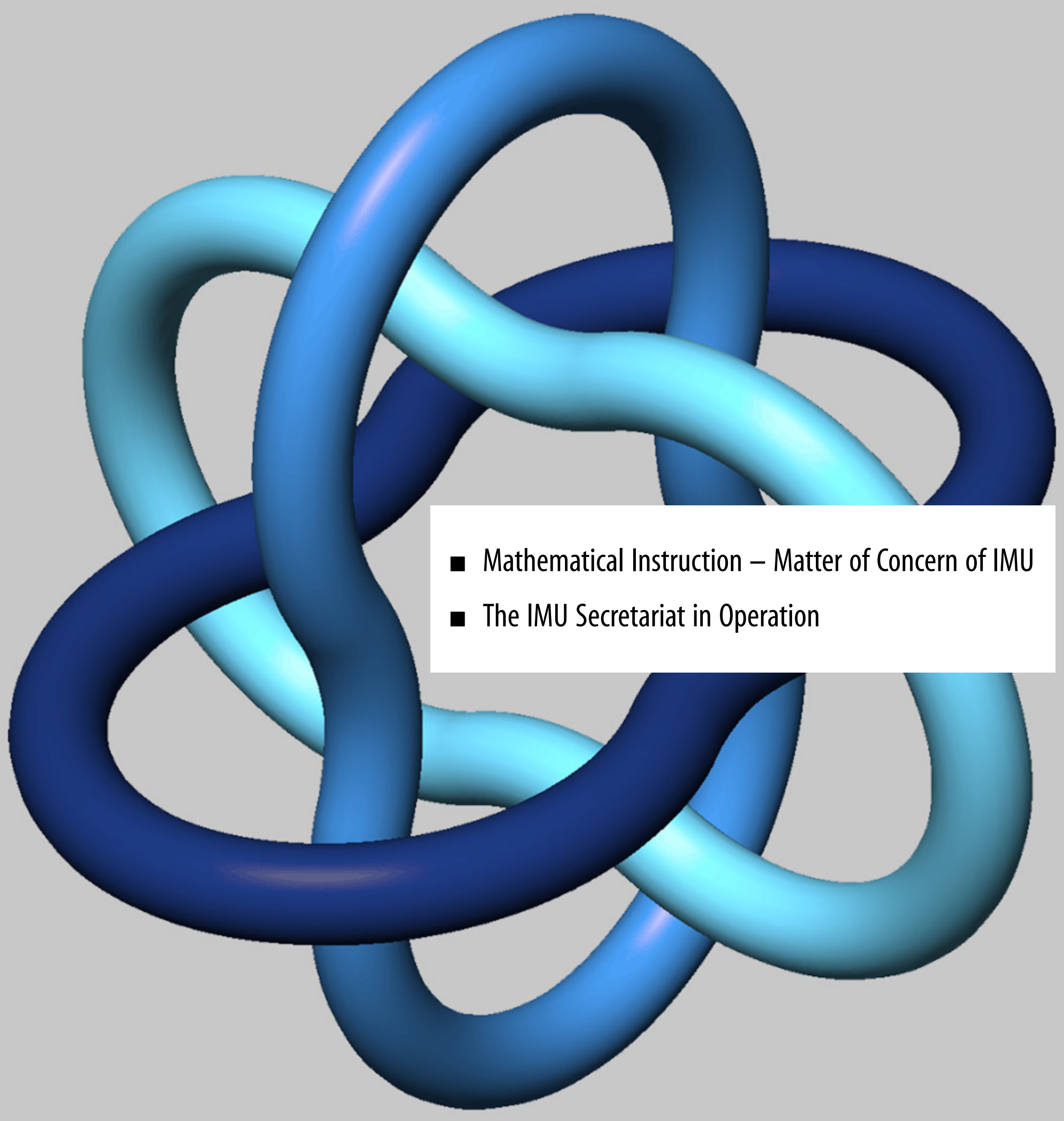
[2] S.L.M. van Mensfoort, S.I.E. Vulto, R.A.J. Janssen, R. Coehoorn, *Hole transport in polyfluorene-based sandwich-type devices: Quantitative analysis of the role of energetic disorder*, Phys. Rev. B, **78** (2008), pp. 085208/1–085208/10.

[3] M. Shaw, V. Mitin, E. Schöll, H. Grubin, *The Physics of Instabilities in Solid State Electron Devices*, Plenum Press, New York, 1992.

[4] A. Fischer, P. Pahner, B. Lüssem, K. Leo, R. Scholz, T. Koprucki, J. Fuhrmann, K. Gärtner, A. Glitzky, *Self-heating effects in organic semiconductor crossbar structures with small active area*, Org. Electron., **13(11)** (2012), pp. 2461–2468.

[5] A. Fischer, P. Pahner, B. Lüssem, K. Leo, R. Scholz, T. Koprucki, K. Gärtner, A. Glitzky, *Self-heating, bistability, and thermal switching in organic semiconductors*, Phys. Rev. Lett., **110** (2013), pp. 126601/1–126601/5.

3 IMU@WIAS



- Mathematical Instruction – Matter of Concern of IMU
- The IMU Secretariat in Operation

3.1 Mathematical Instruction – Matter of Concern of IMU

Lena Koch and Sylwia Markwardt

The International Commission on Mathematical Instruction, a commission of IMU

The International Mathematical Union (IMU) fosters mathematics education through its International Commission on Mathematical Instruction (ICMI). This commission is organized similarly to IMU with its own Executive Committee and General Assembly, see `http://www.mathunion.org/icmi`.

Overview ICMI:

Fig. 1: *ICMI Survey Poster*

ICMI (Figure 1) is a global network designed to improve and support mathematical education and instruction from pre-primary to university level.

ICMI was founded in 1908 at the International Congress of Mathematicians in Rome, and reconstituted in 1952 as an official commission of the International Mathematical Union.

The objective of ICMI is to improve the quality of mathematical instruction by connecting mathematics educators, teachers of mathematics, mathematicians, educational researchers, curriculum designers as well as educational policy makers and others interested in mathematical education worldwide.

Current projects:

- The Klein Project (inspired by Felix Klein's famous book "Elementary Mathematics from an Advanced Standpoint", published in 1908 and 1909) was launched in 2008 and supports mathematics teachers to connect the mathematics they teach with recent developments in the field of mathematics. A book will be published in several languages which will include sample mathematical problems suitable for students. A wiki based web site has already been launched for the many people who wish to contribute to the project in an ongoing way. ICMI will hold a workshop related to the project in Berlin in September 2013.
- The Database Project, launched in 2011, has as its ultimate goal a free-access database of mathematics curricula from all over the world.
- The Pipeline Project is an international study focusing on the supply and demand of mathematics students and personnel in educational institutions and workplaces. The study provides data for policy decision making and promotes a better understanding of the international situation. The following countries have supplied data to the study: Australia, Finland, France, Korea, New Zealand, Portugal, the UK, and the USA (2012).
- The ICMI Digital Library Project aims to provide open access to all ICMI publications and thematic studies.

Outreach to developing countries:

ICMI supports developing countries to become part of the international community of mathematical educators and supports local and regional development through projects and activities. Current projects include the Capacity and Network Project (CANP), the ICME Grant Program, and the ICMI Solidarity Fund.

Fig. 2: *ICMI's Capacity and Network Project*

Capacity and Network Project (CANP):

The project is a response to "Current Challenges in Basic Mathematics Education" (UNESCO, 2011). CANP (Figure 2) aims to develop the educational capacity of those responsible for mathematics teachers in developing countries, and to create sustained and effective regional networks of teachers, mathematics educators, and mathematicians. The project consists of an ongoing series of programs in a different developing region each year.

The first program was held in Mali in September 2011 and encompassed the Sub-Saharan region of Africa. The second was held in Costa Rica in August 2012 and encompassed Central America and the Caribbean. The third will be in South-East Asia in 2013.

Each program includes a two-week workshop of roughly 40 participants, half from the host country and half from regional neighbors. It is primarily aimed at the educators of mathematics teachers, but each program also includes mathematicians, researchers, policy-makers, and teachers. Each workshop has associated activities such as public lectures, satellite workshops for students, and exhibitions. CANP is the major development project of ICMI and is supported by IMU, UNESCO, and ICSU as well as regional governments and institutions.

Conferences:

Three main series of conferences are organized on a regular basis by ICMI or under its auspices.

The **International Congress on Mathematical Education (ICME)** is a quadrennial conference which gathers more than 3,000 participants from all over the world. An International Programme Committee (IPC) forms the scientific program and selects speakers, as well as oversees the progress of the congress preparations. ICME-12 (Figure 3) was held in Seoul, Korea, in 2012, and ICME-13 will be held in Hamburg, Germany, in 2016.

The **ICMI Study Programme**. Each ICMI Study has an international conference that is associated with this study that focuses on a topic or issue of prominent current interest in mathematics education with the main emphasis being on analytical and action-oriented aspects. A published study volume is intended to promote and assist discussion and action at the international, regional, or institutional levels. (See "ICMI Studies" below.)

ICMI Regional Conferences are held on various topics in mathematical education. Four ICMI Regional Conferences are held regularly:

- *AFRICME*. The Africa Regional Congress of ICMI on Mathematical Education
- *CIAEM*. The Inter-American Conference on Mathematical Education
- *EARCOME* is the name given to the ICMI East Asia Regional Conferences in Mathematics Education.
- *EMF* was launched by the French Sub-Commission for ICMI on the occasion of the World Mathematical Year 2000. The biennial series of *E*space *M*athématique *F*rancophone conferences is defined in linguistic terms, French being a common language among participants.

Fig. 3: *ICME-12 Visitors*

ICMI Studies:

Each study initiated by ICMI addresses an issue or topic of significance in contemporary mathematical education, and is conducted by an international team of leading scholars and practitioners. More than twenty volumes have already been published between 1986 and 2012. The latest edition, launched in 2012, covered the topic "Proof and Proving in Mathematics Education".

Publications:

There are various publications made by or under the auspices of ICMI:

- The ICMI Bulletin is published twice a year and available in paper or online.
- ICMI News, the ICMI electronic newsletter is published six times a year. Subscription is free and can be made from the ICMI web site.
- ICME Proceedings
- ICMI Studies
- L'Enseignement Mathématique

Exhibitions:

ICMI has supported the international UNESCO exhibition "Experiencing Mathematics!", which has been traveling the world since 2004 and has reached the eyes of over 800,000 pupils, students, teachers, and parents, in more than fifty cities from twenty countries. Future locations for the exhibition include Equatorial and East Africa as well as the United Arab Emirates. The exhibition is managed by the French Centre de Culture Scientifique, Technique et Industrielle Orléans.

Awards:

In 2003 ICMI created two awards in mathematics education research: the *Felix Klein Award*, for lifelong achievement in mathematics education research, and the *Hans Freudenthal Award*, for a major program of research on mathematics education. These awards are announced every two years and conferred at the opening ceremonies of ICMEs (ICME-12, Figure 4).

Fig. 4: *ICME-12 Prize Awardees*

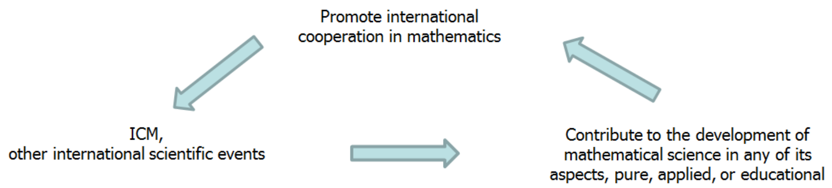
IMU's involvement:

ICMI's projects and activities are supported by the IMU through an annual grant, human resources, and participation in selected events and activities. This ongoing support ensures ICMI's effectiveness as an organization and the continued work to improve international mathematics education.

3.2 The IMU Secretariat in Operation

The IMU Secretariat finished successfully its second year at the Weierstrass Institute, completely in accordance with the Memorandum of Understanding concluded between the IMU and the Forschungsverbund Berlin that defines the following general provision, see below.

"The Secretariat will facilitate the activities of the IMU and support its committees and officers by providing it with a stable legal, administrative and financial structure. ..."



The work of the IMU Secretariat comprises, in general, the following areas:

- Meetings of the IMU Executive Committee
- Meetings of the IMU General Assembly
- The International Congress of Mathematicians (ICM)
- Administration of membership of countries in IMU
- Communication of/within the IMU Executive Committee
- IMU web site, bulletins, newsletter
- IMU finance, managing financial and legal aspects

Some examples. The web page of IMU's Commission for Developing Countries (CDC) was redesigned and relaunched this year. The web page of the Committee on Electronic Information and Communication (CEIC) was moved to the IMU server at WIAS and redesigned. Preparations have started to install a web page called "Women and Mathematics" that will be designed as an information site. A video conference system was installed in the conference room of the secretariat thus facilitating international communication.

An important event in 2012 was ICMI's 12th International Congress on Mathematical Education (ICME-12), held in Seoul, Korea. A booth run jointly by IMU and ICMI contributed to improving public relations activities for mathematics. Accompanying activities of ICME-12 were a special workshop of the 2014 ICM Local Organizing Committee to which were invited the OC presidents of ICMs 2010, 2006, 2002, 1998, as well as a site visit of the 2014 IMU General Assembly venue.

This year, the IMU Office Committee, whose purpose is to monitor the performance of the IMU Secretariat on behalf of the IMU Executive Committee (EC) and the IMU Adhering Organizations and to report to the EC, made its first visit to the secretariat (Figure 1). In a two-day workshop, the staff of the secretariat and others involved in IMU Secretariat "business" comprehensively informed the Office Committee about everything going on in the secretariat.

Fig. 1: *IMU Office Committee visit*

IMU won ICSU grant

IMU's application to ICSU (International Council for Science) for a €30,000 grant was successful. The grant project was entitled "Capacity and Network Project (CANP) Central America and the Caribbean", supporting applicants were ICMI, UNESCO, the Comité Interamericano de Educación Matemática (CIAEM), and regional universities.

The CANP proposal addressed ICSU's strategic priority of supporting Capacity Building and Science Education and Outreaching to Teachers and Young Scientists as well as ICSU's scientific priority "Mathematics Education" for Latin America and The Caribbean. Through fostering regional development and capacity building for mathematics teacher educators and forming self-sustainable networks concerned with mathematics education in Central America and the Caribbean, CANP aims to strengthen mathematical education and contribute to the further development of a regional professional community involving mathematicians, educationalists, teachers, policy makers, and institutions.

IMU supports Heidelberg Laureate Forum

Starting in September 2013, the "Heidelberg Laureate Forum" will bring together winners of the Abel Prize, the Fields Medal, the Nevanlinna Prize, and the Turing Award with young scientists from all over the world. The meeting is held in Heidelberg, it is established and sponsored by the Klaus Tschira Foundation and organized in collaboration with the Association for Computing Machinery (ACM; Turing Award), the International Mathematical Union (IMU; Fields Medal and Nevanlinna Prize), and the Norwegian Academy of Science and Letters (DNVA; Abel Prize). The meeting is modeled after the Lindau Nobel Laureate Meetings.

Guests of the IMU Secretariat. The table below gives an overview of guests who visited the IMU Secretariat this year.

Date	Guests	Event
Feb 7, 2012	Bernard Saint-Donat, USA; Yuri Tschinkel, USA	Individual visit
June 4–6, 2012	Bill Barton, New Zealand; Bernard Hodgson, Canada	ICMI Archive, ICMI issues

July 19–20, 2012	Thierry Bouche, France; Olga Caprotti, Finland; James Davenport, UK; Carol Hutchins, USA; László Lovász, Hungary; Peter Olver, USA; Ravi Vakil, USA	CEIC Meeting
Aug 23, 2012	Robert E. Bixby, USA; William Cook, USA, Gérard Cornuéjols, USA; Richard W. Cottle, USA; William H. Cunningham, Canada; Matthias Ehrgott, New Zealand; Robert Fourer, USA; David S. Johnson, USA; Eberhard Knobloch, Germany; Robert Mifflin, USA; Rolf Möhring, Germany; George Nemhauser, USA; Jaroslav Nešetřil, Czech Republic; Hans Josef Pesch, Germany; Claudia Sagastizábal, Brazil; Klaus Truemper, USA; Laurence Wolsey, Belgium; Margaret Wright, USA; Yinyun Ye, China/USA; Ya-xiang Yuan, China; Günter Ziegler, Germany	ISMP 2012
Sep 18–21, 2012	Abraham Arcavi, Israel; Ferdinando Arzarello, Italy; Bill Barton, New Zealand; Jaime Carvalho e Silva, Portugal; Bernard Hodgson, Canada	ICMI issues
Oct 5, 2012	Helge Holden, Norway	Individual visit
Nov 2–3, 2012	Bernard Hodgson, Canada; Ragni Piene, Norway; John Toland, UK; Wendelin Werner, France	IMU Office Committee
Nov 26, 2012	Mireille Chaleyat-Maurel, France	MPE2013
Dec 12/14, 2012	Ingrid Daubechies, USA	IMU issues, MATHEON
Dec 19, 2012	Anatoly Vershik, Russia	Invidual visit


Fig. 2: *Left: IMU Booth at 6ECM. Right: IMU President at ICME-12 Opening Ceremony.*

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

- 5th International Conference on Science and Mathematics Education, Phnom Penh, Cambodia (L. Koch)
- IMU EC meeting, Rio de Janeiro, Brazil (M. Grötschel, S. Markwardt; A. Mielke via skype)
- Abel Prize events, Oslo, Norway (M. Grötschel)
- 6th European Congress of Mathematics (6ECM), Krakow, Poland (S. Markwardt, A. Mielke, B. Seeliger), (Figure 2, left).
- 12th International Congress on Mathematical Education (ICME-12), Seoul, Korea (M. Grötschel, L. Koch, S. Markwardt), (Figure 2, right).

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*
- YSG *Modeling of Damage Processes*
- LG 3 *Mathematical Models for Lithium-ion Batteries*

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 physically motivated energetic formulations
- Qualitative methods for evolutionary systems such as Hamiltonian systems and gradient flows or suitable coupled systems
- Multiscale methods for deriving effective large-scale models 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.

Semiconductors

Photovoltaics. The group continued its cooperation with the Institute for Heterogeneous Materials Systems and the Institute for Silicon Photovoltaics of the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB). Based on a research and development contract with HZB, Reiner Nürnberg carried out two-dimensional and three-dimensional simulations with `WIAS-TeSCA` for a new concept of $CuInS_2$-chalcopyrite-based thin-film solar cells with a point contact/defect passivation structure at the hetero-interface; see Figure 1.

Within the MATHEON project D22 "Modeling of electronic properties of interfaces in solar cells", the group participates in the "Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin" (PVcomB), which is coordinated by HZB and financed by the Federal Ministry of Education and Research and the Federal State of Berlin. In thin-film solar cells, the electronically active interfaces have an essential impact on the device performance. One central point in the MATHEON project is the rigorous derivation of bulk interface models as limits of bulk models with thin layers. These results, using methods of variational convergence, like Γ-convergence, are contained in the Ph.D. thesis of Matthias Liero [1], defended in December 2012. Results concerning existence, uniqueness, and boundedness of solutions to electronic models for photovoltaic cells, which take into account active interfaces and energy-resolved defect densities, can be found in [2].

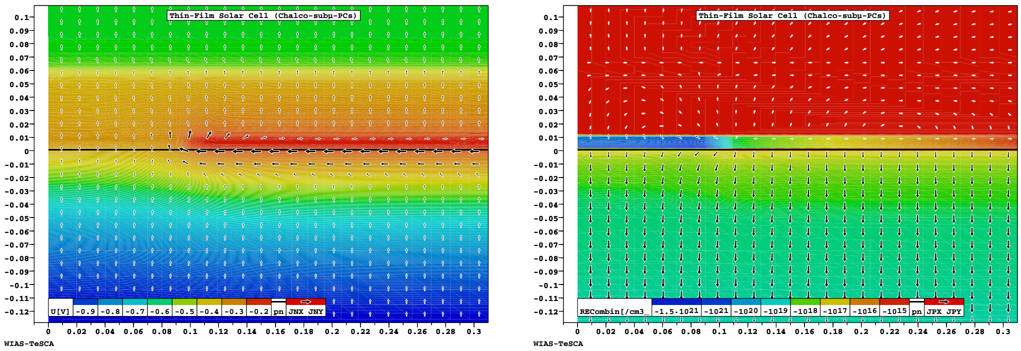


Fig. 1: *WIAS-TeSCA simulations of a thin-film solar cell based on chalcopyrite. Left: electric potential and electron flux. Right: recombination and hole flux.*

Together with the Research Group *Numerical Mathematics and Scientific Computing* (RG 3), first results with respect to amorphous organic semiconductors were obtained in close cooperation with the Institut für Angewandte Photophysik (IAPP) of Technische Universität Dresden. One of the main differences to crystalline semiconductors is the presence of significant self-amplifying effects. The feedback loop with respect to temperature was studied in a qualitative approach. The predictions were used to verify the previously unknown hysteresis effect by suitably designed experiments. For details, see the Scientific Highlights article "Self-heating, Hysteresis, and Thermal Switching of Organic Semiconductors" on page 44.

Halbleiter-Nanophotonik SFB 787

Discretization scheme for drift-diffusion equations for non-Boltzmann statistics. The modeling of the carrier transport in semiconductor lasers requires the use of the Fermi–Dirac statistical distribution function. The aim is to carry over the analytic properties of the equations and to handle the rapidly varying coefficient functions analogously to the Boltzmann case. Hence, one is looking for a generalization of the Scharfetter–Gummel scheme for the spatial discretization of the drift-diffusion operator originally derived for the Boltzmann (i.e. exponential) distribution function. For the special family of distribution functions $\mathcal{F}(\eta) = 1/(\exp(-\eta) + \gamma)$, a generalized Scharfetter–Gummel scheme was derived in cooperation with RG 3. The result is a nonlinear fixed-point problem for the current, which has a unique solution [4]. The result can be used for laser applications requiring a limited argument range and is an asymptotic limit of the Gauss–Fermi distributions describing hopping transport in amorphous organic semiconductors.

Scattering theory for cylindrically symmetric nanowires. The R-matrix formalism is a powerful tool for a realistic and quantitative description of the scattering process in cylindrically symmetric nanowire heterostructures. A numerical approach, based on the finite-volume method, was developed for computing the eigenvalues and eigenvectors of the Schrödinger operator on a three-dimensional cylindrically symmetric bounded domain with mixed boundary conditions, i.e., the Wigner–Eisenbud problem. It was studied how the anisotropy of the effective mass tensor acts on the uniform approximation of the first K eigenvalues and eigenvectors and their sequential arrangement [3]. There exists an optimal uniform Delaunay discretization with matching anisotropy

$(h_z/h_r)_{\text{opt}} = (m_r^*/m_z^*)^{1/2}$, which yields best accuracy also in the presence of mildly varying scattering potentials. The second-order convergence of the eigenvalues can be recovered only on uniform grids with an anisotropy correction; see Figure 2.

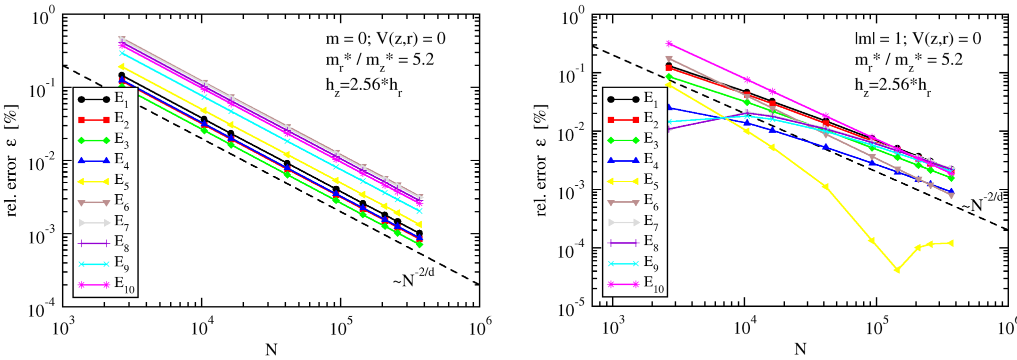


Fig. 2: *Relative errors for the lowest ten eigenvalues considering a grid with the optimal aspect ratio* $h_z/h_r = 2.56 \simeq 2.28 = (m_r^*/m_z^*)^{1/2}$ *for* $m = 0$ *(left) and* $|m| = 1$ *(right)*

Landauer–Büttiker formula and models for solar cells and LEDs. The goal of this research was to extend existing and well-analyzed quantum transport models to models taking into account electron-photon interaction. The main tool to analyze electron transport problems is the so-called *Landauer–Büttiker formula*. Hence, the first step was to extend the usual Landauer–Büttiker formula to systems with photon interaction, which was achieved by proving an abstract Landauer–Büttiker formula in an operator-theoretical framework; cf. [5]. The next step was to find suitable models describing quantum transport as well as electron-photon interaction to which the abstract Landauer–Büttiker formula can be applied. Two such models were found and analyzed in the Ph.D. thesis of Lukas Wilhelm, namely the Jaynes–Cummings model coupled to two leads and the Pauli–Fierz model in one space dimension.

Material modeling

The research in this field deals with the mathematical modeling and the analysis of the elastic behavior of solids undergoing dissipative processes. It includes chemical reaction and diffusion processes on the one hand and, on the other hand, dissipative phenomena that can be described with the aid of internal variables, such as plastic deformations, phase transformations in shape memory alloys, or damage and delamination processes. The latter are investigated in collaboration with the Young Scientists' Group *Modeling of Damage Processes* (YSG).

Shape memory alloys, elastoplasticity, and damage. In the MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape memory alloys", a collaboration with Sören Bartels (Universität Freiburg) and Tomáš Roubíček (Charles University, Prague) provided numerical approaches to elastoplasticity without hardening. Furthermore, mathematical methods for homogenization and dimension reduction in rate-independent systems were developed.

The modeling and analysis of microstructure evolution is the central topic of the subproject P5 "Regularizations and relaxations of time-continuous problems in plasticity" within the DFG Research Unit FOR *797* "Analysis and Computation of Microstructure in Finite Plasticity". A joint work [6] with Klaus Hackl (Ruhr-Universität Bochum) studies the evolution of laminate-type microstructures and shows the existence of solutions to time-incremental minimization problems.

In the application area of damage, a model for the rate-independent evolution of brittle delamination in thermoviscoelastic materials was analyzed as the limit of adhesive contact models. To carry out this limit passage in presence of rate-dependent effects requires the study of the fine properties of the internal variables solving the approximating problems.

Effective equations for slowly diffusing substances. The project A5 "Pattern formation in systems with multiple scales" within the Collaborative Research Center 910 "Control of self-organizing nonlinear systems" investigates the homogenization of semilinear parabolic PDEs. Of particular interest are reaction-diffusion systems with two subsystems, one with slowly diffusing substances and one with faster diffusing substances, coupled via nonlinear reactions. Spatial patterns occur on two very different scales and lead via two-scale convergence to an effective system defined on the physical domain times the periodicity cell.

Analysis of multiscale systems driven by functionals

The ERC project "Analysis of multiscale systems driven by functionals" 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, which couple Hamiltonian and dissipative effects. In this project, several topics in the focus areas of the Research Group *Partial Differential Equations* interact, such as the thermomechanical modeling and analysis of dissipative effects in solids, the investigation of the coupling of Maxwell–Bloch equations and the evolution systems for semiconductors in a GENERIC framework, the multi-scale analysis for Wasserstein gradient flows, and the study of reaction-diffusion systems. In [7], a general method is provided for proving the geodesic convexity of energy or entropy functionals if the dissipations metric of the corresponding gradient flow is expressed explicitly in terms of an Onsager operator. It is shown that this method applies to chemical reaction kinetics of mass-action type, diffusion equations, and coupled linear and nonlinear reaction-diffusion systems.

Further activities

International Workshop "Mathematics for Semiconductor Heterostructures: Modeling, Analysis, and Numerics". This workshop took place at WIAS from September 24–28, 2012 and was organized by Klaus Gärtner (RG 3), Annegret Glitzky, Hans-Christoph Kaiser (both RG 1), and Francis Nier (Rennes, France). Besides two key-note presentations, 32 talks and a poster session were held. The conference covered analytical and numerical aspects of the relevant mathematical models for semiconductor devices and the design of efficient numerical algorithms. The five-day event was devoted to the modeling of micro-, nano-, and optoelectronic devices by classical drift-diffusion and energy models, by semi-classical and quantum transport models as well as by asymptotic models. The main topics were organic semiconductors, spintronics, quantum dots, wires, wells, and wave guides. The multi-physics problems were discussed from the mathematical point of view up to the simulation of real-world devices.

Fig. 3: *MSH 2012: Berlin, September 24–28*

Leibniz Mentoring Program. In 2011/12, Marita Thomas participated in the pilot project "Mentoring for women scientists in Leibniz institutions". With this one-year program, the Leibniz Association coaches highly qualified female postdocs in obtaining essential skills required for scientific leadership positions. The program combines a mentor-mentee partnership with individual coaching and with a series of workshops and lectures. These seminars provide an insight into legal aspects of the German scientific system and equip the mentees with a variety of tools for future career pathing, project and science management. After its successful pilot phase in Berlin and Brandenburg, the Leibniz Mentoring Program will be perpetuated as a nationwide Leibniz program.

References

[1] M. Liero, *Variational methods for evolution*, Ph.D. Thesis, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, 2012.

[2] A. Glitzky, *An electronic model for solar cells including active interfaces and energy resolved defect densities*, SIAM J. Math. Anal., **44** (2012), pp. 3874–3900.

[3] P. N. Racec, S. Schade, H.-C. Kaiser, *Eigensolutions of the Wigner–Eisenbud problem for a cylindrical nanowire within finite volume method*, WIAS Preprint no. 1709, 2012, to appear in: J. Comp. Phys.

[4] T. Koprucki, K. Gärtner, *Discretization scheme for drift-diffusion equations with a generalized Einstein relation*, WIAS Preprint no. 1738, 2012, submitted.

[5] H. Cornean, H. Neidhardt, L. Wilhelm, V. Zagrebnov, *Cayley transform applied to non-interacting quantum transport*, arXiv:1212.4965, Cornell University Library, arXiv.org, Ithaca, USA, 2012, submitted.

[6] K. Hackl, S. Heinz, A. Mielke, *A model for the evolution of laminates in finite-strain elastoplasticity*, Z. Angew. Math. Mech., **92** (2012), pp. 888–909.

[7] M. Liero, A. Mielke, *Gradient structures and geodesic convexity for reaction-diffusion systems*, WIAS Preprint no. 1701, 2012, to appear in: Phil. Trans. Royal Soc. A.

4.2 Research Group 2 “Laser Dynamics”

The research of this group is devoted to 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*. External funding is received within the DFG Research Center MATHEON (projects D8 and D14), the Collaborative Research Center (SFB) 787 (projects B4 and B5), and the Marie Curie Initial Training Network PROPHET. In 2012, also a new DFG Individual Grant has been approved (details below).

Dynamics of semiconductor lasers

The research in this field is characterized by its close relations to various experimental partners, and it presently covers a particularly wide range of different types of devices. An important event was the Workshop “Nonlinear Dynamics in Semiconductor Lasers” where new trends in laser technology as well as theoretical concepts were discussed.

Mode-locking. In the field of mode-locking, a detailed study of the locking range in a hybrid mode-locked two-section device was performed. The basis for these numerical and analytical investigations was a system of delay-differential equations that had been developed in this research group earlier. Moreover, the influence of optical feedback from an external mirror on a passively mode-locked semiconductor ring laser was investigated. It turned out that a reduction of the timing jitter is possible if the delay time is chosen close to an integer multiple of the inter-spike interval time of the laser without external feedback. Outside the main resonant regimes, the timing jitter is drastically increased by the feedback.

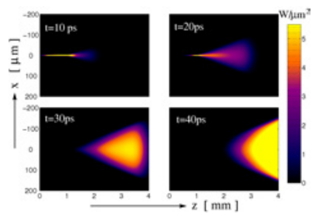


Fig. 1: Simulated intensity distributions of a pulse in a tapered amplifier

Broad-area lasers and amplifiers. For broad-area lasers the stabilization by an injected optical beam and the shaping of the output beam were investigated. Moreover, for tapered and broad-area amplifiers the propagation and amplification of short optical pulses was investigated [2]. Simulations were performed with the code “BALASER” executed on the parallel compute cluster “Euler” at WIAS.

Wavelength conversion in ring lasers. All-optical simultaneous wavelength conversion of multiple channels via four-wave mixing in semiconductor ring lasers was theoretically studied using a semi-classical traveling wave model.

VCSEL (vertical cavity surface emitting lasers). As a part of the long-term goal of developing a simulation tool for VCSELs with quantum dot active materials, pursued within the project B4 in the Collaborative Research Center (SFB) 787, the Coulomb scattering processes between bound states in semiconductor quantum dots and delocalized states of the surrounding carrier reservoir were calculated. This work was part of the Ph.D. thesis of Alexander Wilms that was successfully defended in the last year.

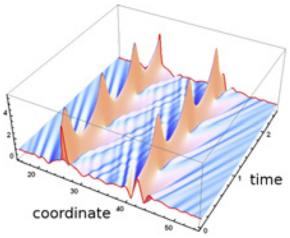


Fig. 2: *Anti-phase bound state of two oscillating cavity solitons*

Cavity solitons. The interaction of well-separated oscillating localized structures of light was studied within the framework of the Lugiato–Lefever model [3]. These structures emit weakly decaying dispersive waves leading to the formation of bound states due to harmonic synchronization; see Figure 2. An Andronov–Hopf bifurcation of stationary localized structures leads to a drastic increase in their interaction strength.

Pulses in nonlinear optical media

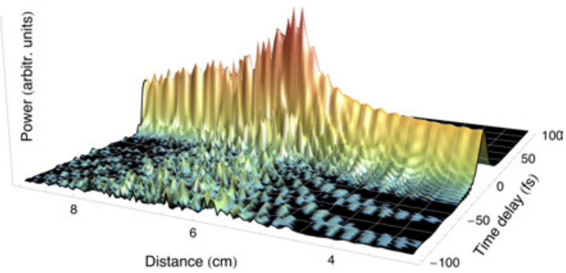


Fig. 3: *Spontaneous formation of a short-living large pulse in an optical fiber*

The research in this field is concerned with mathematical questions related to nonlinear phenomena in optics that can be observed in optical fibers or in self-organized optical filaments in transparent media.

The new project "Ab-initio description of optical nonlinearities in femtosecond filaments", submitted by Carsten Brée, has been positively evaluated by the German Research Foundation DFG. It is aiming at a theoretical understanding of the light-matter interaction processes that are responsible for the appearance of femtosecond filaments in corresponding experiments. In addition to nonlinear optics, it also invokes time-dependent density functional theory to describe these processes on the level of quantum theory.

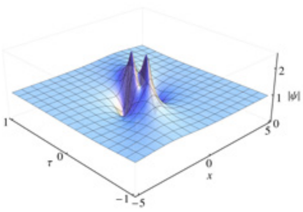


Fig. 4: *Rogue wave of the Sasa–Satsuma equation*

An important activity in 2012 was related to optical rogue waves, i.e., unexpected, extremely powerful pulses that suddenly appear in optical supercontinuum and then quickly disappear. A new mechanism of rogue waves formation was found [5]. The mechanism is based on a very special realization of the common cross-phase-modulation interactions between optical solitons and dispersive wave packets. The mechanism explains both birth and death of the extreme solitons and, as expected, provides heavy-tailed statistics of the extreme events. Moreover, this kind of interaction is generic, since it is based on only two simple preconditions: (i) nonlinearity and (ii) presence of a zero-dispersion point.

Furthermore, for a specific integrable system called *Sasa–Satsuma equation*, an explicit multi-parameter family of solitons on a background has been presented [4]. The solution contains a set of several free parameters that control the background amplitude as well as the soliton itself. This family of solutions admits a few nontrivial limiting cases that are considered in detail. Among these special cases are the nonlinear Schrödinger equation limit and the limit of rogue wave solutions.

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. In the last year, a major focus was on complex dynamics in large coupled systems and on the formation and interaction of patterns.

An important event was the Workshop "Coupled Networks, Patterns, and Complexity" that was organized at WIAS with the support of the DFG Research Center MATHEON, the Collaborative Research Center (SFB) 910, and the International Research Training Group (IRTG) 1740. The large response to this workshop, leading to the number of 80 participants, pointed out the ongoing relevance of this mathematical topic. Its importance for various fields of application was underlined by contributions concerning a variety of practical questions, including, e.g., the stability of power grids, the modeling of excitation waves in the human heart, or spintronics.

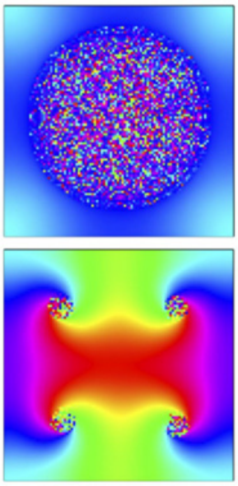


Fig. 5: *Two-dimensional coherence-incoherence patterns in a system of coupled oscillators*

The research group's activities in the the field of *dynamical systems* included new results for coupled phase oscillators and coherence-incoherence patterns, so-called *chimera states*, that had already been studied intensively in the previous years. A major breakthrough was the discovery of non-universal transitions to synchrony in the Sakaguchi–Kuramoto model [5]. It was obtained by a new approach to the bifurcation problem in the infinite-dimensional thermodynamic limit problem. Moreover, the research on collective dynamics and pattern formation was successfully extended to irregular networks.

Fig. 6: *Participants of the Workshop "Coupled Networks, Patterns and Complexity"*

References

[1] A. Demircan, S. Amiranashvili, C. Brée, Ch. Mahnke, F. Mitschke, G. Steinmeyer, *Rogue events in the group velocity horizon*, Sci. Rep., **2** (2012), pp. 00850/1–00850/6.

[2] D.R. Herrero, M. Botey, M. Radziunas, K. Staliunas, *Beam shaping in spatially modulated broad area semiconductor amplifiers*, Opt. Lett., **37** (2012), pp. 5253–5255.

[3] D. Turaev, A.G. Vladimirov, S. Zelik, *Long range interaction and synchronization of oscillating dissipative solitons*, Phys. Rev. Lett., **108** (2012), pp. 263906/1–263906/5.

[4] U. Bandelow, N. Akhmediev, *Sasa–Satsuma equation: Soliton on a background and its limiting cases*, Phys. Rev. E., **86** (2012), pp. 026606/1–026606/8.

[5] O. Omel'chenko, M. Wolfrum, *Nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, Phys. Rev. Lett., **109** (2012), pp. 164101/1–164101/4.

4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

The research group works on the development of numerical methods, their analysis, and the implementation of software tools for the numerical solution of partial differential equations and differential-algebraic systems. Many of the research topics have been inspired by the solution of problems coming from applications. Here, a short overview of selected fields of the group's research will be presented.

Tetrahedral mesh generation

Many numerical methods, such as finite element or finite volume methods, require a partition of a given domain. The quality of the partition affects the accuracy and convergence of simulations.

The goal of the research on tetrahedral mesh generation consists in developing robust and efficient algorithms for automatically generating high-quality tetrahedral meshes. A good quality, i.e., with respect to the elements' shape, size, and orientation, is a prerequisite for the high accuracy and the efficiency of the numerical methods used. In particular, the Voronoi finite volume method that was developed in the group requires a boundary-conforming Delaunay mesh to exhibit its most favorable properties.

Tetrahedral mesh generation is an active topic of research. It still faces many challenges in designing provable and efficient algorithms and in robust software implementation. For example, one of the fundamental difficulties is the preservation of boundaries in tetrahedral meshes. Once boundaries are properly represented, the quality of the tetrahedral mesh can be improved by inserting new vertices together with mesh optimizations. Another challenge is to conform special geometric configurations such as the sharp features, which are acute angles in input boundaries. They may prevent algorithms from converging, or they might result in a large number of unnecessary tetrahedra. Finally, the problem of generating quality meshes that involve anisotropically shaped elements is far from being well understood.

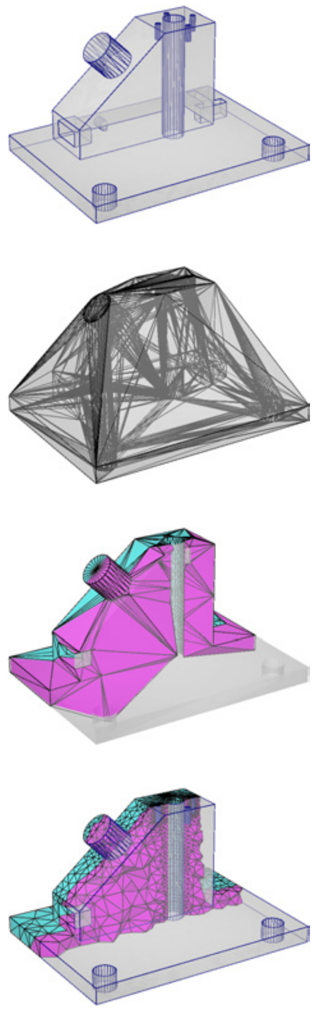


Fig. 1: *TetGen work flow: (a) input domain – a 3D piecewise linear complex (PLC), (b) Delaunay tetrahedralization of the vertices of the PLC, (c) constrained Delaunay tetrahedral mesh, (d) quality tetrahedral mesh of the PLC. Cut views in (c) and (d) show the internal tetrahedra.*

The development of the software TetGen [3] in the group faces two goals. First, it provides a research tool for evaluating state-of-the-art algorithms and technologies for quality tetrahedral mesh generation. Second, it provides a robust, efficient, and easy-to-use software for various applications. TetGen is written in C++. Its source code is available under a dual-licensing policy. It can be used freely for academic purposes. Commercial licenses are provided for a fee. TetGen includes efficient algorithms for generating Delaunay tetrahedralizations, constrained Delaunay tetrahedralizations, and good quality tetrahedral meshes. These algorithms can tetrahedralize three-dimensional objects of arbitrary complexity. Specific input constraints, such as edges and triangles, can be preserved in the generated meshes. Extensive local mesh modification operations have been implemented for refining and optimizing meshes to efficiently improve the quality and the adaptivity. If the input does not contain sharp features, TetGen is able to generate quality meshes whose dihedral angles are between 20^o and 155^o. TetGen uses advanced techniques in computational geometry. Figure 1 illustrates a work flow of TetGen for quality tetrahedral mesh generation.

Velocity-pressure reduced-order modeling for flow problems

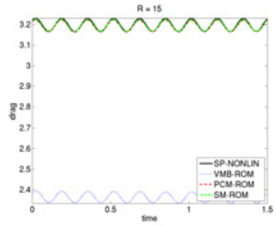


Fig. 2: *Flow around cylinder, Re = 100. VBM-ROM: ROM pressure based on velocity POD basis, PCM-ROM and SM-ROM: ROM pressure based on pressure POD basis, SP-NONLIN: reference values*

Reduced-order modeling (ROM) performs simulations in spaces with very low dimension to compute the most important features of the solution to some problem. This technique is used, e.g., in optimization problems that require the repeated solution of partial differential equations. Proper orthogonal decomposition (POD) is one of the most successful techniques in the context of ROM. The main goal of POD consists in finding an orthonormal basis of low dimension that captures the most dominant features of the input data. The input data of POD are the so-called *snapshots*. These data can be, e.g., the numerical solution of a problem at different time instances or even experimental data. In other fields, the same procedure is often called *singular value decomposition*, *Karhunen–Loève decomposition*, or *principal components analysis*. Within the framework of flow problems, POD was introduced by Lumley about 45 years ago.

The standard way of deriving a ROM is by performing the Galerkin projection of the governing equations onto the POD basis. In the case of the incompressible Navier–Stokes equations, this approach leads to a ROM only for velocity, if it is assumed that the snapshots and, consequently, the POD basis functions, are discretely divergence-free. This is a common assumption in the literature. However, there exist important reasons why the computation of pressure is of great interest, e.g., computation of relevant quantities such as drag and lift coefficients, particular flows with boundary conditions depending on the pressure, or the need of residuals' computation for stabilized discretizations.

One can find in the literature already different proposals for incorporating the pressure (or an approximation of the pressure) into the ROM. Some suggest to represent the ROM pressure solely by the velocity POD basis functions and ROM coefficients. Within the other methods, the computation of the ROM pressure relies on the pressure POD basis. However, no numerical comparison of the methods exists so far. In the group, detailed numerical studies were accomplished, involving some of the existing methods and a new one that is motivated by the residual-based stabilization for the incompressible Navier–Stokes equations. These studies were performed for a laminar flow in order to avoid possible interference with other aspects like turbulence modeling. Concerning the computing time and the accuracy, the pressure ROM methods based on the pressure POD basis performed better; see Figure 2.

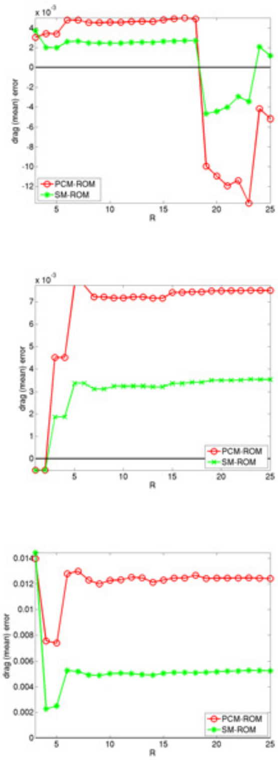


Fig. 3: *Flow around cylinder, Re = 100. Top: accurate POD basis, middle: moderately accurate POD basis, bottom: inaccurate POD basis.*

The crucial factor of ROMs is the computational efficiency. For this reason, simplified, and therefore potentially inaccurate, numerical schemes are usually incorporated into the ROMs, e.g., avoiding the accurate solution of nonlinear systems and considering, if possible, explicit time integration schemes. Hence, it can be expected that the accuracy of the ROM simulations will not be better than the accuracy of the snapshots. However, the interesting question is the following: Is the accuracy of the ROM simulations dominated by the involvement of the simple numerical methods in the ROM or by the accuracy of the underlying POD modes? To investigate this issue, ROM simulations were performed using three types of POD bases: accurate, moderately accurate, and inaccurate ones. It turned out that the accuracy of the ROM simulations correlated strongly with the accuracy of the POD basis; see Figure 3. For more details on the numerical studies; see [1].

A robust a posteriori error estimator for scalar convection-diffusion equations

A posteriori error estimates are estimates that are computed during the numerical solution of a partial differential equation. These estimates aim at two goals. First, a global upper estimate in some norm should give information about the error of the numerical solution and thus serve as a stopping criterion for the solution process. Second, local lower estimates should control an adaptive grid refinement. The theory of a posteriori error estimators and adaptive finite element methods is well developed for many problems. However, for scalar convection-diffusion equations

$$-\varepsilon\Delta u + \mathbf{b}\cdot\nabla u + cu = f \quad \text{in } \Omega, \tag{1}$$

there are still open questions. These questions are connected with the robustness of the a posteriori error estimates, i.e., with the dependence of the constants in the estimates on the data of the problem. For problems of type (1), the data are characterized by the ratio between the diffusion coefficient ε and the convection $\|\mathbf{b}\|$, where $\|\cdot\|$ is some norm. The practically interesting case is $0 < \varepsilon < \|\mathbf{b}\| = \mathcal{O}(1)$. In this case, solutions to (1) typically exhibit layers, i.e., there are subregions in which the value of the solution changes rapidly. Depending on the type of layer, their thickness is $\mathcal{O}(\varepsilon)$ or $\mathcal{O}(\varepsilon^{1/2})$.

Numerical simulations of convection-diffusion equations face the difficulty that usually the layer widths are much smaller than the mesh width such that the layers cannot be resolved. It is known that in this situation the use of stabilized discretizations becomes necessary that introduce a well-dosed amount of numerical diffusion. The most popular stabilized finite element method is the Streamline-Upwind Petrov–Galerkin (SUPG) method, which was proposed by Hughes and Brooks more than 30 years ago. The a priori error analysis of this method is well understood. Considering the a posteriori error analysis of the SUPG method, two situations could be distinguished so far. First, a posteriori error estimates in standard norms could be derived; however, they have been proved not to be robust, i.e., a reliable estimate of the global error is not possible with these estimators. And second, robust estimates were derived in norms that are not of practical interest.

In [2], the a posteriori error estimation of the SUPG method was considered in the same norm as the one used for the a priori error analysis, which is the SUPG norm. The analysis in [2] relies on some hypotheses that relate the SUPG solution to the best interpolation of the analytical solution into the finite element space. The derivation of realistic hypotheses was a central issue in this work. In the numerical studies presented in [2], it was demonstrated that the hypotheses were usually satisfied. Based on these hypotheses, which clearly restrict the mathematical generality of the error estimates, a residual-based a posteriori error estimator was derived, and an upper bound for the global error in the SUPG norm was proved. The weights in the individual terms of this estimator differ from the weights of residual-based estimators known from the literature. Numerical studies show the robustness of the error estimator; see Figure 4. Local lower estimates for the new estimator were proved in [2] without the hypotheses needed for the global upper estimate. Comparing the weights of residual-based error estimators for different norms, one finds that the new estimator tends to refine the mesh cells at the strongest layers longer than other estimators. This way of refinement reduces the error in the SUPG norm most; however, it is of disadvantage if the solution possesses layers of different type and if all of them should be computed accurately. In this situation, other residual-based estimators have been shown to work better; see Figure 5.

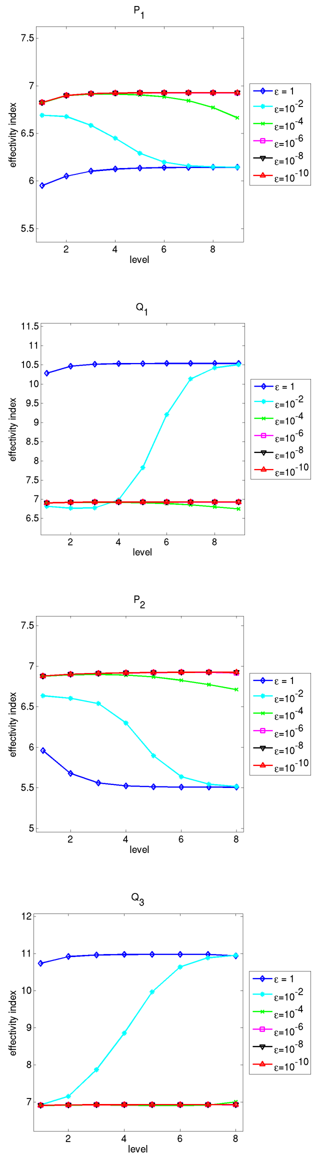


Fig. 4: *Example with analytical solution with $\|\mathbf{b}\| = \mathcal{O}(1)$. The effectivity index for different finite elements. The effectivity index is the ratio of estimated error and real error.*

Parameter calibration for multiple measurement points in gas turbine modeling

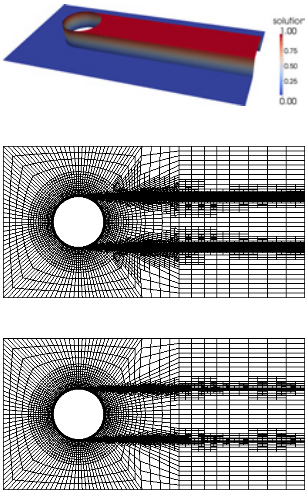


Fig. 5: *Hemker problem. Top: solution, middle: adaptive grid obtained with a residual-based error estimator for the error in $L^2(\Omega)$, bottom: adaptive grid obtained with the new residual-based error estimator for the error in the SUPG norm, both simulations with the Q_1 finite element.*

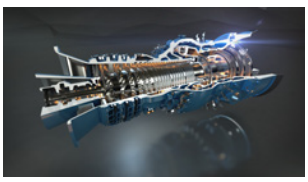


Fig. 6: *Gas Turbine GT26 (ALSTOM Power Ltd)*

The process simulator BOP provides different modes for steady-state, transient, Monte Carlo, correction-curve, homotopy, and script simulations to treat large-scale systems of differential-algebraic equations arising in process simulation problems. A recently developed optimization add-on of the process simulator may be used for the parameter calibration in gas turbine models.

The BOP optimization add-on was implemented as an algorithm of Levenberg–Marquardt type. It permits the prediction of input parameters of a process while matching certain output values, like sensory measurements, within certain tolerance bounds.

In 2012, a two-stage deterministic model calibration approach was implemented for a dataset of multiple measurement points of heat balance data for gas turbine models. In the first stage, the measurement points and the model parameters were corrected individually by use of the further developed least-squares methodology. An additional stabilization strategy was established particularly for part-load points that can cause unstable behavior of the solver in the vicinity of the least-squares estimate. Then, in the second stage, a nonparametric statistical method (like local polynomial regression) was applied to the whole dataset of corrected measurement points of the first stage. This dataset was used to interpolate important calibration parameters for process units, like for compressor efficiency or mass flow, in order to compute a new calibrated process model. Additionally to the above-mentioned deterministic approach, a stochastic calibration approach based on a Bayesian analysis for multiple measurement points was implemented as well. This approach is based on an extension of the BOP script mode and should help to gain a better insight into the problem.

The recently introduced script mode of BOP itself was extended by numerous features. Now, it provides a flexible tool for the performance of simulation sequences, e.g., for complex simulation scenarios with varying settings for parameters, initial conditions, or numerical control. Amongst other things, it can be used for process model validation or for comparative simulation runs with the detection of significant differences in the result data.

Beside the new numerical features, the process description interpreter of BOP was extended, e.g., concerning the hierarchical process description (the so-called *MACRO feature*), the treatment of global parameter arrays, and an optional user-defined scaling of process variables.

The version BOP2.9, including new features and improvements, will be released in March 2013.

References

[1] A. Caiazzo, T. Iliescu, V. John, S. Schyschlowa, *A numerical investigation of pressure reduced order models for incompressible flows*, WIAS Preprint no. 1765, 2013, submitted.

[2] V. John, J. Novo, *A robust SUPG norm a posteriori error estimator for stationary convection-diffusion equations*, Comput. Methods Appl. Mech. Engrg., **255** (2013), pp. 289–305.

[3] H. Si, *TetGen, A quality tetrahedral mesh generator*, WIAS Preprint no. 1762, 2013, submitted.

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 2012, the group continued its participation in the DFG Priority Program SPP 1204. 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 98 ff.

A special highlight result of last year's work was achieved in PDE-constrained optimal control. In a collaboration with the Research Group *Partial Differential Equations*, Klaus Krumbiegel and Joachim Rehberg were able to extend known one-dimensional results for second-order sufficient optimality conditions for control problems with semilinear parabolic partial differential equations and pointwise state and control constraints to two- and three-dimensional problems, thereby solving a long-standing problem [5].

In the following, further scientific achievements of the research group in 2012 are detailed.

Optimization and optimal control

Stochastic Optimization is a major research topic in the group. The application background is given by optimization problems arising in the generation, the management, and the trade of energy. These problems are typically affected by random parameters such as demand, prices, or meteorological uncertainty (wind, precipitation). The group's research is anchored in the MATHEON projects C7 "Stochastic optimization models for electricity production in liberalized markets" and B20 "Optimization of gas transport", as well as in an industry project on gas network optimization. Here, the mathematical objects of primary interest are optimization problems with probabilistic constraints or with equilibrium constraints. The progress of the group's work in this field led to a participation in the *Gaspard Monge Program for Optimization and Operations Research*, launched by Electricité de France (EDF) and the Jacques Hadamard Mathematical Foundation. As a part of the project "Stochastic optimization for unit-commitment problems" in this program, a Ph.D. thesis at EDF is currently co-supervised.

Probabilistic constraints represent a well-established model for finding decisions that are robust against uncertainty and can be interpreted in a probabilistic sense. A major challenge in optimization problems with probabilistic constraints is the approximation of function values and gradients.

Therefore, a principal concern of the group's research was to find analytical reductions of gradients to function values [3] that allowed to employ available codes for the latter in order to cope with gradients at the same time and without introducing additional inaccuracy. This approach is a key for employing appropriate nonlinear optimization methods.

Figure 1 illustrates the solution to such a problem involving a coupled system of a wind farm and a water reservoir that together are supposed to satisfy at high probability a given demand profile. Randomness enters here via the uncertain amount of wind energy that has to be complemented by hydro energy. The surplus hydro energy is sold at the market. By the possibility to store water, the selling profile can be adjusted in a way to follow as much as possible a certain given price profile under the probabilistic constraint of demand satisfaction and the constraint of respecting the reservoir capacity.

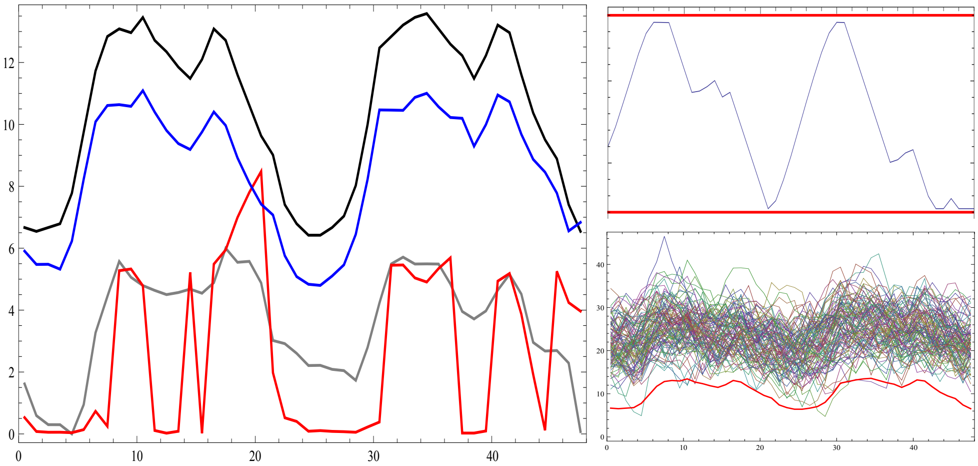


Fig. 1: *Optimal management of a water reservoir coupled with a wind farm. Left: Hydro energy (blue) complemented by random wind energy to satisfy demand (black) and surplus hydro energy (red) sold at market according to price (grey). Right top: Filling level profile of the reservoir within capacity limits. Right bottom: Satisfaction of demand (red) for 100 simulated scenarios (wind + hydro).*

In the MATHEON project C11 "Modeling and optimization of phase transitions in steel" , the work on the shape optimization of a sharp interface model to describe distortion compensation was continued, where changing the interface allows to control the outer workpiece shape. Using a reformulation as a transmission problem, shape differentiability could be proved. Moreover, even in view of the low regularity of the solution to the mixed-type elliptic system it was possible to use the so-called *Lagrange method* to calculate the shape derivative. Using the expression for the shape derivative, a numerical solution strategy was developed employing a spline representation of the interface.

Based on modeling experience in solid-solid phase transitions, the identification of thermal growth parameters for tissue coagulation models was investigated [4].

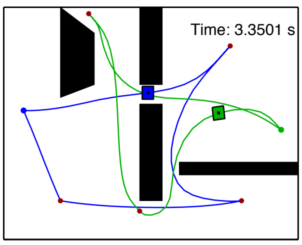


Fig. 2: *Snapshot of the optimal task assignment and motion planning of two robots where the red dots are the task location*

The MATHEON project C30 "Automatic reconfiguration of robotic welding cells" is divided into a discrete and a continuous part. The first focus of the continuous part is to compute for each robot the fastest trajectory that connects two weld points and avoids obstacles. This goal was achieved in 2011 by developing a time-optimal control problem. In 2012, heuristics were developed to find an efficient initialization of the control variables and to automatically set a value to all parameters (e.g., the number of time steps). Moreover, an algorithm detecting the existence of collisions between the trajectories of the robots was developed. These two accomplishments enabled the coupling with the discrete part of the project, developed by Martin Skutella (Technische Universität Berlin). The resulting algorithm is an efficient interplay between continuous and discrete optimization, which was tested on a two-dimensional example.

Inverse problems

The work on elastic wave scattering by diffraction gratings and rough surfaces [2] was continued within a DFG Individual Grant Project, which was successfully completed in July 2012. For the details about the results on direct and inverse scattering problems, see the Scientific Highlights article “Recent Progress in Elastic Wave Scattering” by Johannes Elschner and Guanghui Hu on page 22. As another success, the new project “Direct and inverse interaction problems with unbounded interfaces between acoustic, electromagnetic and elastic waves” within the DFG’s Research Grants Programme could be acquired. This project is devoted to the mathematical analysis and numerical treatment of the scattering of time-harmonic acoustic and electromagnetic waves by an unbounded elastic body that can be modeled by transmission problems for the Helmholtz (or Maxwell) equations coupled with the Navier equation through a periodic or non-periodic unbounded interface. Moreover, in cooperation with Andreas Kirsch (KIT Karlsruhe) and Mourad Sini (RICAM Linz), the recovery of bounded obstacles from the far-field pattern of elastic shear or pressure waves was investigated, leading to new uniqueness results and a reconstruction algorithm based on the factorization method.

The numerical analysis of the group’s methods for the simulation and optimization of the scattering by biperiodic surface structures was continued. The unique solvability of a variational equation was shown that couples Fourier-mode expansions over unbounded half spaces with classical variational forms over finite computational domains. This result allows the treatment of boundary value problems without the exclusion of Rayleigh frequencies and, as shown in a subsequent paper, enables the convergence analysis of finite element methods coupled with truncated Fourier-mode expansions.

For surface structures with stochastic features, the scattering of plane waves by rough interfaces was analyzed in [1]. Following ideas of Stearns, in the low contrast regime of extreme ultraviolet wavelengths, a class of interfaces was fixed, and approximate formulas for the scattered electric field and the corresponding far-field were derived. In cooperation with the Physikalisch-Technische Bundesanstalt in Berlin, the numerical simulation of lithographic line-space structures with stochastic deviations (line-width and line-edge roughness) was continued, and improved methods for the reconstruction algorithm of scatterometric measurements were discussed; cf. Figure 3.

The theoretical and algorithmic work on the integral equation solver for conical diffraction was intensified in connection with the collaborative project “Grating simulation in field tracing” together with LightTrans GmbH Jena. The project is supported by the Federal Ministry of Economics and Technology within the framework of the Central Innovation Program for small and medium-sized enterprises (ZIM). The aim is the development of an enhanced and robust simulation method of diffraction gratings based on the integral method and its subsequent adaption to the field tracing approach and software of the project partner.

To this end, spline discretizations of the occurring integral operators were studied, and the convergence of spline collocation for the system of singular integral equations for conical diffraction was established. Collocation algorithms with cubic splines were implemented for the special case of one-profile gratings, which provide higher accuracy compared with trigonometric collocation or Nyström methods. First numerical tests for multi-profile gratings indicate that the spline methods can treat extremely difficult diffraction problems, including thin layers and large period-over-wavelength ratios. Optimal quadrature rules to compute the integrals of splines have to be developed to speed up these methods.

The integral equation solver for multi-profile gratings where the interfaces between adjacent materials cannot be separated by horizontal planes [6] has now the same functionality as the solver for gratings with separable interfaces. Much effort has been spent on the adaptation of the software to a common platform for the cooperation with the project partner. Here, new types of grating profiles and interfaces between different materials were introduced and pre- and postprocessing algorithms were implemented, allowing for the integration of the grating simulation into the field tracing approach.

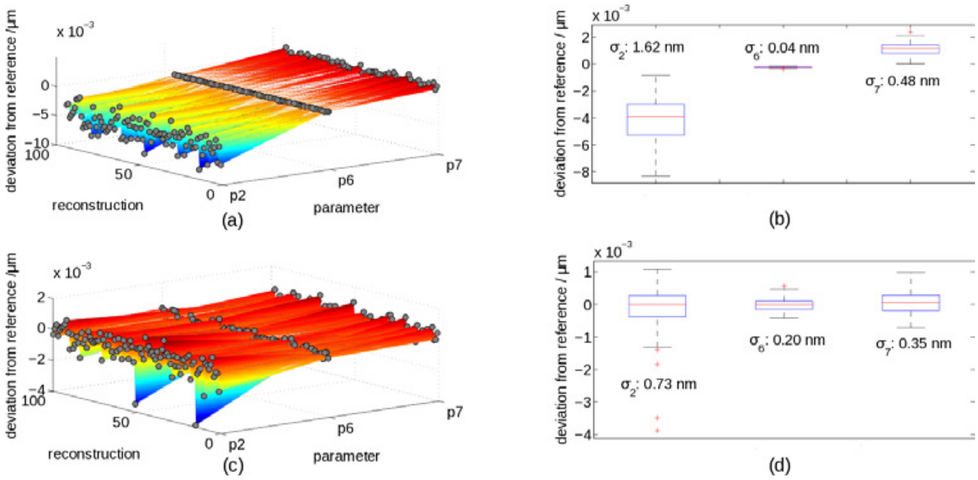


Fig. 3: *Reconstruction of top and bottom width (p2 and p7) and of height (p6) of absorber lines from "measured" efficiency data with random noise (line-edge and line-width roughness). (a)/(b): Deviation of reconstructed values using an inverse algorithm designed for unperturbed data. (c)/(d): Deviation using an inverse algorithm with a special bias correction of the perturbed efficiency data.*

References

[1] T. Arnold, A. Rathsfeld, *Reflection of plane waves by rough surfaces in the sense of Born approximation*, WIAS Preprint no. 1725, 2012, to appear in: Math. Methods Appl. Sci.

[2] J. Elschner, G. Hu, *Elastic scattering by unbounded rough surfaces*, SIAM J. Math. Anal., **6** (2012), pp. 4101–4127.

[3] R. Henrion, A. Möller, *A gradient formula for linear chance constraints under Gaussian distribution*, Math. Oper. Res., **37** (2012), pp. 475–488.

[4] D. Hömberg, J. Liu, N. Togobytska, *Identification of the thermal growth characteristics of coagulated tumor tissue in laser-induced thermotherapy*, Math. Methods Appl. Sci., **35** (2012), pp. 497–509.

[5] K. Krumbiegel, J. Rehberg, *Second order sufficient optimality conditions for parabolic optimal control problems with pointwise state constraints*, SIAM J. Control Optim., **51** (2013), pp. 304–331.

[6] G. Schmidt, *Conical diffraction by multilayer gratings: A recursive integral equations approach*, Appl. Math., **58** (2013), pp. 279–307.

4.5 Research Group 5 "Interacting Random Systems"

The group continued its research activities on a number of topics like mobile ad-hoc networks (see the Scientific Highlights article on page 33), spectra of random Schrödinger operators, interacting many-body systems, and the topics described below. In this way, a number of timely applications of large interacting random systems are under study in various fields like kinetic theory, statistical mechanics, and telecommunication networks. In connection with the latter topic, a strategic partnership with the Leibniz-Institut für innovative Mikroelektronik (Frankfurt/Oder) was initiated. Furthermore, the group became also a member of the newly installed nationwide DFG Priority Program (SPP) 1590 "Probabilistic Structures in Evolution", where the group studies branching processes in random environment.

As one activity of WIAS on the way to a more systematic combination of the fields of analysis and stochastics, the group co-organized with Research Groups RG 1 *Partial Differential Equations* and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* a WIAS Workshop, combined with two minicourses delivered by eminent experts, on the subject "From Particle Systems to Differential Equations". Further such workshops are to come in the future, and some strategic decisions about joint research positions were made. Three students of Wolfgang König, the head of the group, successfully continued their studies in 2012 and will be finishing their Ph.D.s early in 2013 on topics that each have a strong analysis component. Moreover, the head of the group was a member of the organizing commitee of the prestigeous Workshop on "Mathematics of Many-particle Systems" on the occasion of Elliott Lieb's 80th birthday and co-organized an Oberwolfach Workshop on the "Interplay of Analysis and Probability in Physics".

The nationwide DFG Research Unit FOR 718 *Analysis and Stochastics in Complex Physical Systems*, headed by Wolfgang König, also continued its activities, among which there were two group meetings and several public talks and workshops at various places. Unfortunately, this unit is close to its end, and the funding terminates in 2013. The Springer Festschrift on the occasion of the birthdays of Profs. Bolthausen and Gärtner, co-edited by the head of the group, finally appeared in 2012. The regular bi-weekly seminar of the Berlin probability community took place at WIAS in the winter term this year, featuring a number of prestigeous speakers.

The Center for Mathematics and Science Education and Hands-on Museum "INSPIRATA", located in Leipzig and chaired by Wolfgang König, continued its long way to consolidation and to strong and positive mindfulness; the visitor numbers steadily increase, and in November there was a successful vernissage for an exhibition of paintings on the subject of Pythagoras' theorem.

A closer description of some of the group's achievements in 2012 follows.

Stochastic particle methods for kinetic equations

Nonlinear kinetic equations are closely related to stochastic interacting particle models. These connections provide the basis both for analytical studies and for numerical approximations. A challenging field of application is chemical engineering, where population balance equations are used to describe the dynamic processes of growth and evolution of particles. Stochastic particle methods offer an attractive choice of solution method as they are capable of tracking high-dimensional systems and provide information about the history of individual particles.

A class of stochastic algorithms for the numerical treatment of multidimensional population balance equations has been developed in recent years. These 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. A spatially resolved stochastic weighted particle method for coagulation-advection problems with inception was presented in [6]. Convergence of stochastic particle systems to a deterministic limit was studied in another work of the group. A particular challenge was the treatment of bounded domains with realistic boundary conditions.

Several new results were obtained in collaboration with the Department of Chemical Engineering and Biotechnology (University of Cambridge, UK). A mathematical model for the formation and growth of silica nanoparticles was introduced. Each particle is described by its constituent primary particles and the connectivity between these primaries (see Figure 1). Each primary in turn has internal variables that describe its chemical composition. In [5], stochastic weighted algorithms were applied to this multidimensional particle model. 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. Convergence properties were studied, and it was demonstrated that stochastic weighted algorithms can be successfully used with complex coagulation kernels and high-dimensional particle models.

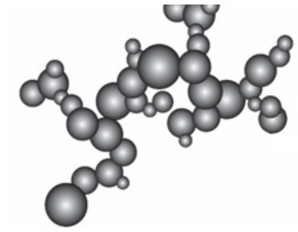


Fig. 1: *Schematic of a soot particle*

Another field of application of stochastic particle methods is electron transport and heat generation in semiconductor devices. An improved version of the electrothermal Monte Carlo method was presented by the group as well. This modification has better approximation properties due to reduced statistical fluctuations.

Out-of-equilibrium dynamics of complex disordered systems

One of the most important classes of disordered systems that has been studied both experimentally and theoretically are spin glasses. Experimentally, the dynamics of spin glasses exhibits striking decorrelation properties such as aging, rejuvenation, and memory effects. On the theoretical side, a crucial and intriguing phenomenon of the statistical properties of spin glasses is that in the thermodynamic limit the energy landscape has a hierarchical organization. Hence, it is important to understand the dynamics of spin glasses having such a hierarchical structure. With this goal in mind, the group introduced GREM-like trap models, where “GREM” stands for “generalized random energy model”. This model describes a dynamical spin glass model in which the hierarchy of the energy landscape is given through a finite tree. Carefully using techniques from the theory of point processes, the group was able in [2] to analyze the limiting decorrelation behavior of the model over large two-time windows, to prove that the system ages, and to identify the limiting aging functions on all possible time scales.

This GREM-like model is adequate for spin glass models in which the limiting hierarchical structure of the energy landscape has finite levels, such as p-spin models. However, in the case of the most important spin glass model, the Sherrington–Kirkpatrick model, the limiting hierarchical structure of the energy landscape has infinite levels. Hence, the group introduced so-called *CREM-like trap models*, which have infinite levels of hierarchy and can be seen as a limit of GREM-like trap models. Studying this model, the group discovered a connection with the theory of branching processes, more precisely, with continuous-state branching processes (CSBP). In [3], the group identified the limiting decorrelation functions of the CREM-like trap models as the genealogical structures of a certain CSBP, namely Neveu's CSBP, and proved aging. The group expects that this infinite-level model exhibits rejuvenation and memory effects on certain time scales of observation and is working on developing the necessary tools to carry out such an analysis.

Branching random walks in random environment

The group studies systems of particles that randomly migrate in space, are randomly killed, and randomly produce offspring, according to random space-dependent killing/branching rates. The main question concerns the main flow of the particles when the system evolves for a long time. An intermittency effect is expected to determine the long-time behavior of the system, i.e., a huge number of particles are expected to accumulate at certain places with extremely good killing/branching rates, and a mass migration occasionally takes place between these preferable places. The goal of the study is to deeper understand this picture and to find methods to prove it. A first step is the consideration of the moments of the total number of particles, where the expectation of the n-th power of the population size is taken over the migration and the killing/branching, for fixed rates. Afterwards, the expectation of its p-th power is taken over the randomness of the rates, and the long-time limit is studied.

The first step in this program is to find and prove a formula for the former expectation, and this is one of the main results of [4]. Indeed, a Feynman–Kac-like formula is found and proved there with the help of spine techniques from the theory of branching processes, as an alternate strategy to PDE methods that were used before. The value of these new formulas is demonstrated in [4] by deriving the first two terms of the long-time asymptotics of the p-th moments, taken over the environment. The entire research project strongly benefits from the group's long-term expertise on the parabolic Anderson model, a famous model that describes the mass flow through a random environment of sinks and sources.

Effective conductance in random electrical networks

The random conductance model describes current flow and diffusion in an inhomogeneous medium. In the rectangular lattice, each bond is assigned a random positive value, the conductance. The effective conductance, associated with a domain and a set of boundary conditions, is the amount of current that flows in and out of the boundary of this domain if the voltage on the boundary is kept at a value prescribed by the boundary conditions. The main question here is in what way electric conductance is averaged out if the inhomogeneities are on very small scales. For convenience, one usually considers the equivalent notion of inhomogeneities on unit scale and a "blown-up" domain. At least for linear boundary conditions, the effective conductance is of volume order. It is reasonably well known that, normalized by volume, it converges to a certain average that depends on the distribution of the conductances. The group's goal is to derive a central limit theorem under most general conditions, as the scale tends to infinity, i.e., to show that the random fluctuations of the effective conductance are comparable to the square root of volume times a Gaussian random variable.

In [1], the group achieved this goal under three critical assumptions: (1) The boundary conditions are given by a linear function, (2) the region is box-shaped, and (3) the conductances are close to a constant. The latter condition is needed for controlling the distance between gradients of finite-volume correctors on the one hand and those of the infinite-volume counterpart on the other hand, in some L^p sense with $p > 4$. These two objects are essential in describing effective conductance in terms of minimal Dirichlet energy and are well known to be close in a corresponding L^2 sense. Based on Meyers' estimate and the Calderón–Zygmund regularity theory, the group was able to establish this result. In future work, the group will be trying to avoid the assumption (3), and hopefully also to weaken the other two assumptions.

References

[1] M. Biskup, M. Salvi, T. Wolff, *A central limit theorem for the effective conductance: I. Linear boundary data and small ellipticity contrasts*, WIAS Preprint no. 1739, 2012, submitted.

[2] V. Gayrard, O. Gün, *Aging for GREM-like trap models*, in preparation.

[3] V. Gayrard, O. Gün, *Trap models with infinite levels and genealogies of continuous state branching processes*, in preparation.

[4] O. Gün, W. König, O. Sekulović, *Moment asymptotics for branching random walks in random environment*, WIAS Preprint no. 1729, 2012, to appear in: Electron. J. Probab.

[5] W.J. Menz, R.I.A. Patterson, W. Wagner, M. Kraft, *Application of stochastic weighted algorithms to a multidimensional silica particle model*, Preprint no. 120, University of Cambridge, Cambridge Center for Computational Chemical Engineering, 2012, submitted.

[6] R.I.A. Patterson, W. Wagner, *A stochastic weighted particle method for coagulation-advection problems*, SIAM J. Sci. Comput., **34** (2012), pp. B290–B311.

4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

The research group focuses on the research projects Statistical Data Analysis and Applied Mathematical Finance. Applications are mainly in economics, financial engineering, medical imaging, life sciences, and mathematical physics. Special interest is in 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 DFG Research Center MATHEON projects F10 and E5 and the SFB 649 project B5; see page 99. 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 100). 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".

Scientific highlights achieved by the research group in 2012 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 2012:

- Continuation of the mega-grant with the Moscow Institute of Physics and Technology
- Successful defense of the B5 project "Structural adaptive data analysis" within the Collaborative Research Center (SFB) 649 and the prolongation of the Center for the next four years
- Participation in the Research Unit 1735 "Structural Inference in Statistics: Adaptation and Efficiency" with the project "Semiparametric approach to structural adaptive estimation"
- Ph.D. thesis of Hilmar Mai

Modern statistical analysis faces numerous challenges due to model complexity and uncertainty leading to a small or limited sample size and very complicated parametric models with a huge number of parameters. The classical asymptotic theory is hardly applicable in such a situation, new methods and approaches are called for. The paper [2] offered a novel approach to studying a general statistical problem that can be viewed as an extension of the famous Le Cam *Local Asymptotic Normality* theory to the nonparametric situation, which has been an open problem for more than 60 years. The main features of the approach that make it different from the classical one are: (1) the study is non-asymptotic, that is, the sample size is fixed and does not tend to infinity; (2) the parametric assumption is possibly misspecified, and the underlying data distribution can lie beyond the given parametric family. These two features enable to bridge the gap between parametric and nonparametric theory and to build a unified framework for statistical estimation.

The main results include a *large deviation bound* for the (quasi) maximum likelihood and a *local bracketing* result for the log-likelihood process. The latter yields a number of important corollaries for statistical inference: concentration, confidence and risk bounds, expansion of the maximum likelihood estimate, etc. All these corollaries are stated in a non-classical way, admitting a model misspecification and finite samples. However, the classical asymptotic results including the efficiency bounds can be easily derived as corollaries of the non-asymptotic statements obtained. At the same time, the new bracketing device works well in the situations with large or growing parameter dimension in which the classical parametric theory fails.

The Bayesian approach becomes more and more popular in statistical applications in the recent years. The theoretical foundation of this approach is given by the prominent Bernstein–von Mises (BvM) theorem, which claims asymptotic normality of the posterior distribution. The bracketing device of [2] appears very useful for proving and extending the BvM result to the cases with a possible model misspecification and a limiting sample size. It helps to address the important question of a *critical dimension*, which is the largest possible dimension of the parameter space for which the BvM result still applies; [3].

Quantile regression is a popular technique to estimate conditional quantile curves. It provides a comprehensive picture of a response contingent on explanatory variables. In a flexible modeling framework, a specific form of the conditional quantile curve is not a priori fixed. This fact motivates a local parametric rather than a global model-fitting approach. A nonparametric smoothing estimator of the conditional quantile curve requires to balance between local curvature and stochastic variability. A local model selection technique that provides an adaptive estimator of the conditional quantile regression curve at each design point was suggested. Theoretical results claim that the proposed adaptive procedure performs as good as an oracle, which would minimize the local estimation risk for the problem at hand.

Stochastic differential equations that allow solutions with discontinuous trajectories enjoy increasing popularity in many fields of applications as, for example, in mathematical finance or system biology. Their discontinuities allow for sudden changes in market behavior or biological systems that lead to a more realistic description of empirical data and a better understanding of the underlying market mechanisms or natural processes. Classical statistical theory usually fails to produce accurate results when applied in this more flexible jump process setting. The new challenges that appear are twofold. The first step requires the separation of continuous and jump components of the process under investigation. The second step consists usually of semi- or non-parametric estimation problems for the characteristics of the system that often involves inverse problems. The group developed efficient approaches for both problems, recently focusing on the separation step. It was demonstrated that jump filtering techniques lead to feasible estimation methods that produce optimal results for very general model classes.

Interesting results were obtained at the interface between classical regularization theory and sta-

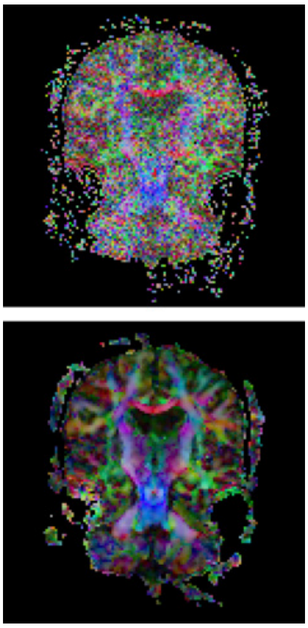


Fig. 1: *Comparison of color coded FA estimates in ultra-high resolution dMRI. Top: voxelwise estimates, bottom: exploiting spatial structure.*

tistical inverse problems. An attempt was made to base model selection on the discrepancy (data misfit). In classical regularization, the related *discrepancy principle* is the standard tool for the parameter choice, whereas a similar procedure was not available in statistics. In a series of papers, see e.g. [1], variants for the discrepancy principle were developed with a theoretical justification, and preliminary numerical studies show their robustness in applications.

Problems from Neuroimaging are investigated within the MATHEON project F10 in close collaboration with partners from university hospitals and neuroscience research institutes. Research concentrates on improvements of data quality and novel modeling techniques in experiments at the current technical borderline. These are characterized by high resolution, extremely low signal-to-noise ratio, and complex models needed to describe the structures of interest.

In collaboration with the biometrics department at the University of St. Andrews and the Leibniz Institute for Zoo and Wildlife Research in Berlin, a new project was initiated that strives for the application of these tools to obtain a better understanding of ecosystems with a focus on the behavior of endangered animal species and wildlife diseases.

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. In particular, in the project there is a strong expertise in the application of these methods and solutions to interest rate modeling and valuation.

Highlights 2012:

- Continuation of the cooperation contract with HSH Nordbank
- Successful defense of the MATHEON E5 project "Statistical and numerical methods in modeling of financial derivatives and valuation of risk"

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. In 2011, 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. As an innovation, the multilevel idea is applied to the number of subsimulations used in the problem of trajectory-wise estimation of conditional expectations that arises in several simulation-based methods for the evaluation of high-dimensional American options.

Before, the multilevel idea was virtually exclusively applied to the size of the time steps used in the simulation of stochastic differential equations. Now, a multilevel version of the Kolodko–Schoenmakers-2005 policy iteration is developed. In this context, it is shown that the bias rate of simulation-based policy iteration equals one under mild conditions. The proof of this statement required parts of large deviation theory and was rather involved. Nowadays, rough path theory is emerging more and more in finance. In this respect, new simulation schemes for rough financial quantities are constructed and also put into a multilevel framework.

As a new topic, a generic approach for the simulation of conditional diffusions is in development. This approach turns out to be very useful, for example, in the evaluation of derivatives that involve the traded variance of underlying assets. The method is based on forward-reverse simulation (due to Milstein–Schoenmakers–Spokoiny 2004) and, as such, may be considered a completely new access to the problem of conditional simulation.

Another line of research is the use of asymptotic expansions for option pricing. Even for relatively simple models, like local volatility models or the Black–Scholes model, the pricing of high-dimensional basket/index or spread options is difficult using non-simulation-based algorithms due to the curse of dimensionality. For such products extremely accurate formulas based on heat kernel expansions were derived that allow for very fast approximations in high-dimensional environments [5].

In the area of interest-rate modeling, the focus this year was on a new expiry-wise stochastic volatility LIBOR model that allows for a more stable and more fast calibration, in particular in times of crisis. Moreover, a new method for coupling local currency LIBOR models to FX LIBOR models was provided. The successful continuation of the contract with HSH Nordbank was partially due to the latter developments and partially due to the extensive implementation work done by Marcel Ladkau and Jianing Zhang.

The research on optimal dual martingales for American options and generalized multiple stopping for options in energy markets (swing options) in the preceding year required mayor revisions in the reporting year, but now it has culminated in [6] and [4], respectively.

References

[1] G. Blanchard, P. Mathé, *Discrepancy principle for statistical inverse problems with application to conjugate gradient iteration*, Inverse Problems, in press, doi:10.1088/0266-5611/28/11/115011.

[2] V. Spokoiny, *Parametric estimation. Finite sample theory*, Ann. Statist., **40** (2012), pp. 2877–2909.

[3] V. Spokoiny, *Roughness penalty, Wilks phenomenon, and Bernstein–von Mises theorem*, arXiv:1205.0498, Cornell University Library, arXiv.org, Ithaca, USA, 2012, submitted.

[4] C. Bender, J. Schoenmakers, J. Zhang, *Dual representations for general multiple stopping problems*, WIAS Preprint no. 1665, to appear in: Math. Finance.

[5] C. Bayer, P. Laurence, *Asymptotics beats Monte Carlo: The case of correlated local vol baskets*, to appear in: Commun. Pure Appl. Math.

[6] J. Schoenmakers, J. Zhang, J. Huang, *Optimal dual martingales, their analysis and application to new algorithms for Bermudan products*, SIAM J. Financial Math., **4** (2013), pp. 86–116.

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

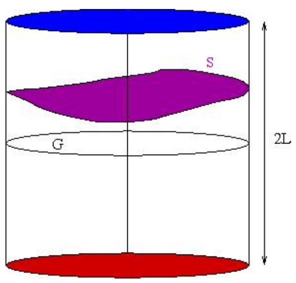
The topics of the research group may be found within three essential categories:

- Production and application of modern materials
- Energy technology
- Multiscale problems and 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, transport of matter, diffusion problems in gases, liquids, and crystals, as well as nucleation of droplets and bubbles. An essential part of the current issues addresses problems in the context of electrochemical energy storage systems.

The complexity of the problems treated arises from various strong couplings, for example, interface motion producing mechanical stresses, quasi-electrostatic fields influencing diffusion of charged particles in electrolytic solutions, chemical reactions producing mechanical stresses, the appearance of precipitates in crystals leading to lattice deformations, long-range energetic and entropic interactions leading to nonlocal PDEs, and pattern formation of nano-scale films.

Highlights



1. Significant progress was achieved in the analysis of phase transitions in the Stefan–Gibbs–Thompson setting and the related control problem. The results are of large importance for industrial crystal growth processes. In a series of three papers, Pierre-Étienne Druet studies the optimization of the stationary temperature distribution and the equilibrium shape of the solid-liquid interface in a two-phase system subjected to a temperature gradient. The interface is described by a geometric equation that follows from the minimization of an interfacial free energy.

$$\mathrm{div}_S(\sigma_q(x,\nu)) + \sigma_x(x,\nu)\cdot\nu = \theta\,. \tag{1}$$

The heat conduction problem consists of the PDE

$$\mathrm{div}(k_S \nabla\theta) = f \quad \text{in} \quad \Omega\backslash S \tag{2}$$

and of the boundary conditions

$$[[\theta]]_S = 0, \quad [[-k_S\nabla\theta\cdot\nu]] = 0 \quad \text{on } S \qquad -k_S\nabla\theta\cdot\nu = \beta(\theta^4-\theta_{\text{ext}}^4) \quad \text{on} \quad \partial\Omega. \tag{3}$$

The paper [1] identifies the mathematical requirements such that classical solutions exist. In the WIAS Preprint no. 1708 *"Some mathematical problems related to the second order optimal shape of a crystallization interface"*, Pierre-Étienne Druet derives a new first-order optimality system for a class of objective functionals that account for the second surface derivatives and for the surface temperature gradient.

2. The fast charging regime of lithium-ion batteries involves a phase transition that may be described by a coupled diffuse-interface PDE system including the viscous Cahn–Hilliard equation. In order to illustrate an observed thermodynamic inconsistency context, Wolfgang Dreyer and Clemens Guhlke considered a single viscous Cahn–Hilliard equation.

Diffuse- and sharp-interface models represent two alternatives to describe phase transitions with an interface between two coexisting phases. The two model classes can be independently formulated. Thus there arises the problem whether the sharp limit of the diffuse model fits into the setting of a corresponding sharp-interface model. A diffuse model is called *admissible* if its sharp limit produces interfacial jump conditions that are consistent with the interfacial balance equations and the second law of thermodynamics for sharp interfaces. Special cases of the viscous Cahn–Hilliard equation show that there are admissible as well as non-admissible diffuse-interface models. The details are extensively described in [5].

3. In 2012, the analysis of a new model for diffusive phase segregation due to Paolo Podio-Guidugli (Rome) was extended to phase field systems of the form

$$(\varepsilon + 2g(\rho))\,\mu_t \;+\; \mu\, g'(\rho)\,\rho_t \;-\; \operatorname{div}(\kappa(\mu,\rho)\,\nabla\mu) = 0\,, \tag{4}$$

$$\delta\rho_t \;-\; \sigma\,\Delta\rho \;+\; \partial f_1(\rho) + f_2'(\rho) \ni \mu\, g'(\rho). \tag{5}$$

Here, ρ is an order parameter (typically, the fraction of one of the phases), μ is the chemical potential, ε, δ, and σ are positive physical constants, and κ stands for a nonnegative diffusivity. g is a smooth nonnegative function, and the coarse-grain free energy f is of the form $f = f_1 + f_2$, where f_2 is smooth and f_1 is a proper, convex, and lower semicontinuous function. In this sense, ∂f_1 stands for the set-valued *subdifferential* of f_1, and (2) is an inclusion. Typical cases are the *logarithmic potential* $f_1(\rho) = \rho\,\ln(\rho) + (1-\rho)\,\ln(1-\rho)$ or the *indicator function* of the interval $[0,1]$, $f_1(\rho) = I_{[0,1]}(\rho)$ $(= 0$ if $\rho \in [0,1]$, and $= +\infty$ otherwise).

The system (1), (2) is a highly nonlinearly coupled system of singular partial differential equations whose analysis requires delicate estimates and advanced 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 $0 \le \rho \le 1$.

In [3], global existence was shown for the non-degenerate case that $\kappa(\mu,\rho) \ge \kappa_* > 0$, while the submitted WIAS Preprint no. 1713 *"Global existence and uniqueness for a singular/degenerate Cahn–Hilliard system with viscosity"* also addressed the degenerate case when κ may become zero. In the WIAS Preprint no. 1742 *"Continuous dependence for a nonstandard Cahn–Hilliard system with nonlinear atom mobility"*, the continuous dependence on initial data was investigated for the case $\kappa(\mu,\rho) = \kappa(\mu) \ge \kappa_* > 0$. The asymptotic behavior as $\varepsilon \searrow 0$ and $\sigma \searrow 0$ was rigorously analyzed in [4] and in the WIAS Preprint no. 1758 *"A vanishing diffusion limit in a nonstandard system of phase field equations"*, respectively. Finally, optimal distributed and boundary control problems were treated for the differentiable case of the logarithmic potential.

Funded under Priority Programs of the German Research Foundation

Barbara Wagner participates 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"*. In 2012, she successfully submitted a new proposal on *"Mathematical modeling, analysis and numerical simulation of thin liquid bilayers"* and obtained a funding for the second three-year period of the SPP.

In 2012, Sebastian Jachalski, in collaboration with Dirk Peschka and Andreas Münch from the University of Oxford, developed new thin film models for systems of two immiscible liquid films on a solid substrate. By introducing new kinds of slip conditions, they could predict new patterns of dewetting thin films. The significance of variations of the slip condition is carefully described and illustrated in the WIAS Preprint no. 1743 *"Impact of interfacial slip on the stability of liquid two-layer polymer films"*.

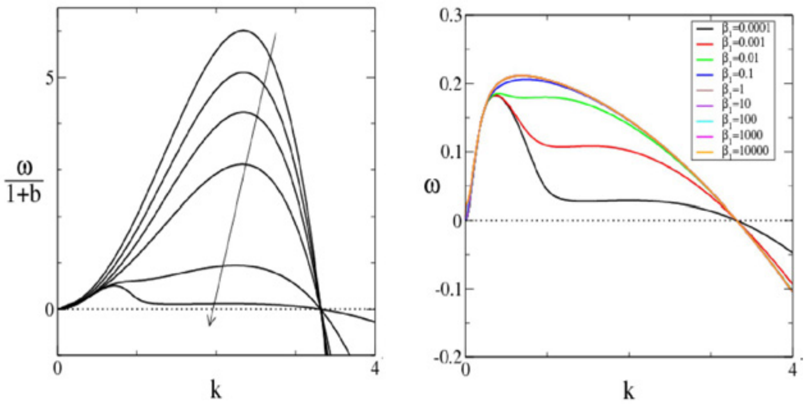


Fig. 1: *Dispersion relations reflect the stability of thin films encoded by wave number k and the frequency of the film height disturbances. Negative frequencies indicate stability. $1/\omega_{max}$ determines the time of rupture. For various slip lengths: weak slip (left) and strong slip (right).*

DFG-CNRS research group

Within the framework of a German-French research group on liquid-vapor flow, Wolfgang Dreyer and Christiane Kraus from the Young Scientists' Group *Modeling of Damage Processes* jointly guided an interdisciplinary project on diffuse-interface models and their sharp-interface limits.

In 2012, Jan Giesselmann formulated and studied a hierarchy of new diffuse-interface models for compressible two-phase mixtures without and with electrically charged constituents. The most important achievements concern a decoupling of the diffuse-interface thickness and the surface tension by the introduction of an artificial phase field and a special scaling. Usually, both quantities are linearly coupled, which leads to extreme numerical difficulties because, in this case, numerically resolvable interfaces imply unrealistically large surface tensions. Moreover, the new diffuse models exhibit again the following peculiar property: Only diffuse models with weak viscosities lead in the sharp limit to physically reasonable interface conditions describing the phase transition. Currently, it is not clear if this is a generic feature of diffuse models.

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"

The project C10, guided by Barbara Wagner, may serve as an example of a typical MATHEON research project. Dirk Peschka studied a two-dimensional multiphase Stokes flow with finite elements.

A multiphase flow of two viscous Newtonian liquids is generated by surface tension. The variational formulation of the problem is based on a gradient flow structure with energy

$$E = \sum_{i=1}^{3} \sigma_i \int_{\Gamma_i} d\Gamma \,.$$

The dissipated energy production reads

$$D = \int_{\Omega} \tau(\mathbf{u}) : \tau(\mathbf{u}) \, d\Omega \,,$$

where τ is the shear stress tensor in the space of volume-preserving deformations $\mathbf{u}$. Upon variation $\mathbf{u} = \operatorname{argmin}_u(\frac{1}{2}D + E)$, this approach results in the weak formulation

$$\sum_j \frac{1}{2\mu_j} \int_{\Omega_j} \tau(\mathbf{u}) : \tau(\mathbf{v}) \, d\Omega + \sum_i \int_{\Gamma_i} \sigma_i \left(\nabla_{\|}\mathrm{id}\right) : \left(\nabla_{\|}\mathbf{v}\right) d\Gamma = 0 \,,$$

which is discretized applying P_2 (velocity) and $P_1 + P_0$ (pressure)-extended Taylor–Hood elements. Using the Laplace–Beltrami technique via $\sigma_i\left(\nabla_{\|}\mathrm{id}\right) : \left(\nabla_{\|}\mathbf{v}\right)$ is sufficient to introduce curvature by employing a piecewise C^1 representation of boundary. Since no in-/outflows are present, mesh motion via $\dot{x} = \mathbf{u}$ is sufficient if the mesh quality is controlled (remeshing).

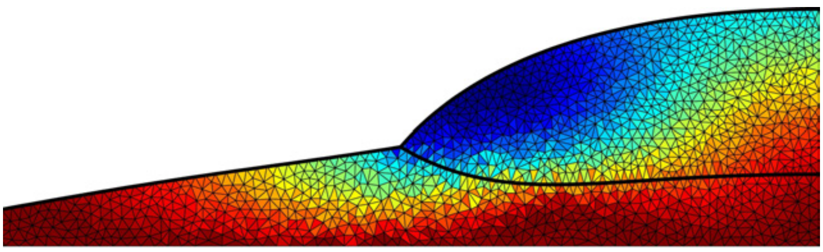


Fig. 2: *Motion of a (half) liquid droplet on another liquid from a 2D FEM simulation. Colors indicate the modulus of the velocity, thick black lines are the liquid/liquid, liquid/air interfaces, respectively. Thin black lines show the triangulation.*

Ph.D. students

Wolfgang Dreyer, Jürgen Sprekels, and Barbara Wagner, jointly with other partners, guide and supervise five 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. Mainly initial-boundary value problems for nonlinear coupled systems of partial differential equations are involved.

In May 2012, Robert Huth very successfully defended his Ph.D. thesis at the Humboldt-Universität zu Berlin *"On a Fokker–Planck equation coupled with a constraint"*, which is strongly related to the topics of the Leibniz Group *Mathematical Models for Lithium-Ion Batteries*. The Ph.D. thesis contains analysis and numerics of a model for many-particle electrodes. The model describes the intercalation of lithium atoms in an electrode consisting of many nanosized FePO4 particles and predicts an unexpected behavior of the charging process of lithium-ion batteries. The mathematical core of the model is a new nonlinear and nonlocal Fokker–Planck equation. The nonlinearity in this partial differential equation results from a coefficient that depends on the solution first nonlocally and secondly in a higher order, i.e., it depends on the solution as a function in $C(\bar{\Omega})$ and not only in $L^2(\Omega)$. Interpolation spaces and semigroup generated from sectorial operators are used to show the existence and uniqueness of solutions locally in time. Moreover, positivity and regularity properties of solutions are also derived. Jointly with Alexander Mielke and Joachim Rehberg from the Research Group *Partial Differential Equations* and Michael Winkler from the Universität Paderborn, the analytical results were described in [2]. The numerical part of the Ph.D. study can be found in [6].

Miscellaneous

In 2012, Wolfgang Dreyer, jointly with Daniel Balzani (Duisburg-Essen), organized the Section "Material modelling in solid mechanics" at the 83rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM) in Darmstadt.

References

[1] P.-E. DRUET, *The classical solvability of the contact angle problem for generalized equations of mean curvature type*, Port. Math., **69** (2012), pp. 233–258.

[2] W. DREYER, R. HUTH, A. MIELKE, J. REHBERG, M. WINKLER, *Blow-up versus boundedness in a nonlocal and nonlinear Fokker–Planck equation*, WIAS Preprint no. 1604, 2011, submitted.

[3] P. COLLI, G. GILARDI, P. PODIO-GUIDUGLI, J. SPREKELS, *Global existence for a strongly coupled Cahn–Hilliard system with viscosity*, Boll. Unione Mat. Ital. (9), **5** (2012), pp. 495–513.

[4] P. COLLI, G. GILARDI, P. PODIO-GUIDUGLI, J. SPREKELS, *An asymptotic analysis for a nonstandard viscous Cahn–Hilliard system*, Discrete Contin. Dyn. Syst. Ser. S, **6** (2013), pp. 387–400.

[5] W. DREYER, C. GUHLKE, *Sharp limit of the viscous Cahn–Hilliard equation and thermodynamic consistency*, WIAS Preprint no. 1771, 2013, submitted.

[6] R. HUTH, *Numerical convergence for semilinear parabolic equations*, WIAS Preprint no. 1747, 2012, submitted.

4.8 Young Scientists' Group "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 provided the basis for the Young Scientists' Group. 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. In addition, the group develops multi-scale damage models that reflect the evolution of microdefects in effective models on the macroscopic level in a mathematically justified way.

In general, the resulting models consist of strongly coupled, nonlinear, and nonsmooth time-dependent systems of PDEs. The analytical investigation of these systems requires tools from calculus of variations for nonlinear and nonsmooth evolution systems and from geometric measure theory.

In classical damage models, the dependence of the elastic parameters on the damage state is given by phenomenological constitutive relations. Based on a multi-scale approach, a macroscopic damage model was developed that reflects the evolution of microdefects. The starting point is a time-dependent model with periodically distributed microdefects that individually evolve with respect to applied loadings. Using two-scale convergence techniques, an effective evolution model was derived, where the dependence of the macroscopic elasticity tensor on the spatially varying damage state is given by a cell formula known from periodic homogenization theory. The analysis required the definition of a suitable discrete gradient and a compactness result for piecewise constant functions, inspired by similar constructions in the context of discrete Galerkin methods.

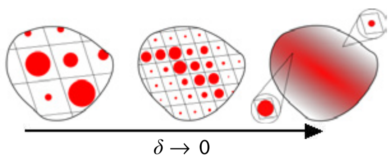


Fig. 1: *Sketch of a body with periodically distributed microdefects of different sizes and its two-scale limit*

Analytical and numerical investigations on a nonlocal Cahn–Hilliard system with damage were continued within the DFG Research Center MATHEON project C32. There, the damage process is incorporated in a multi-component Cahn–Hilliard system by considering the damage process as a diffusion of vacancies, being nothing but some special type of noninteracting particles of the multi-component system.

Complete damage in elastic solids appears when the material looses all its integrity due to high exposure. In the case of alloys, the situation is quite involved since spinodal decomposition and coarsening phenomena also occur at sufficiently low temperatures. Complete damage theories and degenerating parabolic differential systems lead to several mathematical problems since, for instance, coercivity properties of the free energy are lost.

To describe complete damage processes and phase separation phenomena in a more realistic way, a new degenerating phase field model of Cahn–Hilliard type coupled with complete damage was developed. Because of the doubly degenerating character and the doubly nonlinear differential inclusion for the damage process, a suitable notion of weak solutions had to be introduced. For the proposed system, existence of weak solutions was shown via suitable variational techniques. In addition, the classical differential inclusion can be regained under certain regularity assumptions, which is a novelty in the theory of complete damage models of this type.

As a further topic, phase field models for flows of two incompressible fluids were investigated. In particular, a new thermodynamically consistent diffuse phase field model for two-component flows of incompressible fluids was deduced and physically admissible sharp interface limits were investigated by asymptotic techniques. Depending on the scaling regimes, the Euler equations or the Navier–Stokes equations can be recovered in the bulk phases equipped with admissible interfacial conditions in the sharp interface limit.

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 "Evolution Problems in Damage, Plasticity and Fracture: Mathematical Models and Numerical Analysis" organized by Dorothee Knees (YSG) and Rodica Toader (U Udine), took place at University of Udine, September 19–21, 2012. The lectures focused on the modeling of the mechanisms that lead to the occurrence of damage phenomena, plasticity and crack propagation, on the mathematical analysis of these highly nonlinear models, and on issues in numerical simulations.
Within the Winter School "Modeling Complex Physical Systems with Nonlinear (S)PDE" at the Technische Universität Dortmund, Dorothee Knees gave a course on "Modeling and mathematical analysis of elasto-plastic phenomena".

Fig. 2: *Participants of the workshop "Evolution Problems in Damage, Plasticity and Fracture", Udine*

References

[1] G. Aki, J. Daube, W. Dreyer, J.Giesselmann, M. Kränkel, C. Kraus, *A diffuse interface model for quasi-incompressible flows: Sharp interface limits and numerics*, ESAIM Proceedings, **38** (2012), pp. 54–77.

[2] G. Aki, W. Dreyer, J.Giesselmann, C. Kraus, *A quasi-incompressible diffuse model with phase transition – Modeling and sharp interface limits*, WIAS Preprint no. 1706, 2012, to appear in: Math. Models Methods Appl. Sci.

[3] R. Haller-Dintelmann, D. Knees, J. Rehberg, *On elliptic and parabolic regularity for mixed boundary value problems*, WIAS Preprint no. 1706, 2012, submitted.

[4] H. Hanke, D. Knees, *Derivation of an effective damage model with evolving micro-structure*, WIAS Preprint no. 1749, 2012, submitted.

[5] C. Heinemann, C. Kraus, *Complete damage in linear elastic materials – Modeling, weak formulation and existence results* , WIAS Preprint no. 1722, 2012, submitted.

[6] C. Heinemann, C. Kraus, *A degenerating Cahn–Hilliard system coupled with complete damage processes*, WIAS Preprint no. 1759, 2012, submitted.

4.9 Leibniz Group 3 "Mathematical Models for Lithium-ion Batteries"

The Leibniz group is externally funded with 616,200 Euros for three years. The funding results from a successful proposal by Wolfgang Dreyer within the competition procedure of the Leibniz Association in the Pact for Research and Innovation.

The group started in July 2012. It is working on the modeling, the analysis, the scientific computing, and simulations of various components of lithium-ion batteries, particularly

- Many-particle electrodes
- Graphite electrodes
- Electrolytes
- Electrolyte-electrode interfaces

The involved electrochemical processes and transport phenomena are modeled by partial differential equations in the bulk regions and by jump conditions across the interfaces.

Highlights

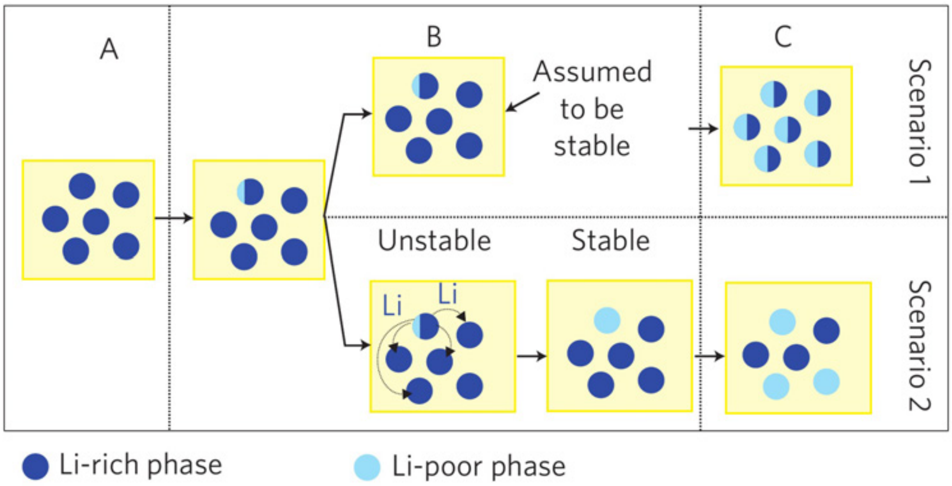


Fig. 1: *Two possible scenarios of the charging process within the many-particle cathode*

The new many-particle model. This new model has received worldwide attention because it led to a groundbreaking change of the chemical model of the storage process within many-particle electrodes. In the slow-charging regime, the many-particle model predicts: (i) The storage particles are not simultaneously loaded, but, according to the rule, *"one after the other"*. (ii) The phase transition happens in the ensemble, but not in the individual particles. In 2012, these predictions were confirmed by William C. Chueh and his group from the Sandia National Laboratories, Livermore, California. The details are found in their experimental paper *Probing Surface & Transport Phenomena in Energy Materials Under Operating Conditions* [6].

The chemical essentials of the many-particle model are described in the papers "The thermodynamic origin of hysteresis in insertion batteries" [4] and "The behavior of a many-particle electrode in a lithium-ion battery" [1]. The corresponding mathematical model and numerical simulations are treated in the article "Hysteresis and phase transition in many-particle storage systems" [5], and the mathematical analysis is found in the preprint "Blow-up versus boundedness in a nonlocal and nonlinear Fokker–Planck equation" [3].

The new electrolyte model. A study of the literature on existing electrolyte models reveals that they exhibit various serious shortcomings. A coupling of diffusion and mechanical motion is either missing or introduced in a thermodynamically incorrect way [2]. In particular, the still very popular Nernst–Planck model from 1890 shows a further problem. For a mixture of N constituents the Nernst–Planck model proposes N diffusion equations and does not take care of the fact that the sum of these equations over all constituents must give the equation of continuity, i.e, the conservation law of mass for the total mixture. Due to this fact, the Nernst–Planck model cannot guarantee bounded partial mass densities of the constituents. In the article "Overcoming the shortcomings of the Nernst–Planck model" [2], the Leibniz group proposed a new electrolyte model with a thermodynamically consistent coupling of the diffusion equations and the momentum balance that removes the deficiencies of the classical models. An iterative fixed-point method was designed to solve the finite element discretization of the coupled nonlinear system, allowing the spatial resolution of boundary layers and offering an independent possibility to predict the plateau height inside of the electrolyte.

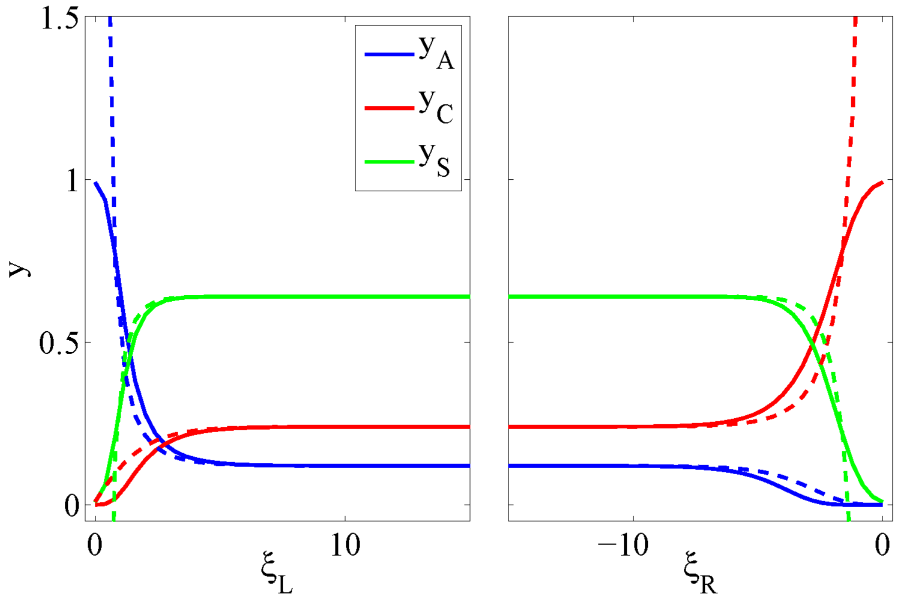


Fig. 2: *Comparison of the mole fractions* $(y_\alpha)_{\alpha\in\{C,A,S\}}$ *according to the new electrolyte model (solid) with the Poisson–Boltzmann equation (dashed) of the Nernst–Planck model. Note that the latter does not guarantee* $0 \leq y_\alpha \leq 1$.

Collaborations

The group has started a collaboration with the *Virtual Vehicle Competence Center*, Graz, on the pre-development of battery components.

There is a strong collaboration with the DFG Research Center MATHEON. One of the topics within the MATHEON project C26 "Storage of hydrogen in hydrides" concerns a joint research on the catalytic dissociation of hydrogen.

Perspectives

The ongoing work of the Leibniz group includes the following topics:

- Rational derivation of improved boundary conditions within the Butler–Volmer setting
- Rational derivation of the Lippmann equation relating the surface tension of electrodes to their electrical voltage
- New model for electrical double layers relying on asymptotic methods
- Charging simulation of a lead-acid battery including dissociation reactions and electrolyte convection

Miscellaneous

In 2012, Wolfgang Dreyer was invited by the President of the Leibniz Association to present his new research results on lithium-ion batteries at the Innovation Days "Research meets Business" in Munich.

References

[1] W. DREYER, C. GUHLKE, R. HUTH, *The behavior of a many-particle electrode in a lithium-ion battery*, Phys. D, **240** (2011), pp. 1008–1019.

[2] W. DREYER, C. GUHLKE, R. MÜLLER, *Overcoming the shortcomings of the Nernst–Planck model*, Phys. Chem. Chem. Phys., **15** (2013), pp. 7075–7086.

[3] W. DREYER, R. HUTH, A. MIELKE, J. REHBERG, M. WINKLER, *Blow-up versus boundedness in a nonlocal and nonlinear Fokker–Planck equation*, WIAS Preprint no. 1604, 2011, submitted.

[4] 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.

[5] W. DREYER, C. GUHLKE, M. HERRMANN, *Hysteresis and phase transition in many-particle storage systems*, Contin. Mech. Thermodyn., **23(3)** (2011), pp. 211–231.

[6] W.C. CHUEH, F. EL GABALY, A.H. MCDANIEL, K.F. MCCARTY, *Probing Surface & Transport Phenomena in Energy Materials Under Operating Conditions*, Sandia Report no. SAND2012-8027, Sandia National Laboratories, 2012, to appear in: Nano Lett.

A Facts and Figures

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

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

A.1.1 Awards and Distinctions

1. M. Becker, *University Medal of the Leipzig University*, December 3, 2012.
2. S. Becker, K. Tabelow, *Third prize for the best posters at the 3rd Annual Scientific Symposium "Ultrahigh Field Magnetic Resonance: Clinical Needs Research Promises and Technical Solutions", Max Delbrück Communications Center in Berlin*, June 8.
3. A. Mielke, *Head of the Secretariat of the International Mathematical Union (IMU)*.
4. ———, *Member of the Executive Committee of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
5. ———, *Member of the IMU Berlin Einstein Foundation Program Committee*.
6. ———, *Treasurer of IMU*.
7. H. Si, *Software Award for Excellence achieved in developing the free software TetGen to greatly affect the scientific progress in the field of Geometry Processing*, July 17.
8. V. Spokoiny, *Mega-Grant of the Russian Government to establish a Research Group "Predictive Modeling" at the University of Physics and Technology in Moscow*.
9. A.G. Vladimirov, *E.T.S. Walton Visitor Award of the Science Foundation Ireland for "Theoretical modelling of quantum dot mode-locked and frequency swept Fourier domain mode-locked lasers"*, 2012–2013.

A.1.2 Ph.D. Theses

1. B. Nehring, *Point processes in statistical mechanics. A cluster expansion approach*, Universität Potsdam, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. W. König, November 9.
2. V. Panov, *Abelian theorem for stochastic volatility models and semiparametric estimation of the signal space*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. V. Spokoiny, January 26.
3. W. Wang, *Adaptive methods for risk calibration*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, August 2.
4. R. Huth, *On a Fokker–Planck equation coupled with a constraint*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisors: Prof. Dr. A. Mielke, Prof. Dr. W. Dreyer, Prof. Dr. R. Denk, May 31.
5. M. Liero, *Variational methods for evolution*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, December 7.
6. H. Mai, *Drift estimation for jump diffusions: Time-continuous and high-frequency observations*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. V. Spokoiny, September 28.
7. A. Wilms, *Coulomb induced interplay of localized and reservoir carriers in semiconductor quantum dots*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. U. Bandelow, December 12.

A.1.3 Undergraduate-degree Supervision

1. T. Fluschnik, *Kritisches Verhalten eines verdünnten zufälligen Polymers* (bachelor's thesis), Technische Universität Berlin, Faukultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 12.
2. Th. Frenzel, *Geodätische Konvexität für reversible Markov-Ketten* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, October 15.
3. P. Gussmann, *Die linearisierte Elastizität als Grenzwert finiter Elastizität im Falle von Schlitzgebieten* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. A. Mielke, January 19.
4. S. Käbisch, *Phase field methods in shape optimization* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, September 10.
5. Ch. Klausen, *The largest step of a far-traveling random walk* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 23.
6. Y. Liu, *Ray-Knight-Theorem für Irrfahrten in stetiger Zeit* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, November 21.
7. P. Pietzner, *Kritische Phänomene im Boole'schen Modell* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, November 1.
8. M. Reinbacher, *The moments of a branching random walk in random medium: Feynman–Kac formula and asymptotics* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 23.
9. K. Retzlaff, *Ein zufälliges Polymer zwischen zwei attrahierenden undurchlässigen Schichten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 9.
10. L. Sammüller, *Kritische Eigenschaften der Trennlinie zwischen Lokalisation und Delokalisation eines zufälligen Kopolymers* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 15.
11. M.K. Sol, *Interaction with a penetrable surface* (master's thesis), Delft University of Technology, Faculty of Electrical Engineering, Mathematics and Computer Science, Delft Institute of Applied Mathematics, supervisor: Prof. Dr. W. König, January 17.
12. Y. Sun, *Statistische Analyse der Konnektivität in mobilen Ad-hoc-Netzwerken* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 13.
13. M.-C. Vidovic, *Analysis of learning models for motif recognition in DNA sequences* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, December 13.
14. F. Walter, *Ein Phasenübergang bei weit entferntem Massefluss durch ein zufälliges Potential* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 19.

A.2 Grants[1]

European Union, Brussels

- **Seventh Framework Programme**

  ERC Starting Independent Researcher Grant "Rough path theory, differential equations and stochastic analysis" (P. Friz in RG 6)

  ERC Advanced Researcher Grant "AnaMultiScale – Analysis of multiscale systems driven by functionals" (A. Mielke in RG 1)

  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)

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 subproject "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 "Gittersimulation im Field Tracing" (Grating simulation in field tracing), subproject "Entwicklung der Integralmethode für die konische Diffraktion mit Anwendung beim Field Tracing" (Development of an integral method for conical diffraction with application in field tracing; 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)

[1] The groups (RGs, LG, or YSG) involved in the respective projects are indicated in brackets.

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)

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)

D27: “Numerical methods for coupled micro- und nanoflows with strong electrostatic forces” (in RG 3)

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)

- **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 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)

- **Research Unit FOR 1735 "Structural Inference in Statistics: Adaptation and Efficiency"**, Humboldt-Universität zu Berlin

  "Semiparametric approach to structural adaptive estimation" (in RG 6)

- **Normalverfahren (Individual Grants)**

  "Ab initio Beschreibung optischer Nichtlinearitäten in Femtosekunden-Filamenten" (Ab-initio description of optical nonlinearities in femtosecond filaments; in RG 2)

  "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)

  "Direkte und inverse Kopplungsprobleme mit unbeschränkten Grenzflächen zwischen akustischen, elektromagnetischen und elastischen Wellen" (Direct and inverse interaction problems with unbounded interfaces between acoustic, electromagnetic and elastic waves; G. Hu)

- **Bilateral cooperation:** "Martingale approach in pricing European options under regime-switching" (in RG 6)

Leibniz-Gemeinschaft (Leibniz Association), Bonn and Berlin

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

  "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)

"SMATH – Mathematische Software für Wissenschaft und Anwendungen" (SMATH – Mathematical software for sciences and applications), joint project of Mathematisches Forschungsinstitut Oberwolfach, FIZ Karlsruhe – Leibniz Institute for Information Infrastructure, DFG Research Center MATHEON, Zuse Institute Berlin, Felix Klein Center for Mathematics in Kaiserslautern, and WIAS

"Mathematische Modelle für Lithium-Ionen-Batterien" (Mathematical models for Lithium-ion batteries; in LG 3)

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

- 1 Friedrich Wilhelm Bessel awardee (in RG 1)
- 1 scholarship holder (in RG 6); see page 153

International projects

- E.T.S. Walton Research Grant of Science Foundation Ireland to Cork Institute of Technology for "Theoretical modelling of quantum dot mode-locked and frequency swept Fourier domain mode-locked lasers" (Principal Investigator A.G. Vladimirov in RG 2)
- Mega-Grant of the Russian Government to establish a Research Group "Predictive Modeling" at the University of Physics and Technology in Moscow for the head of RG 6, V. Spokoiny.

Mission-oriented research (examples)

- Alstom (Switzerland) Ltd., Baden: "Prozesssimulation bei industriellen Gasturbinen" (Process simulation for industrial gas turbines; in RG 3 and RG 6)
- 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)
- Max Planck Institute for Physics, Munich, and Max Planck Institute for Extraterrestrial Physics, Garching: agreement to collaborate in the field of the simulation of semiconductor devices for radiation detectors (in RG 3)
- Nippon Steel & Sumitomo Metal Corporation, Chiba, Japan: "Optimization of steel microstructures on a mesoscopic scale" (in RG 4)
- PAR Medizintechnik GmbH, Berlin: "Automatische Blutdruckmessung mit Störsignalen" (Automatic blood pressure measuring with noisy signals; in RG 6)
- 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, suborder 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, Stochastic Processes and Applications, Elsevier, Oxford, UK.
3. ———, Editorial Board, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
4. ———, Editorial Board, International Journal of Stochastic Analysis, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, Pennsylvania, USA.
5. R. Henrion, Editorial Board, Nonlinear Analysis: Theory, Methods & Applications, Elsevier, Amsterdam, The Netherlands.
6. ———, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, The Netherlands.
7. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, The Netherlands.
8. ———, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
9. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
10. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
11. D. Knees, Editorial Board, Discrete and Continuous Dynamical Systems — Series S (DCDS-S), American Institute of Mathematical Sciences, Springfield, Missouri, USA.
12. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
13. P. Mathé, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
14. ———, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
15. A. Mielke, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
16. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
17. ———, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
18. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin, Heidelberg.
19. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
20. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
21. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
22. ———, Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
23. H. Neidhardt, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russia.

[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, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
25. ———, Editorial Board, Journal of Operators, Hindawi Publishing Corporation, New York, USA.
26. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
27. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
28. J.G.M. Schoenmakers, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
29. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
30. ———, Editorial Board, International Journal of Portfolio Analysis and Management, Inderscience Enterprises Limited, Genèva, Switzerland.
31. J. Sprekels, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
32. ———, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest, Romania.
33. ———, Editorial Board, Applied Mathematics and Optimization, Springer-Verlag, New York, USA.
34. ———, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
35. 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 "From Particle Systems to Differential Equations"
Berlin, February 21–23
Organized by: WIAS (RG 1, RG 5, and RG 7)
Supported by: FOR 718

This workshop was one of the measures taken by WIAS to strengthen the links between the analytic and the probabilistic fields of expertise that are present at the institute. It focused on a current subject, the question how a macroscopic picture arises from microscopically defined random interacting particle systems. Answers to this question, on the one hand, are expected to give a rigorous motivation for the study of many well-known types of partial differential equations that have been under study at WIAS for decades. On the other hand, they show the way to an understanding of the global behavior of certain random interacting particle systems by making them amenable to an analysis in terms of differential equations. In this way, the subject builds a bridge between research topics that have been studied in the three organizing groups for decades.

About 50 scientists, mainly from various research groups of WIAS, participated in the workshop. In two mini-courses, two eminent experts surveyed the analytical and probabilistic aspects of the subject. In seven more invited talks, more specific research results were presented and discussed.

2nd Structural Inference Day
Berlin, April 23
Organized by: FOR 1735, WIAS (RG 6)
Supported by: DFG, WIAS

The Second Structural Inference Day marked the beginning of the work of the DFG Research Unit FOR 1735 "Structural Inference in Statistics: Adaptation and Efficiency". It showed the scope of the unit's research and brought together researchers from different fields of statistics and machine learning. The speakers—among which were five members of the research unit FOR 1735—gave high-quality talks and presented recent results. Topics ranged from multiple testing and multi-task learning to testing for Poisson processes and the analysis of random walks on graphs to nonparametric regression and finite sample semiparametrics.

The workshop was attended by 34 participants. Two invited and six contributed talks were given.

Adaptive Methods with Applications in Fluid Dynamics
Berlin, April 26–27
Organized by: WIAS (RG 3)
Supported by: DFG Research Center Matheon, DFG SPP 1276 "MetStröm: Multiple Scales in Fluid Mechanics and Meteorology"

The workshop aimed to bring together researchers who are working on different aspects of adaptive methods in Computational Fluid Mechanics. Altogether, 42 scientists from six countries participated in it, and 16 invited talks were given. Topics of the talks included, e.g., the theory of a posteriori error estimation and adaptive methods, the use of adaptive methods in science and applications, scientific computational aspects of adaptive methods, and reduced order modeling.

Simulation in Industrial Process Engineering
Berlin, September 6
Organized by: WIAS (RG 3)

The simulator BOP (Block Oriented Process Simulator) is a software package for the static and dynamic simulation of complex tasks in process engineering, which can be modeled by differential-algebraic equations. It is developed and maintained by the the Research Group 3 *Numerical Mathematics and Scientific Computing* in cooperation with the Research Group 6 *Stochastic Algorithms and Nonparametric Statistics*. The simulation concept of BOP is based on a hierarchical, modularly structured process model and provides an efficient solution strategy also for large-scale systems. It allows to perform steady state and transient simulations, Monte Carlo, correction-curve, optimization, and homotopy calculations.

Based on this simulator, a long-term industrial cooperation between the Weierstrass Institute and Alstom Power Ltd. could be sustained. The workshop gave an insight into the industrial requirements and challenges and discussed possible future directions of the algorithmic development in this field.

NONLINEAR DYNAMICS IN SEMICONDUCTOR LASERS
Berlin, September 12–14
Organized by: WIAS (RG 2), Technische Universität Berlin
Supported by: WIAS, DFG Research Center MATHEON, Marie Curie Initial Training Network PROPHET

The aim of the workshop was to bring together applied mathematicians and scientists from semiconductor physics and to give them the opportunity to exchange experience in the field of nonlinear phenomena in semiconductor lasers. The main topics of the workshop were analytical and numerical methods in optoelectronics, quantum dot lasers, mode-locked lasers, dynamics of ring and multi-section lasers, high-power tapered and broad-area lasers and amplifiers. The workshop was attended by more than 50 participants from 11 countries. Thirty-eight talks were given.

MATHEMATICS FOR SEMICONDUCTOR HETEROSTRUCTURES – MODELING, ANALYSIS, AND NUMERICS
Berlin, September 24–28
Organized by: WIAS (RG 1 and RG 3), IRMAR (Rennes/France)
Supported by: DFG, WIAS

New generations of electronic semiconductor devices play a crucial role in spurring technological advance. Miniaturization, nanostructuring, new materials and technologies require a permanent progress in modeling, mathematical treatment, and simulation tools.

This international workshop was devoted to analytical and numerical aspects of the relevant mathematical models for semiconductor devices and to the design of efficient numerical algorithms. It focused on the modeling of micro-, nano-, and optoelectronic devices by classical drift-diffusion and energy models, by semiclassical and quantum-transport models, as well as by asymptotic models. Main topics were organic semiconductors, spintronics, quantum dots, wires, wells, and wave guides. The multi-physics problems were discussed from the mathematical point of view up to the simulation of real-world devices. 56 scientists participated in the workshop. Two key-note lectures, 32 talks, and several posters were presented.

WORKSHOP PARALLELES RECHNEN
Berlin, October 25
Organized by: WIAS (RG 3)

This workshop on Parallel Computing was held in German language. A future increase in computational power of computer systems will be mainly due to parallelization, as the decrease of structure width and the increase of core frequencies are approaching physical limits that seem to be impossible to pass. In particular, this situation needs to be accounted for in the design of algorithms and software for numerical computations. The workshop was intended to raise the awareness on this fact among scientists involved in numerical computations and to support the development of a consensus on the future directions of the computing infrastructure of WIAS. In the talks, current competing concepts and software interfaces to parallel execution were critically reviewed. These included OpenCL/CUDA for GPU cards, OpenMP for shared memory systems and MPI for distributed memory systems.

COUPLED NETWORKS, PATTERNS AND COMPLEXITY
Berlin, November 19–21
Organized by: WIAS (RG 2)
Supported by: WIAS, DFG Research Center MATHEON, SFB 910, and International Research Training Group 1740

The workshop was devoted to the dynamics of networks of interacting systems. An important mathematical question is the emergence of nonlinear collective behavior, patterns, or chaos due to the interaction of the elements in networks of different structure. The workshop was intended to address and combine interesting aspects from applications with recent development in corresponding mathematical methods from nonlinear dynamics, such as bifurcation theory, formation and interaction of patterns, and delay systems. The workshop was attended by more than 80 participants from 12 countries. Thirty talks were given, and there was also a poster session.

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

PREMOLAB: MOSCOW–BERLIN STOCHASTIC AND PREDICTIVE MODELING
Moscow, May 31 – June 1
Organized by: WIAS (RG 6), Institute for Information Transmission Problems (Russian Academy of Sciences), Moscow Institute of Physics and Technology
Supported by: RF government grant, ag. 11.G34.31.0073

The Laboratory of Structural Methods of Data Analysis in Predictive Modeling (PreMoLab) was created within the mega-grant program of the Russian government to attract the world's leading scientists to create new research groups in Russia. Interactions of this new group with established international groups are of special importance for the success of this project. The Moscow–Berlin workshop was an important step in this direction, bringing together two groups lead by Prof. V. Spokoiny: the Research Group *Stochastic Algorithms and Nonparametric Statistics* at WIAS and PreMoLab (MITP Moscow). The workshop was attended by 15 members of the research group in Berlin and 25 members of the research group in Moscow. The program included 8 talks on the current research fields from each side and a lot of scientific discussion.

17TH JOINT CZECH-GERMAN-SLOVAK CONFERENCE ON MATHEMATICAL METHODS IN ECONOMY AND INDUSTRY
Berlin, June 24–28
Organized by: WIAS (RG 4), Humboldt-Universität zu Berlin (HU)
Supported by: DFG Research Center MATHEON, HU Berlin, WIAS

This conference series, initiated in 1973 by the renowned Czech mathematician František Nožička, aims at gathering Central European scientists working on the theory and applications of Mathematical Methods in Economy and Industry. The 17th issue of this meeting was organized by René Henrion (WIAS) and Werner Römisch (HU) and attended by around 40 participants. The talks covered topics from discrete, nonlinear, and stochastic optimization, optimal control and finance with applications to, e.g., robotics, process engineering, electricity spot markets, water reservoir management, or equilibrium problems in economy. Seven distinguished speakers gave invited lectures on new trends and challenges in their research areas. The conference succeeded in giving a new impulse for maintaining this traditional series and in "passing the baton" from the pioneers to the next generation of scientists. The following meeting of this series will take place in Bratislava in 2014.

EVOLUTION PROBLEMS IN DAMAGE, PLASTICITY AND FRACTURE: MATHEMATICAL MODELS AND NUMERICAL ANALYSIS
Università degli Studi di Udine/Italy, September 19–21
Organized by: WIAS (YSG), Università degli Studi di Udine (DIMI)
Supported by: GNAMPA/INdAM, WIAS, DIMI Univ. Udine, PRIN Variational problems, ERC grant QuaDynEvoPro

The understanding and modeling of the mechanisms that lead to the occurrence of damage phenomena, plasticity, and crack propagation are of great importance for technological applications. In the last fifteen years, there was a considerable progress in the mathematical foundation of these processes due to new variational formulations based on energy minimization in the framework of appropriate function spaces.

The obvious interplay between damage, plasticity, and fracture has been evidenced by recently proposed mathematical models. Moreover, the mathematical analysis of damage or plasticity models that are coupled with further physical processes, as well as a justification of such models from a microscopic point of view, attracted increasing attention. The workshop provided a platform for intensive discussions on the latest results on these topics.

About 40 scientists mainly from the Czech Republic, France, Italy and Germany participated in the workshop. In four invited lectures, 19 talks, and a poster session, a broad range of topics from modeling, analysis, and simulation were covered.

Stochastic Optimization and Optimal Stopping
Moscow, September 24–28
Organized by: WIAS (RG 6), Institute of Physics and Technology (Russian Academy of Sciences), Steklov Mathematical Institute
Supported by: PreMoLab, Institute of Physics and Technology (Russian Academy of Sciences), Steklov Mathematical Institute

The workshop aimed at bringing together world-renowned experts and younger promising researchers in the field of optimal stopping and control. Vladimir Spokoiny from WIAS and Albert Shiryaev (Steklov Institute) were the co-chairmen of the workshop. John Schoenmakers from WIAS was one of the invited speakers and presented recent developments of his research on multilevel methods for American options.

Hermann Otto Hirschfeld Lecture Series 2012: High Dimensional Statistical Inference
Berlin, October 12–13
Organized by: WIAS (RG 6), SFB 649 “Economic Risk”, C.A.S.E. – Center for Applied Statistics and Economics (Humboldt-Universität zu Berlin, HU)
Supported by: DFG, C.A.S.E., and Wirtschaftswissenschaftliche Gesellschaft of HU Berlin

At this year’s Hermann Otto Hirschfeld Lecture Series, Tony Cai, Professor of Statistics at the Wharton School (University of Pennsylvania), presented an overview on ‘ ‘High-dimensional statistical inference on the covariance structure” with highlights from some of his seminal contributions to this research field. The Lecture started with a historical talk on “Statistics in Berlin – From Richard Böckh to Ladislaus von Bortkiewicz” by Annette Vogt from the Max Planck Institute for the History of Science. Altogether, 49 registered participants from 16 different institutions all over Germany came together at the Weierstrass Institute to attend the lectures.

A.4.3 Oberwolfach Workshops co-organized by WIAS

Workshop “Interplay of Analysis and Probability in Physics”
Mathematisches Forschungsinstitut Oberwolfach, January 22–28
Organized by: Wolfgang König (RG 5), Peter Mörters (Bath), Mark Peletier (Eindhoven), Johannes Zimmer (Bath)

The main purpose of this workshop was to foster interaction between researchers in the fields of analysis and probability with the aim of joining forces to understand difficult problems from physics rigorously. 52 researchers of all age groups and from many parts of Europe and overseas attended. The talks and discussions evolved around five topics on the interface between analysis and probability. The main goal of the workshop, the systematic encouragement of intense discussions between the two communities, was achieved to a high extent.

WORKSHOP “ROUGH PATHS AND PDES”
Mathematisches Forschungsinstitut Oberwolfach, August 19–25
Organized by: Peter Friz (RG 6), Massimiliano Gubinelli (Paris), Dan Crisan (London)

The workshop was attended by more than 25 participants from 10 countries. Altogether, 14 invited and 8 contributed talks were given.

The major topics were:

(1) new solution methods for stochastic partial differential equations via rough paths
(2) numerical methods deriving from rough path theory
(3) physical and financial modeling via rough paths

Researchers with different backgrounds were invited. Martin Hairer (Warwick) gave several lectures on the ground-breaking work “Solving the KPZ equations”; to appear in Annals of Mathematics. Takis Souganidis (Chicago) gave several lectures on his ongoing work with P.L. Lions on a pathwise approach to stochastic viscosity solutions for fully nonlinear stochastic PDEs. The workshop was also attended by a number of Ph.D. students about to finish their degree and early postdocs.

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

1. P. Friz, co-organizer, *Workshop "Rough Paths and PDEs"*, Mathematisches Forschungsinstitut Oberwolfach, August 19–25.
2. U. Bandelow, member of the Organizing Committee, *12th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD12)*, Shanghai, China, August 28–31.
3. W. Dreyer, organizer of Section S6 "Material Modelling in Solid Mechanics", *83rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2012)*, Universität Darmstadt, March 26–30.
4. ———, member of the Scientific Board and organizer of the session "Thermodynamics of Interfaces ", *12th International Conference on Free Boundary Problems: Theory and Applications*, Frauenchiemsee, June 11–15.
5. K. Emich, member of the Local Organizing Committee, *17th International Conference on Mathematical Methods in Economy and Industry (MMEI 2012)*, Schmöckwitz, June 24–28.
6. R. Henrion, member of the Scientific Committee and of the Local Organizing Committee, *17th International Conference on Mathematical Methods in Economy and Industry (MMEI 2012)*, Schmöckwitz, June 24–28.
7. ———, co-organizer of the cluster "Variational Analysis", *21st International Symposium on Mathematical Programming (ISMP)*, Technische Universität Berlin, August 19–24.
8. D. Hömberg, organizer of the session "Optimization Applications in Industry I–VI", *21st International Symposium on Mathematical Programming (ISMP)*, Technische Universität Berlin, August 19–24.
9. O. Klein, member of the International Steering Committee, *6th International Workshop on Multi-Rate Processes and Hysteresis (MURPHYS 2012)*, Stefan cel Mare University, Suceava, Romania, May 21–24.
10. D. Knees, co-organizer, *International Workshop on Evolution Problems in Damage, Plasticity, and Fracture: Mathematical Models and Numerical Analysis*, University of Udine, Department of Mathematics, Italy, September 19–21.
11. W. König, member of the Local Organizing Committee, *Interplay of Analysis and Probability in Physics*, Mathematisches Forschungsinstitut Oberwolfach, January 22–28.
12. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, WIAS Berlin, April 13.
13. ———, member of the Organizing Committee, *Mathematics of Many-particle Systems, Conference in Honor of Elliott Lieb on the Occasion of his 80th Birthday*, Technische Universität Berlin, Institut für Mathematik, July 12–14.
14. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Universität Leipzig, Mathematisches Institut, October 26.
15. Ch. Landry, organizer of the minisymposium "Mathematical Challenges in Robotics and Automotive Industry", *The 17th European Conference on Mathematics for Industry 2012 (ECMI 2012)*, Lund, Sweden, July 23–27.
16. A. Mielke, co-organizer, *SFB 910 Symposium "Mathematical Methods in Multiscale Systems"*, Technische Universität Berlin, Institut für Mathematik, May 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.

17. ———, member of the International Scientific Committee, *XVIII International ISIMM Symposium on Trends in Applications of Mathematics to Mechanics (STAMM 2012)*, Technion – Israel Institute of Technology, Faculty of Aerospace Engineering, Haifa, September 3–6.

18. A. Möller, member of the Local Organizing Committee, *17th International Conference on Mathematical Methods in Economy and Industry (MMEI 2012)*, Schmöckwitz, June 24–28.

19. V. Spokoiny, co-organizer, *PreMoLab I*, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, February 24.

20. ———, co-organizer, *PreMoLab II*, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, March 16.

21. ———, co-organizer, *PreMoLab: Moscow-Berlin Stochastic and Predictive Modeling*, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, May 31 – June 1.

22. ———, co-organizer, *Stochastic Optimization and Optimal Stopping*, Russian Academy of Sciences and Moscow Institute of Physics and Technology, Moscow, September 24–28.

23. J. Sprekels, member of the Scientific Board and co-organizer of the focus session "Phase Field Models", *12th International Conference on Free Boundary Problems: Theory and Applications*, Frauenchiemsee, June 11–15.

24. M. Thomas, co-organizer, *SFB 910 Symposium "Mathematical Methods in Multiscale Systems"*, Technische Universität Berlin, Institut für Mathematik, May 18.

25. A.G. Vladimirov, co-organizer, *FP7 Marie Curie Initial Training Network PROPHET Workshop: Theory and Modelling in Photonics*, Pavia, Italy, April 11–13.

26. ———, co-organizer, *XVI International Conference-School "Foundations and Advances in Nonlinear Science"*, Belarusian State University, Minsk, September 24–28.

A.6 Publications

A.6.1 Monographs

[1] C. Breé, *Nonlinear Optics in the Filamentation Regime*, Springer Theses Recognizing Outstanding Ph. D. Research, Springer, Berlin Heidelberg, 2012, 125 pages.

[2] O. Kastner, W.H. Müller, St. Seelecke, H. Struchtrup, M. Torrilhon, W. Weiss, eds., *Special Issue: Trends in Thermodynamics and Materials Theory*, vol. 24, issue 4–6, of Continuum Mechanics and Thermodynamics, Springer, Berlin Heidelberg, 2012, 470 pages.

A.6.2 Editorship of Proceedings and Collected Editions

[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, 2012, 512 pages.

Editorship of Proceedings and Collected Editions (to appear)

[1] G. Dal Maso, A. Mielke, U. Stefanelli, eds., *Rate-independent Evolutions*, Discrete and Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences.

A.6.3 Outstanding Contributions to Monographs

[1] K. Gärtner, H. Si, A. Rand, N. Walkington, *Chapter 11: 3D Delaunay Mesh Generation, in: Combinatorial Scientific Computing*, U. Naumann, O. Schenk, eds., Computational Science Series, CRC Computational Science/Chapman & Hall, Boca Raton, 2012, pp. 299–319.

[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., 2012, pp. 65–81.

Outstanding Contributions to Monographs (to appear)

[1] J.G.M. Schoenmakers, *Coupling local currency Libor models to FX Libor models, in: Recent Advances in Computational Finance*, Th. Gerstner, P. Kloeden, eds., World Scientific Publishers, Singapore.

A.6.4 Articles in Refereed Journals[4]

[1] R. Driben, I. Babushkin, *Accelerated rogue waves generated by soliton fusion at the advanced stage of supercontinuum formation in photonic-crystal fibers*, Opt. Lett., 37 (2012), pp. 5157–5159.

[2] P. Friz, J. Diehl, *Backward stochastic differential equations with rough drivers*, Ann. Probab., 40 (2012), pp. 1715–1758.

[4] Articles that have been written by scholarship holders during their stay at WIAS have been listed in front of those written by the WIAS staff members.

[3] U.K. Sapaev, I. Babushkin, J. Herrmann, *Quasi-phase-matching for third harmonic generation in noble gases employing ultrasound*, Optics Express, 20 (2012), pp. 22753–22762.

[4] G. Aki, J. Daube, W. Dreyer, J. Giesselmann, M. Kränkel, Ch. Kraus, *A diffuse interface model for quasi-incompressible flows: Sharp interface limits and numerics*, ESAIM Proc., 38 (2012), pp. 54–77.

[5] S. Amiranashvili, U. Bandelow, A. Mielke, *Calculation of ultrashort pulse propagation based on rational approximations for medium dispersion*, Opt. Quantum Electron., 44 (2012), pp. 241–246.

[6] A. Demircan, S. Amiranashvili, C. Brée, Ch. Mahnke, F. Mitschke, G. Steinmeyer, *Rogue events in the group velocity horizon*, Sci. Rep., 2 (2012), pp. 00850/1–00850/6.

[7] U. Bandelow, N. Akhmediev, *Persistence of rogue waves in extended nonlinear Schrödinger equations: Integrable Sasa–Satsuma case*, Phys. Lett. A, 376 (2012), pp. 1558–1561.

[8] ———, *Sasa–Satsuma equation: Soliton on a background and its limiting cases*, Phys. Rev. E (3), 86 (2012), pp. 026606/1–026606/8.

[9] M. Becker, W. König, *Self-intersection local times of random walks: Exponential moments in subcritical dimensions*, Probab. Theory Related Fields, 154 (2012), pp. 585–605.

[10] S. Becker, K. Tabelow, H.U. Voss, A. Anwander, R.M. Heidemann, J. Polzehl, *Position-orientation adaptive smoothing of diffusion weighted magnetic resonance data (POAS)*, Med. Image Anal., 16 (2012), pp. 1142–1155.

[11] C. Brée, A. Demircan, G. Steinmeyer, *Kramers–Kronig relations and high order nonlinear susceptibilities*, Phys. Rev. A, 85 (2012), pp. 033806/1–033806/8.

[12] C. Brée, S. Amiranashvili, U. Bandelow, *Spatio-temporal pulse propagation in nonlinear dispersive optical media*, Opt. Quantum Electron., (2012), pp. 012963/1–012963/7.

[13] M. Natale, A. Caiazzo, E.M. Bucci, E. Ficarra, *A novel Gaussian extrapolation approach for 2D gel electrophoresis saturated protein spots*, Genomics Proteomics Bioinformatics, 10 (2012), pp. 336–344.

[14] W. Dreyer, F. Duderstadt, M. Hantke, G. Warnecke, *Bubbles in liquids with phase transition*, Contin. Mech. Thermodyn., 24 (2012), pp. 461–483.

[15] W. Dreyer, P.-É. Druet, O. Klein, J. Sprekels, *Mathematical modeling of Czochralski type growth processes for semiconductor bulk single crystals*, Milan J. Math., 80 (2012), pp. 311–332.

[16] W. Dreyer, J. Giesselmann, Ch. Kraus, Ch. Rohde, *Asymptotic analysis for Korteweg models*, Interfaces Free Bound., 14 (2012), pp. 105–143.

[17] P.-E. Druet, *The classical solvability of the contact angle problem for generalized equations of mean curvature type*, Port. Math., 69 (2012), pp. 233–258.

[18] J. Elschner, G. Hu, *Elastic scattering by unbounded rough surfaces*, SIAM J. Math. Anal., 44 (2012), pp. 4101–4127.

[19] ———, *An optimization method in inverse elastic scattering for one-dimensional grating profiles*, Commun. Comput. Phys., 12 (2012), pp. 1434–1460.

[20] ———, *Scattering of plane elastic waves by three-dimensional diffraction gratings*, Math. Models Methods Appl. Sci., 22 (2012), pp. 1150019/1–1150019/34.

[21] G. Faraud, Y. Hu, Z. Shi, *Almost sure convergence for stochastically biased random walk on trees*, Probab. Theory Related Fields, 154 (2012), pp. 621–660.

[22] Ch. Batallion, F. Bouchon, C. Chainais-Hillairet, J. Fuhrmann, E. Hoarau, R. Touzani, *Numerical methods for the simulation of a corrosion model in a nuclear waste deep repository*, J. Comput. Phys., 231 (2012), pp. 6213–6231.

[23] T. Girnyk, M. Hasler, Y. Maistrenko, *Multistability of twisted states in non-locally coupled Kuramoto-type models*, Chaos Solitons Fractals, 22 (2012), pp. 013114/1–013114/10.

[24] A. Glitzky, *An electronic model for solar cells including active interfaces and energy resolved defect densities*, SIAM J. Math. Anal., 44 (2012), pp. 3874–3900.

[25] G. BenArous, O. Gün, *Universality and extremal aging for the dynamics of spin glasses on subexponential time scales*, Comm. Pure Appl. Math., 65 (2012), pp. 77–127.

[26] K. Hackl, S. Heinz, A. Mielke, *A model for the evolution of laminates in finite-strain elastoplasticity*, ZAMM Z. Angew. Math. Mech., 92 (2012), pp. 888–909.

[27] R. Henrion, *Gradient estimates for Gaussian distribution functions: Application to probabilistically constrained optimization problems*, Numer. Algebra Control Optim., 2 (2012), pp. 655–668.

[28] G. Colombo, R. Henrion, N.D. Hoang, B.S. Mordukhovich, *Optimal control of the sweeping process*, Dyn. Contin. Discrete Impuls. Syst. Ser. B Appl. Algorithms, 19 (2012), pp. 117–159.

[29] R. Henrion, J. Outrata, Th. Surowiec, *Analysis of M-stationary points to an EPEC modeling oligopolistic competition in an electricity spot market*, ESAIM Control Optim. Calc. Var., 18 (2012), pp. 295–317.

[30] ———, *On regular coderivatives in parametric equilibria with non-unique multiplier*, Math. Program., 136 (2012), pp. 111–131.

[31] M. Gerdts, R. Henrion, D. Hömberg, Ch. Landry, *Path planning and collision avoidance for robots*, Numer. Algebra Control Optim., 2 (2012), pp. 437–463.

[32] R. Henrion, A. Möller, *A gradient formula for linear chance constraints under Gaussian distribution*, Math. Oper. Res., 37 (2012), pp. 475–488.

[33] D. Hömberg, J. Liu, N. Togobytska, *Identification of the thermal growth characteristics of coagulated tumor tissue in laser-induced thermotherapy*, Math. Methods Appl. Sci., 35 (2012), pp. 497–509.

[34] G. Hu, *Inverse wave scattering by unbounded obstacles: Uniqueness for the two-dimensional Helmholtz equation*, Appl. Anal., 91 (2012), pp. 703–717.

[35] G. Hu, F. Qu, B. Zhang, *A linear sampling method for inverse problems of diffraction gratings of mixed type*, Math. Methods Appl. Sci., 35 (2012), pp. 1047–1066.

[36] S. Jansen, W. König, *Ideal mixture approximation of cluster size distributions at low density*, J. Statist. Phys., 147 (2012), pp. 963–980.

[37] V. John, J. Novo, *On (essentially) non-oscillatory discretizations of evolutionary convection-diffusion equations*, J. Comput. Phys., 231 (2012), pp. 1570–1586.

[38] V. John, F. Thein, *On the efficiency and robustness of the core routine of the quadrature method of moments (QMOM)*, Chem. Engng. Sci., 75 (2012), pp. 327–333.

[39] R. Bordás, V. John, E. Schmeyer, D. Thévenin, *Measurement and simulation of a droplet population in a turbulent flow field*, Comput. Fluids, 66 (2012), pp. 52–62.

[40] W. Hackbusch, V. John, A. Khachatryan, C. Suciu, *A numerical method for the simulation of an aggregation-driven population balance system*, Internat. J. Numer. Methods Fluids, 69 (2012), pp. 1646–1660.

[41] O. Klein, *Representation of hysteresis operators acting on vector-valued monotaffine functions*, Adv. Math. Sci. Appl., 22 (2012), pp. 471–500.

[42] ———, *Representation of hysteresis operators for vector-valued inputs by functions on strings*, Phys. B, 407 (2012), pp. 1399–1400.

[43] A. Fiaschi, D. Knees, U. Stefanelli, *Young measure quasi-static damage evolution*, Arch. Ration. Mech. Anal., 203 (2012), pp. 415–453.

[44] D. Knees, A. Schröder, *Global spatial regularity for elasticity models with cracks, contact and other non-smooth constraints*, Math. Methods Appl. Sci., 35 (2012), pp. 1859–1884.

[45] W. König, M. Salvi, T. Wolff, *Large deviations for the local times of a random walk among random conductances*, Electron. Comm. Probab., 17 (2012), pp. 1–11.

[46] A. Fischer, P. Pahner, B. Lüssem, K. Leo, R. Scholz, Th. Koprucki, J. Fuhrmann, K. Gärtner, A. Glitzky, *Self-heating effects in organic semiconductor crossbar structures with small active area*, Organic Electronics, 13 (2012), pp. 2461–2468.

[47] K. Krumbiegel, I. Neitzel, A. Rösch, *Regularization error estimates for semilinear elliptic optimal control problems with pointwise state and control constraints*, Comput. Optim. Appl., 52 (2012), pp. 181–207.

[48] M. Liero, Th. Roche, *Rigorous derivation of a plate theory in linear elastoplasticity via Γ-convergence*, NoDEA Nonlinear Differential Equations Appl., 19 (2012), pp. 437–457.

[49] 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*, Comput. Methods Appl. Mech. Engrg., 237–240 (2012), pp. 166–176.

[50] R. Eymard, Th. Gallouët, R. Herbin, A. Linke, *Finite volume schemes for the biharmonic problem on general meshes*, Math. Comp., 81 (2012), pp. 2019–2048.

[51] G. Blanchard, P. Mathé, *Discrepancy principle for statistical inverse problems with application to conjugate gradient iteration*, Inverse Problems, 28 (2012), pp. 115011/1–115011/23.

[52] B. Hofmann, P. Mathé, *Parameter choice in Banach space regularization under variational inequalities*, Inverse Problems, 28 (2012), pp. 104006/1–104006/17.

[53] ———, *Some note on the modulus of continuity for ill-posed problems in Hilbert space*, Trudy Inst. Mat. i Mekh. UrO RAN, 18 (2012), pp. 34–41.

[54] A. Mielke, *Emergence of rate-independent dissipation from viscous systems with wiggly energies*, Contin. Mech. Thermodyn., 24 (2012), pp. 591–606.

[55] ———, *Generalized Prandtl–Ishlinskii operators arising from homogenization and dimension reduction*, Phys. B, 407 (2012), pp. 1330–1335.

[56] St. Arnrich, A. Mielke, M.A. Peletier, G. Savaré, M. Veneroni, *Passing to the limit in a Wasserstein gradient flow: From diffusion to reaction*, Calc. Var. Partial Differ. Equ., 44 (2012), pp. 419–454.

[57] S. Bartels, A. Mielke, T. Roubíček, *Quasistatic small-strain plasticity in the limit of vanishing hardening and its numerical approximation*, SIAM J. Numer. Anal., 50 (2012), pp. 951–976.

[58] A. Mielke, R. Rossi, G. Savaré, *BV solutions and viscosity approximations of rate-independent systems*, ESAIM Control Optim. Calc. Var., 18 (2012), pp. 36–80.

[59] ———, *Variational convergence of gradient flows and rate-independent evolutions in metric spaces*, Milan J. Math., 80 (2012), pp. 381–410.

[60] A. Mielke, L. Truskinovsky, *From discrete visco-elasticity to continuum rate-independent plasticity: Rigorous results*, Arch. Ration. Mech. Anal., 203 (2012), pp. 577–619.

[61] A. Mielke, T. Roubíček, M. Thomas, *From damage to delamination in nonlinearly elastic materials at small strains*, J. Elasticity, 109 (2012), pp. 235–273.

[62] M. Malamud, H. Neidhardt, *Sturm–Liouville boundary value problems with operator potentials and unitary equivalence*, J. Differential Equations, 252 (2012), pp. 5875–5922.

[63] O. Omel'chenko, M. Wolfrum, *Nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, Phys. Rev. Lett., 109 (2012), pp. 164101/1–164101/4.

[64] O. Omel'chenko, M. Wolfrum, S. Yanchuk, Y. Maistrenko, O. Sudakov, *Stationary patterns of coherence and incoherence in two-dimensional arrays of non-locally coupled phase oscillators*, Phys. Rev. E (3), 85 (2012), pp. 036210/1–036210/5.

[65] R.I.A. Patterson, W. Wagner, *A stochastic weighted particle method for coagulation-advection problems*, SIAM J. Sci. Comput., 34 (2012), pp. B290–B311.

[66] A. Pimenov, T.C. Kelly, A. Korobeinikov, M.J.A. O'Callaghan, A.V. Pokrovskii, D. Rachinskii, *Memory effects in population dynamics: Spread of infectious disease as a case study*, Math. Model. Nat. Phenom., 7 (2012), pp. 204–226.

[67] R. Herrero, M. Botey, M. Radziunas, K. Staliunas, *Beam shaping in spatially modulated broad area semiconductor amplifiers*, Opt. Lett., 37 (2012), pp. 5253–5255.

[68] V. Tronciu, S. Schwertfeger, M. Radziunas, A. Klehr, U. Bandelow, H. Wenzel, *Numerical simulation of the amplification of picosecond laser pulses in tapered semiconductor amplifiers and comparison with experimental results*, Opt. Commun., 285 (2012), pp. 2897–2904.

[69] H. Gross, M.-A. Henn, S. Heidenreich, A. Rathsfeld, M. Bär, *Modeling of line roughness and its impact on the diffraction intensities and the reconstructed critical dimensions in scatterometry*, Appl. Optics, 51 (2012), pp. 7384–7394.

[70] M.-A. Henn, S. Heidenreich, H. Gross, A. Rathsfeld, F. Scholze, M. Bär, *Improved grating reconstruction by determination of line roughness in extreme ultraviolet scatterometry*, Opt. Lett., 37 (2012), pp. 5229–5231.

[71] C. Pfüller, M. Ramsteiner, O. Brandt, F. Grosse, A. Rathsfeld, G. Schmidt, L. Geelhaar, H. Riechert, *Raman spectroscopy as a probe for the coupling of light into ensembles of sub-wavelength-sized nanowires*, Appl. Phys. Lett., 101 (2012), pp. 083104/1–083104/4.

[72] A. ter Elst, J. Rehberg, *L^∞-estimates for divergence operators on bad domains*, Anal. Appl. (Singap.), 10 (2012), pp. 207–214.

[73] L. Goray, G. Schmidt, *Analysis of two-dimensional photonic band gaps of any rod shape and conductivity using a conical-integral-equation method*, Phys. Rev. E (3), 85 (2012), pp. 036701/1–036701/12.

[74] J.G.M. Schoenmakers, *A pure martingale dual for multiple stopping*, Finance Stoch., 16 (2012), pp. 319–334.

[75] A. Papapantoleon, J.G.M. Schoenmakers, D. Skovmand, *Efficient and accurate log-Lévy approximations to Lévy driven LIBOR models*, J. Comput. Finance, 15 (2012), pp. 3–44.

[76] A. Mahayni, J.G.M. Schoenmakers, *Minimum return guarantees with funds switching rights — An optimal stopping problem*, J. Econom. Dynam. Control, 35 (2012), pp. 1880–1897.

[77] V. Spokoiny, *Parametric estimation. Finite sample theory*, Ann. Statist., 40 (2012), pp. 2877–2909.

[78] P. Colli, G. Gilardi, J. Sprekels, *Analysis and optimal boundary control of a nonstandard system of phase field equations*, Milan J. Math., 80 (2012), pp. 119–149.

[79] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Continuous dependence for a nonstandard Cahn–Hilliard system with nonlinear atom mobility*, Rend. Semin. Mat. Univ. Politec. Torino, 70 (2012), pp. 27–52.

[80] ———, *Distributed optimal control of a nonstandard system of phase field equations*, Contin. Mech. Thermodyn., 24 (2012), pp. 437–459.

[81] ———, *Global existence for a strongly coupled Cahn–Hilliard system with viscosity*, Boll. Unione Mat. Ital. (9), 5 (2012), pp. 495–513.

[82] T. Streckenbach, *Parameter determination of an evolution model for phase transformations in steel*, ZAMM Z. Angew. Math. Mech., 92 (2012), pp. 217–235.

[83] K. Tabelow, H.U. Voss, J. Polzehl, *Modeling the orientation distribution function by mixtures of angular central Gaussian distributions*, J. Neurosci. Meth., 203 (2012), pp. 200–211.

[84] M. Tlidi, E. Averlant, A.G. Vladimirov, K. Panajotov, *Delay feedback induces a spontaneous motion of two-dimensional cavity solitons in driven semiconductor microcavities*, Phys. Rev. A, 86 (2012), pp. 033822/1–033822/8.

[85] D. Turaev, A.G. Vladimirov, S. Zelik, *Long range interaction and synchronization of oscillating dissipative solitons*, Phys. Rev. Lett., 108 (2012), pp. 263906/1–263906/5.

[86] M. Lichtner, V.Z. Tronciu, A.G. Vladimirov, *Theoretical investigations of striped and non-striped broad area lasers with off-axis feedback*, IEEE J. Quantum Electron., 48 (2012), pp. 353–360.

[87] T. Habruseva, S.P. Hegarty, A.G. Vladimirov, A. Pimenov, D. Rachinskii, N. Rebrova, E.A. Viktorov, G. Huyet, *Bistable regimes in an optically injected mode-locked laser*, Opt. Express, 20 (2012), pp. 25572–25583.

[88] Ch. Otto, K. Lüdge, A.G. Vladimirov, M. Wolfrum, E. Schöll, *Delay induced dynamics and jitter reduction of passively mode-locked semiconductor lasers subject to optical feedback*, New J. Phys., 14 (2012), pp. 113033/1–113033/29.

[89] S. Shekar, W.J. Menz, A.J. Smith, M. Kraft, W. Wagner, *On a multivariate population balance model to describe the structure and composition of silica nanoparticles*, Comput. Chem. Engng., 43 (2012), pp. 130–147.

[90] I. Müller, W. Weiss, *Thermodynamics of irreversible processes — Past and present*, Eur. Phys. J. H, 37 (2012), pp. 139–236.

[91] A. Wilms, D. Breddermann, P. Mathé, *Theory of direct capture from two- and three-dimensional reservoirs to quantum dot states*, Phys. Status Solidi C, 9 (2012), pp. 1278–1281.

[92] M. Wolfrum, *The Turing bifurcation in network systems: Collective patterns and single differentiated nodes*, Phys. D, 241 (2012), pp. 1351–1357.

[93] B. Fiedler, C. Rocha, M. Wolfrum, *A permutation characterization of Sturm global attractors of Hamiltonian type*, J. Differential Equations, 252 (2012), pp. 588–623.

[94] ———, *Sturm global attractors for S^1 -equivariant parabolic equations*, Networks Heterogeneous Media, 7 (2012), pp. 617–659.

Articles in Refereed Journals (to appear)

[1] D. Crisan, J. Diehl, P. Friz, H. Oberhauser, *Robust filtering: Correlated noise and multidimensional observation*, Ann. Appl. Probab.

[2] J.D. Deuschel, P. Friz, A. Jacquier, S. Violante, *Marginal density expansions for diffusions and stochastic volatility: Part I*, Comm. Pure Appl. Math.

[3] ———, *Marginal density expansions for diffusions and stochastic volatility: Part II*, Comm. Pure Appl. Math.

[4] P. Friz, H. Oberhauser, *Rough path stability of (semi-)linear SPDEs*, Probab. Theory Related Fields.

[5] P. Friz, S. Riedel, *Convergence rates for the full Gaussian rough paths*, Ann. Inst. H. Poincare Probab. Statist.

[6] P. Friz, A. Shekhar, *Doob–Meyer for rough paths*, Ann. Probab.

[7] G. Aki, W. Dreyer, J. Giesselmann, Ch. Kraus, *A quasi-incompressible diffuse interface model with phase transition*, Math. Models Methods Appl. Sci.

[8] R. Arkhipov, A. Pimenov, M. Radziunas, D. Rachinskii, A.G. Vladimirov, D. Arsenijevic, H. Schmeckebier, D. Bimberg, *Hybrid mode-locking in semiconductor lasers: Simulations, analysis and experiments*, IEEE J. Select. Topics Quantum Electron.

[9] Ch. Bayer, P. Laurence, *Asymptotics beats Monte Carlo: The case of correlated local vol baskets*, Comm. Pure Appl. Math.

[10] Ch. Bayer, R.L. Loeffen, P. Friz, *Semi-closed form cubature and applications to financial diffusion models*, Quant. Finance.

[11] P. Friz, Ch. Bayer, *Functional convergence of the cubature tree on Wiener space*, Appl. Math. Optim.

[12] 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*, Quart. Appl. Math.

[13] P.-É. Druet, *Global Lipschitz continuity for elliptic transmission problems with a boundary intersecting interface*, Math. Bohem.

[14] J. Fuhrmann, *Some abstract error estimates of a finite volume scheme*, Appl. Math.

[15] A. Glitzky, A. Mielke, *A gradient structure for systems coupling reaction-diffusion effects in bulk and interfaces*, ZAMP Z. Angew. Math. Phys.

[16] K. Götze, *Strong solutions for the interaction of a rigid body and a viscoelastic fluid*, J. Math. Fluid Mech.

[17] M. Geissert, K. Götze, M. Hieber, *L^p-theory for strong solutions to fluid-rigid body interaction in Newtonian and generalized Newtonian fluids*, Trans. Amer. Math. Soc.

[18] Ch. Heinemann, Ch. Kraus, *Existence results for diffuse interface models describing phase separation and damage*, European J. Appl. Math.

[19] R. Henrion, A. Kruger, J. Outrata, *Some remarks on stability of generalized equations*, J. Optim. Theory Appl.

[20] D. Hömberg, K. Krumbiegel, J. Rehberg, *Boundary coefficient control — A maximal parabolic regularity approach*, Appl. Math. Optim.

[21] R. Haller-Dintelmann, W. Höppner, H.-Chr. Kaiser, J. Rehberg, G. Ziegler, *Optimal elliptic Sobolev regularity near three-dimensional, multi-material Neumann vertices*, Funct. Anal. Appl.

[22] V. John, J. Novo, *A robust SUPG norm a posteriori error estimator for stationary convection-diffusion equations*, Comput. Methods Appl. Mech. Engrg.

[23] R. Bordás, V. John, E. Schmeyer, D. Thévenin, *Numerical methods for the simulation of a coalescence-driven droplet size distribution*, Theor. Comput. Fluid Dyn.

[24] Th.I. Seidman, O. Klein, *Periodic solutions of isotone hybrid systems*, Discrete Contin. Dyn. Syst. Ser. B.

[25] Ch. Kudla, A.T. Blumenau, F. Büllesfeld, N. Dropka, Ch. Frank-Rotsch, F. Kiessling, O. Klein, P. Lange, W. Miller, U. Rehse, U. Sahr, M. Schellhorn, G. Weidemann, M. Ziem, G. Bethin, R. Fornari, M. Müller, J. Sprekels, V. Trautmann, P. Rudolph, *Crystallization of 640 kg mc-silicon ingots under traveling magnetic field by using a heater-magnet module*, J. Crystal Growth.

[26] D. Knees, R. Rossi, Ch. Zanini, *A vanishing viscosity approach to a rate-independent damage model*, Math. Models Methods Appl. Sci.

[27] D. Knees, A. Schröder, *Computational aspects of quasi-static crack propagation*, Discrete Contin. Dyn. Syst. Ser. S.

[28] A. Fiaschi, D. Knees, S. Reichelt, *Global higher integrability of minimizers of variational problems with mixed boundary conditions*, J. Math. Anal. Appl.

[29] K. Krumbiegel, J. Rehberg, *Second order sufficient optimality conditions for parabolic optimal control problems with pointwise state constraints*, SIAM J. Control Optim.

[30] M. Ladkau, J.G.M. Schoenmakers, J. Zhang, *Libor model with expiry-wise stochastic volatility and displacement*, Int. J. Portfolio Analysis and Management.

[31] T. Jacob, M. Landstorfer, *Mathematical modeling of intercalation batteries at the cell level and beyond*, Chem Soc Rev, (2012).

[32] M. Liero, *Passing from bulk to bulk/surface evolution in the Allen–Cahn equation*, NoDEA Nonlinear Differential Equations Appl.

[33] M. Liero, U. Stefanelli, *The elliptic-regularization principle in Lagrangian mechanics*, J. Nonlinear Sci.

[34] ———, *Weighted Inertia-Dissipation-Energy functionals for semilinear equations*, Boll. Unione Mat. Ital. (9).

[35] M. Liero, A. Mielke, *Gradient structures and geodesic convexity for reaction-diffusion systems*, Phil. Trans. R. Soc. A.

[36] S. Lu, P. Mathé, *Heuristic parameter selection based on functional minimization: Optimality and model function approach*, Math. Comp.

[37] A. Mielke, *Geodesic convexity of the relative entropy in reversible Markov chains*, Calc. Var. Partial Differ. Equ.

[38] ———, *Thermomechanical modeling of energy-reaction-diffusion systems, including bulk-interface interactions*, Discrete Contin. Dyn. Syst. Ser. S.

[39] A. Mielke, E. Rohan, *Homogenization of elastic waves in fluid-saturated porous media using the Biot model*, Math. Models Methods Appl. Sci.

[40] A. Mielke, R. Rossi, G. Savaré, *Nonsmooth analysis of doubly nonlinear evolution equations*, Calc. Var. Partial Differ. Equ.

[41] A. Mielke, U. Stefanelli, *Linearized plasticity is the evolutionary Gamma limit of finite plasticity*, J. Eur. Math. Soc. (JEMS).

[42] A. Mielke, S. Zelik, *On the vanishing-viscosity limit in parabolic systems with rate-independent dissipation terms*, Ann. Sc. Norm. Super. Pisa Cl. Sci. (5).

[43] R. Bruggemann, H.-J. Mucha, H.-G. Bartel, *Ranking of polluted regions in south west Germany based on a multi-indicator system*, MATCH Commun. Math. Comput. Chem.

[44] N. Murisic, B. Pausader, D. Peschka, A.L. Bertozzi, *Dynamics of particle setting and resuspension in viscous liquid films*, J. Fluid Mech.

[45] J. Schmidt, R. Prignitz, D. Peschka, A. Münch, B. Wagner, E. Bänsch, W. Peukert, *Conductivity in nonpolar media: Experimental and numerical studies on sodium AOT-hexadecane, lecithin-hexadecane and aluminum(III)-3,5-diisopropyl salicylate-hexadecane systems*, J. Colloid Interface Sci.

[46] A. ter Elst, M. Meyries, J. Rehberg, *Parabolic equations with dynamical boundary conditions and source terms on interfaces*, Ann. Mat. Pura Appl. IV. Ser.

[47] G. Schmidt, *Conical diffraction by multilayer gratings: A recursive integral equations approach*, Appl. Math.

[48] F. Lanzara, V. Maz'ya, G. Schmidt, *Computation of volume potentials over bounded domains via approximate approximations*, J. Math. Sci. (N. Y.).

[49] J.G.M. Schoenmakers, J. Zhang, J. Huang, *Optimal dual martingales, their analysis and application to new algorithms for Bermudan products*, SIAM J. Financial Math.

[50] Ch. Bender, J.G.M. Schoenmakers, J. Zhang, *Dual representations for general multiple stopping problems*, Math. Finance.

[51] V. Spokoiny, W. Wang, W.K. Härdle, *Local quantile regression*, J. Statist. Plann. Inference.

[52] F. Gach, R. Nickl, V. Spokoiny, *Spatially adaptive density estimation by localised Haar projections*, Ann. Inst. H. Poincare Probab. Statist.

[53] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *An asymptotic analysis for a nonstandard Cahn–Hilliard system with viscosity*, Discrete Contin. Dyn. Syst. Ser. S.

[54] M. Thomas, *Quasistatic damage evolution with spatial BV-regularization*, Discrete Contin. Dyn. Syst. Ser. S.

[55] J. Sieber, M. Wolfrum, M. Lichtner, S. Yanchuk, *On the stability of periodic orbits in delay equations with large delay*, Discrete Contin. Dyn. Syst.

A.6.5 Contributions to Collected Editions

[1] R. Arkhipov, *Modelling of hybrid mode-locking in quantum dot lasers*, Section 10 of Proceedings of the XIII School Seminar “Wave Phenomena in Inhomogeneous Media” (in electronic form and in Russian), Lomonosov Moscow State University, Faculty of Physics, Moscow, 2012, pp. 3–6.

[2] R. Arkhipov, M.V. Arkhipov, Y.A. Tolmachev, *Emission of the new frequencies in the resonant medium under the conditions of excitation by an object propagating at superluminal velocity*, Section 11 of Proceedings of the XIII School Seminar “Wave Phenomena in Inhomogeneous Media” (in electronic form and in Russian), Lomonosov Moscow State University, Faculty of Physics, Moscow, 2012, pp. 2–5.

[3] C. Brée, S. Amiranashvili, U. Bandelow, *Spatio-temporal pulse propagation in nonlinear dispersive optical media*, in: Proceedings of the 12th International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD’12, J. Piprek, W. Lu, eds., IEEE Conference Publications Management Group, New Jersey, USA, 2012, pp. 131–132.

[4] W. Dreyer, C. Guhlke, *Hysteresis and phase transition in many-particle storage systems*, in: Hyperbolic Problems: Theory, Numerics and Applications, Vol. 1, T. Li, S. Jiang, eds., vol. 17 of Series in Contemporary Applied Mathematics, Higher Education Press, Beijing, 2012, pp. 196–202.

[5] J. Elschner, G. Hu, *Inverse scattering of elastic waves by diffraction gratings*, in: Inverse Problems for Partial Differential Equations, Workshop, February 19–25, 2012, vol. 11 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2012, pp. 633–634.

[6] K. Götze, *Maximal L^p-regularity of a 2D fluid-solid interaction problem*, in: Spectral Theory, Mathematical System Theory, Evolution Equations, Differential and Difference Equations, W. Arendt, J.A. Ball, J. Behrndt, K.-H. Förster, V. Mehrmann, C. Trunk, eds., vol. 221 of Operator Theory: Advances and Applications, Birkhäuser, Basel, 2012, pp. 373–384.

[7] F. Castell, O. Gün, G. Maillard, *Parabolic Anderson model with finite number of moving catalysts*, in: Probability in Complex Physical Systems, in Honour of Erwin Bolthausen and Jürgen Gärtner, J.-D. Deuschel, B. Gentz, W. König, M. von Renesse, M. Scheutzow, U. Schmock, eds., vol. 11 of Springer Proceedings in Mathematics, Springer, Berlin Heidelberg, 2012, pp. 91–116.

[8] Ch. Heinemann, Ch. Kraus, *Damage processes coupled with phase separation in elastically stressed alloys*, in: Proceedings in Applied Mathematics and Mechanics (PAMM), vol. 12, 2012, pp. 153–154.

[9] R. Henrion, *Stability of chance constrained optimization*, in: Variational Analysis and its Applications, M. Cervinka, ed., Lecture Notes of Spring School in Variational Analysis, MatFyzPress, Prague, 2012, pp. 1–26.

[10] M.J. Fabian, R. Henrion, A. Kruger, J. Outrata, *About error bounds in metric spaces*, Operations Research Proceedings 2011, Springer, Berlin Heidelberg, 2012, pp. 33–38.

[11] W. König, S. Schmidt, *The parabolic Anderson model with acceleration and deceleration*, in: Probability in Complex Physical Systems, in Honour of Erwin Bolthausen and Jürgen Gärtner, J.-D. Deuschel, B. Gentz,

W. König, M. von Renesse, M. Scheutzow, U. Schmock, eds., vol. 11 of Springer Proceedings in Mathematics, Springer, Berlin Heidelberg, 2012, pp. 225–245.

[12] Th. Koprucki, K. Gärtner, *Discretization scheme for drift-diffusion equations with strong diffusion enhancement*, in: Proceedings of the 12th International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD'12, J. Piprek, W. Lu, eds., IEEE Conference Publications Management Group, New Jersey, USA, 2012, pp. 103–104.

[13] H.-J. Mucha, *Method selection in cluster analysis followed by built-in validation*, in: Data Analysis Methods and its Applications, J. Pociecha, R. Decker, eds., Wydawnictwo C. H. Beck, Warszawa, 2012, pp. 125–142.

[14] H.-J. Mucha, H.-G. Bartel, *An accelerated K-means algorithm based on adaptive distances*, in: Challenges at the Interface of Data Analysis, Computer Science, and Optimization — Proceedings of the 34th Annual Conference of the Gesellschaft für Klassifikation e. V., Karlsruhe, July 21–23, 2010, W. Gaul, A. Geyer-Schulz, L. Schmidt-Thieme, J. Kunze, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Heidelberg, 2012, pp. 37–47.

[15] S. Behrendt, H.-J. Mucha, H.-G. Bartel, D.P. Mielke, *Zur Problematik der multivariaten statistischen Analyse umfangreicher P-RFA-Datenmengen phönizischer Keramik*, in: Archäometrie und Denkmalpflege 2012, F. Schlütter, S. Greif, M. Prange, eds., Metalla, Sonderheft 5, Deutsches Bergbau-Museum Bochum, 2012, pp. 157–159.

[16] J. Dolata, H.-J. Mucha, H.-G. Bartel, *Eine neue Referenzgruppe für die römische Ziegelproduktion der I. Thrakerkohorte am Mittelrhein*, in: Archäometrie und Denkmalpflege 2012, F. Schlütter, S. Greif, M. Prange, eds., Metalla, Sonderheft 5, Deutsches Bergbau-Museum Bochum, 2012, pp. 171–173.

[17] C. Morales-Merino, H.-J. Mucha, H.-G. Bartel, *Multivariate statistical analysis of clay and ceramic-data for provenance of Bronze Age pottery from Troia*, in: Archäometrie und Denkmalpflege 2012, F. Schlütter, S. Greif, M. Prange, eds., Metalla, Sonderheft 5, Deutsches Bergbau-Museum Bochum, 2012, pp. 174–176.

[18] A. Pimenov, G. Kozyreff, V.Z. Tronciu, A.G. Vladimirov, *Theoretical analysis of a multi-stripe laser array with external off-axis feedback*, in: Semiconductor Lasers and Laser Dynamics V, K. Panajotov, M. Sciamanna, A. Valle, R. Michalzik, eds., vol. 8432 of Proceedings of SPIE, SPIE, Bellingham, Washington, 2012, pp. 843212/1–843212/10.

[19] M. Radziunas, K. Staliunas, *Spatial "rocking" for improving the spatial quality of the beam of broad area semiconductor lasers*, in: Semiconductor Lasers and Laser Dynamics V, K. Panajotov, M. Sciamanna, A.A. Valle, R. Michalzik, eds., vol. 8432 of Proceedings of SPIE, SPIE, Bellingham, Washington, 2012, pp. 84320Q/1–84320Q/9.

[20] H. Gross, M.-A. Henn, A. Rathsfeld, M. Bär, *Stochastic modeling aspects for an improved solution of the inverse problem in scatterometry*, in: Advanced Mathematical And Computational Tools In Metrology And Testing IX, F. Pavese, M. Bär, J.-R. Filtz, A.B. Forbes, L. Pendrill, K. Shirono, eds., vol. 84 of Series on Advances in Mathematics for Applied Sciences, World Scientific, Singapore, 2012, pp. 202–209.

[21] E. Averlant, M. Tlidi, A.G. Vladimirov, H. Thienpont, K. Panajotov, *Delay induces motion of multipeak localized structures in cavity semiconductors*, in: Semiconductor Lasers and Laser Dynamics V, K. Panajotov, M. Sciamanna, A. Valle, R. Michalzik, eds., vol. 8432 of Proceedings of SPIE, SPIE, Bellingham, Washington, 2012, pp. 84321D/1–84321D/6.

[22] A.G. Vladimirov, D. Rachinskii, M. Wolfrum, *Modeling of passively mode-locked semiconductor lasers*, in: Nonlinear Laser Dynamics: From Quantum Dots to Cryptography, K. Lüdge, ed., Reviews in Nonlinear Dynamics and Complexity, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2012, pp. 183–216.

[23] A. Schnitzler, T. Wolff, *Precise asymptotics for the parabolic Anderson model with a moving catalyst or trap*, in: Probability in Complex Physical Systems, in Honour of Erwin Bolthausen and Jürgen Gärtner, J.-

D. Deuschel, B. Gentz, W. König, M. von Renesse, M. Scheutzow, eds., vol. 11 of Springer Proceedings in Mathematics, Springer, Berlin Heidelberg, 2012, pp. 69–88.

Contributions to Collected Editions (to appear)

[1] S.M.A. Becker, *Regularization of diffusion weighted MRI-data without blurring the geometrical structure*, in: Computational Inverse Problems, Workshop, October 21–27, 2012, Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach.

[2] J. Elschner, G. Hu, *Direct and inverse elastic scattering problems for diffraction gratings*, in: Direct and Inverse Problems in Wave Propagation and Applications, I.G. Graham, U. Langer, J.M. Melenk, M. Sini, eds., no. 14 in Radon Series on Computational and Applied Mathematics, De Gruyter.

[3] R. Henrion, *A critical note on empirical (sample average, Monte Carlo) approximation of solutions to chance constrained programs*, in: System Modeling and Optimization, D. Hömberg, F. Tröltzsch, eds., vol. 391 of IFIP Advances in Information and Communication Technology, Springer, Heidelberg et al.

[4] D. Belomestny, M. Ladkau, J.G.M. Schoenmakers, *Tight bounds for American options via multilevel Monte Carlo*, in: Proceedings of the 2012 Winter Simulation Conference, C. Laroque, J. Himmelspach, R. Pasupathy, O. Rose, A.M. Uhrmacher, eds.

[5] Ch. Landry, M. Gerdts, R. Henrion, D. Hömberg, *Path-planning with collision avoidance in automotive industry*, in: System Modeling and Optimization, D. Hömberg, F. Tröltzsch, eds., vol. 391 of IFIP Advances in Information and Communication Technology, Springer, Heidelberg et al.

[6] A. Mielke, *Dissipative quantum mechanics using GENERIC*, in: Recent Trends in Dynamical Systems, A. Johann, H.-P. Kruse, St. Schmitz, eds., Proceedings in Mathematics, Springer, Heidelberg.

[7] H.-J. Mucha, *Classification, clustering and visualisation based on dual scaling*, in: German-Japanese Interchange of Data Analysis Results, W. Gaul, A. Geyer-Schulz, A. Okada, Y. Baba, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Heidelberg.

[8] ———, *Pairwise data clustering accompanied by validation and visualisation*, in: German-Japanese Interchange of Data Analysis Results, W. Gaul, A. Geyer-Schulz, A. Okada, Y. Baba, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Heidelberg.

[9] H.-J. Mucha, H.-G. Bartel, C. Morales-Merino, *Visualisation of cluster analysis results*, in: Classification and Data Mining, A. Giusti, G. Ritter, M. Vichi, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Berlin.

[10] H.-J. Mucha, J. Dolata, H.-G. Bartel, *Classification of Roman tiles with stamp PARDALIVS*, in: Algorithms from & for Nature and Life, B. Lausen, D. van den Poel, A. Ultsch, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Heidelberg.

[11] C. Morales-Merino, H.-J. Mucha, E. Pernicka, G. Balcazar, R. Tagle, M.E. Espinosa Pesqueira, *Clay sediments diversity in the Troad and the provenance of Troian pottery*, in: Proceedings of the 38th International Symposium on Archaeometry, 10th – 14th May, 2010, Tampa, Springer, New York.

A.7 Preprints, Reports

A.7.1 WIAS Preprints Series[5]

[1] L. Bergé, St. Skupin, Ch. Köhler, I. Babushkin, J. Herrmann, *3D numerical simulations of THz generation by two-color laser filaments*, Preprint no. 1752, WIAS, Berlin, 2012.

[2] D.P. Challa, G. Hu, M. Sini, *Multiple scattering of electromagnetic waves by a finite number of point-like obstacles*, Preprint no. 1745, WIAS, Berlin, 2012.

[3] R. Driben, I. Babushkin, *Accelerated rogue waves generated by soliton fusion at the advanced stage of supercontinuum formation in photonic crystal fibers*, Preprint no. 1754, WIAS, Berlin, 2012.

[4] G. Hu, A. Kirsch, M. Sini, *Some inverse problems arising from elastic scattering by rigid obstacles*, Preprint no. 1727, WIAS, Berlin, 2012.

[5] N. Nefedov, L. Recke, K. Schneider, *On existence and asymptotic stability of periodic solutions with an interior layer of reaction-advection-diffusion equations*, Preprint no. 1683, WIAS, Berlin, 2012.

[6] U. Sapaev, I. Babushkin, J. Herrmann, *Quasi-phase-matching for third harmonic generation in noble gases employing ultrasound*, Preprint no. 1753, WIAS, Berlin, 2012.

[7] G. Aki, J. Daube, W. Dreyer, J. Giesselmann, M. Kränkel, Ch. Kraus, *A diffuse interface model for quasi-incompressible flows: Sharp interface limits and numerics*, Preprint no. 1680, WIAS, Berlin, 2012.

[8] G. Aki, W. Dreyer, J. Giesselmann, Ch. Kraus, *A quasi-incompressible diffuse interface model with phase transition*, Preprint no. 1726, WIAS, Berlin, 2012.

[9] S. Amiranashvili, U. Bandelow, N. Akhmediev, *Few-cycle optical solitons in dispersive media beyond the envelope approximation*, Preprint no. 1723, WIAS, Berlin, 2012.

[10] R. Arkhipov, A. Pimenov, M. Radziunas, A.G. Vladimirov, D. Arsenjević, D. Rachinskii, H. Schmeckebier, D. Bimberg, *Hybrid mode-locking in edge-emitting semiconductor lasers: Simulations, analysis and experiments*, Preprint no. 1734, WIAS, Berlin, 2012.

[11] Th. Arnold, A. Rathsfeld, *Reflection of plane waves by rough surfaces in the sense of Born approximation*, Preprint no. 1725, WIAS, Berlin, 2012.

[12] U. Bandelow, N. Akhmediev, *Persistence of rogue waves in extended nonlinear Schrödinger equations: Integrable Sasa–Satsuma case*, Preprint no. 1696, WIAS, Berlin, 2012.

[13] ———, *Sasa–Satsuma equation: Soliton on a background and its limiting cases*, Preprint no. 1724, WIAS, Berlin, 2012.

[14] C. Brée, S. Amiranashvili, U. Bandelow, *Spatio-temporal pulse propagation in nonlinear dispersive optical media*, Preprint no. 1733, WIAS, Berlin, 2012.

[15] W. Dreyer, M. Hantke, G. Warnecke, *On balance laws for mixture theories of disperse vapor bubbles in liquid with phase change*, Preprint no. 1741, WIAS, Berlin, 2012.

[16] W. Dreyer, P.-É. Druet, O. Klein, J. Sprekels, *Mathematical modeling of Czochralski type growth processes for semiconductor bulk single crystals*, Preprint no. 1689, WIAS, Berlin, 2012.

[17] W. Dreyer, C. Guhlke, R. Müller, *Overcoming the shortcomings of the Nernst–Planck model*, Preprint no. 1730, WIAS, Berlin, 2012.

[18] P.-E. Druet, *Some mathematical problems related to the 2nd order optimal shape of a crystallization interface*, Preprint no. 1708, WIAS, Berlin, 2012.

[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.

[19] J. Elschner, G. Hu, *Direct and inverse elastic scattering problems for diffraction gratings*, Preprint no. 1719, WIAS, Berlin, 2012.

[20] ———, *Elastic scattering by unbounded rough surfaces*, Preprint no. 1677, WIAS, Berlin, 2012.

[21] G. Faraud, St. Goutte, *Bessel bridges decomposition with varying dimension. Applications to finance*, Preprint no. 1707, WIAS, Berlin, 2012.

[22] A. Fiebach, A. Glitzky, A. Linke, *Uniform global bounds for solutions of an implicit Voronoi finite volume method for reaction-diffusion problems*, Preprint no. 1718, WIAS, Berlin, 2012.

[23] T. Girnyk, M. Hasler, Y. Maistrenko, *Multistability of twisted states in non-locally coupled Kuramoto-type models*, Preprint no. 1685, WIAS, Berlin, 2012.

[24] O. Gün, W. König, O. Sekulović, *Moment asymptotics for branching random walks in random environment*, Preprint no. 1729, WIAS, Berlin, 2012.

[25] H. Hanke, D. Knees, *Derivation of an effective damage model with evolving micro-structure*, Preprint no. 1749, WIAS, Berlin, 2012.

[26] Ch. Heinemann, Ch. Kraus, *Complete damage in linear elastic materials – Modeling, weak formulation and existence results*, Preprint no. 1722, WIAS, Berlin, 2012.

[27] ———, *A degenerating Cahn–Hilliard system coupled with complete damage processes*, Preprint no. 1759, WIAS, Berlin, 2012.

[28] S. Heinz, *On the structure of the quasiconvex hull in planar elasticity*, Preprint no. 1736, WIAS, Berlin, 2012.

[29] R. Henrion, A. Kruger, J. Outrata, *Some remarks on stability of generalized equations*, Preprint no. 1678, WIAS, Berlin, 2012.

[30] R. Henrion, J. Outrata, Th. Surowiec, *On regular coderivatives in parametric equilibria with non-unique multipliers*, Preprint no. 1686, WIAS, Berlin, 2012.

[31] R. Henrion, A. Möller, *A gradient formula for linear chance constraints under Gaussian distribution*, Preprint no. 1687, WIAS, Berlin, 2012.

[32] G. Hu, M. Sini, *Elastic scattering by finitely many point-like obstacles*, Preprint no. 1720, WIAS, Berlin, 2012.

[33] G. Hu, A. Rathsfeld, *Scattering of time-harmonic electromagnetic plane waves by perfectly conducting diffraction gratings*, Preprint no. 1694, WIAS, Berlin, 2012.

[34] R. Huth, *Numerical convergence for semilinear parabolic equations*, Preprint no. 1747, WIAS, Berlin, 2012.

[35] S. Jachalski, G. Kitavtsev, R. Taranets, *Weak solutions to lubrication systems describing the evolution of bilayer thin films*, Preprint no. 1746, WIAS, Berlin, 2012.

[36] S. Jachalski, D. Peschka, A. Münch, B. Wagner, *Impact of interfacial slip on the stability of liquid two-layer polymer films*, Preprint no. 1743, WIAS, Berlin, 2012.

[37] S. Jansen, W. König, *Ideal mixture approximation of cluster size distributions at low density*, Preprint no. 1674, WIAS, Berlin, 2012.

[38] G.R. Barrenechea, V. John, P. Knobloch, *A local projection stabilization finite element method with nonlinear crosswind diffusion for convection-diffusion-reaction equations*, Preprint no. 1690, WIAS, Berlin, 2012.

[39] V. John, J. Novo, *A robust SUPG norm a posteriori error estimator for the SUPG finite element approximation of stationary convection-diffusion equations*, Preprint no. 1714, WIAS, Berlin, 2012.

[40] V. JOHN, F. THEIN, *On the efficiency and robustness of the core routine of the quadrature method of moments (QMOM)*, Preprint no. 1697, WIAS, Berlin, 2012.

[41] E. JENKINS, V. JOHN, A. LINKE, L.G. REBHOLZ, *On the parameter choice in grad-div stabilization for incompressible flow problems*, Preprint no. 1751, WIAS, Berlin, 2012.

[42] R. BORDÁS, V. JOHN, E. SCHMEYER, D. THÉVENIN, *Numerical methods for the simulation of an aggregation-driven droplet size distribution*, Preprint no. 1716, WIAS, Berlin, 2012.

[43] O. KLEIN, *Representation of hysteresis operators for vector-valued continuous monotaffine input functions by functions on strings*, Preprint no. 1698, WIAS, Berlin, 2012.

[44] TH.I. SEIDMAN, O. KLEIN, *Periodic solutions of isotone hybrid systems*, Preprint no. 1732, WIAS, Berlin, 2012.

[45] D. KNEES, A. SCHRÖDER, *Global spatial regularity for elasticity models with cracks, contact and other non-smooth constraints*, Preprint no. 1673, WIAS, Berlin, 2012.

[46] R. HALLER-DINTELMANN, A. JONSSON, D. KNEES, J. REHBERG, *On elliptic and parabolic regularity for mixed boundary value problems*, Preprint no. 1706, WIAS, Berlin, 2012.

[47] A. FISCHER, P. PAHNER, B. LÜSSEM, K. LEO, R. SCHOLZ, TH. KOPRUCKI, J. FUHRMANN, K. GÄRTNER, A. GLITZKY, *Self-heating effects in organic semiconductor devices enhanced by positive temperature feedback*, Preprint no. 1693, WIAS, Berlin, 2012.

[48] TH. KOPRUCKI, K. GÄRTNER, *Discretization scheme for drift-diffusion equations with a generalized Einstein relation*, Preprint no. 1738, WIAS, Berlin, 2012.

[49] A. FISCHER, P. PAHNER, B. LÜSSEM, K. LEO, R. SCHOLZ, TH. KOPRUCKI, K. GÄRTNER, A. GLITZKY, *Self-heating, bistability, and thermal switching in organic semiconductors*, Preprint no. 1735, WIAS, Berlin, 2012.

[50] K. KRUMBIEGEL, J. REHBERG, *Second order sufficient optimality conditions for parabolic optimal control problems with pointwise state constraints*, Preprint no. 1700, WIAS, Berlin, 2012.

[51] D. BELOMESTNY, M. LADKAU, J.G.M. SCHOENMAKERS, *Simulation based policy iteration for American style derivatives — A multilevel approach*, Preprint no. 1721, WIAS, Berlin, 2012.

[52] M. LADKAU, J.G.M. SCHOENMAKERS, J. ZHANG, *Libor model with expiry-wise stochastic volatility and displacement*, Preprint no. 1702, WIAS, Berlin, 2012.

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

[54] M. LIERO, A. MIELKE, *Gradient structures and geodesic convexity for reaction-diffusion systems*, Preprint no. 1701, WIAS, Berlin, 2012.

[55] H. MAI, *Efficient maximum likelihood estimation for Lévy-driven Ornstein–Uhlenbeck processes*, Preprint no. 1717, WIAS, Berlin, 2012.

[56] A. MIELKE, *Dissipative quantum mechanics using GENERIC*, Preprint no. 1710, WIAS, Berlin, 2012.

[57] A. MIELKE, E. ROHAN, *Homogenization of elastic waves in fluid-saturated porous media using the Biot model*, Preprint no. 1688, WIAS, Berlin, 2012.

[58] A. MIELKE, R. ROSSI, G. SAVARÉ, *Variational convergence of gradient flows and rate-independent evolutions in metric spaces*, Preprint no. 1704, WIAS, Berlin, 2012.

[59] O. OMEL'CHENKO, M. WOLFRUM, *Nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, Preprint no. 1715, WIAS, Berlin, 2012.

[60] O. OMEL'CHENKO, M. WOLFRUM, S. YANCHUK, Y. MAISTRENKO, O. SUDAKOV, *Stationary patterns of coherence and incoherence in two-dimensional arrays of non-locally coupled phase oscillators*, Preprint no. 1682, WIAS, Berlin, 2012.

[61] R.I.A. Patterson, *Convergence of stochastic particle systems undergoing advection and coagulation*, Preprint no. 1757, WIAS, Berlin, 2012.

[62] A. Pérez-Serrano, J. Javaloyes, S. Balle, *Multi-channel wavelength conversion using four-wave mixing in semiconductor ring lasers*, Preprint no. 1728, WIAS, Berlin, 2012.

[63] ———, *Spectral delay algebraic equation approach to broad area laser diodes*, Preprint no. 1755, WIAS, Berlin, 2012.

[64] N. Murisic, B. Pausader, D. Peschka, A.L. Bertozzi, *Dynamics of particle settling and resuspension in viscous liquids*, Preprint no. 1679, WIAS, Berlin, 2012.

[65] A. Pimenov, V.Z. Tronciu, U. Bandelow, A.G. Vladimirov, *Dynamical regimes of multi-stripe laser array with external off-axis feedback*, Preprint no. 1731, WIAS, Berlin, 2012.

[66] P.N. Racec, St. Schade, H.-Chr. Kaiser, *Eigensolutions of the Wigner–Eisenbud problem for a cylindrical nanowire within finite volume method*, Preprint no. 1709, WIAS, Berlin, 2012.

[67] M. Radziunas, R. Čiegis, A. Mirinavičius, *Compact high order finite difference schemes for linear Schrödinger problems on non-uniform meshes*, Preprint no. 1748, WIAS, Berlin, 2012.

[68] M. Radziunas, K. Staliunas, *Spatial "rocking" for improving the spatial quality of the beam of broad area semiconductor lasers*, Preprint no. 1703, WIAS, Berlin, 2012.

[69] H. Gross, M.-A. Henn, S. Heidenreich, A. Rathsfeld, M. Bär, *Modeling of line roughness and its impact on the diffraction intensities and the reconstructed critical dimensions in scatterometry*, Preprint no. 1711, WIAS, Berlin, 2012.

[70] G. Hu, A. Rathsfeld, *Convergence analysis of the FEM coupled with Fourier-mode expansion for the electromagnetic scattering by biperiodic structures*, Preprint no. 1744, WIAS, Berlin, 2012.

[71] J. Rehberg, *A criterion for a two-dimensional domain to be Lipschitzian*, Preprint no. 1695, WIAS, Berlin, 2012.

[72] A. ter Elst, M. Meyries, J. Rehberg, *Parabolic equations with dynamical boundary conditions and source terms on interfaces*, Preprint no. 1712, WIAS, Berlin, 2012.

[73] L. Goray, G. Schmidt, *Sensitivity analysis of 2D photonic band gaps of any rod shape and conductivity using a very fast conical integral equation method*, Preprint no. 1684, WIAS, Berlin, 2012.

[74] F. Lanzara, V. Maz'ya, G. Schmidt, *Computation of volume potentials over bounded domains via approximate approximations*, Preprint no. 1740, WIAS, Berlin, 2012.

[75] P. Colli, J. Sprekels, *Optimal control of an Allen–Cahn equation with singular potentials and dynamic boundary condition*, Preprint no. 1750, WIAS, Berlin, 2012.

[76] P. Colli, G. Gilardi, J. Sprekels, *Analysis and optimal boundary control of a nonstandard system of phase field equations*, Preprint no. 1681, WIAS, Berlin, 2012.

[77] P. Colli, G. Gilardi, P. Krejčí, J. Sprekels, *A vanishing diffusion limit in a nonstandard system of phase field equations*, Preprint no. 1758, WIAS, Berlin, 2012.

[78] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Continuous dependence for a nonstandard Cahn–Hilliard system with nonlinear atom mobility*, Preprint no. 1742, WIAS, Berlin, 2012.

[79] ———, *Global existence and uniqueness for a singular/degenerate Cahn–Hilliard system with viscosity*, Preprint no. 1713, WIAS, Berlin, 2012.

[80] ———, *Global existence for a strongly coupled Cahn–Hilliard system with viscosity*, Preprint no. 1691, WIAS, Berlin, 2012.

[81] C.P. Niculescu, H. Stephan, *A generalization of Lagrange's algebraic identity and connections with Jensen's inequality*, Preprint no. 1756, WIAS, Berlin, 2012.

[82] R. Rossi, M. Thomas, *From an adhesive to a brittle delamination model in thermo-visco-elasticity*, Preprint no. 1692, WIAS, Berlin, 2012.

[83] M. Tlidi, E. Averlant, A.G. Vladimirov, K. Panajotov, *Spontaneous motion of cavity solitons induced by a delayed feedback*, Preprint no. 1737, WIAS, Berlin, 2012.

[84] M.D. Korzec, A. Münch, B. Wagner, *Anisotropic surface energy formulations and their effect on stability of a growing thin film*, Preprint no. 1705, WIAS, Berlin, 2012.

[85] O. Muscato, V. Di Stefano, W. Wagner, *A variance-reduced electrothermal Monte Carlo method for semiconductor device simulation*, Preprint no. 1699, WIAS, Berlin, 2012.

[86] M. Biskup, M. Salvi, T. Wolff, *A central limit theorem for the effective conductance: I. Linear boundary data and small ellipticity contrasts*, Preprint no. 1739, WIAS, Berlin, 2012.

[87] M. Wolfrum, *The Turing bifurcation in network systems: Collective patterns and single differentiated nodes*, Preprint no. 1675, WIAS, Berlin, 2012.

A.7.2 Preprints/Reports in other Institutions

[1] D. Crisan, J. Diehl, P. Friz, H. Oberhauser, *Robust filtering: Correlated noise and multidimensional observation*, arXiv:1201.1858, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[2] P. Friz, A. Shekhar, *Doob–Meyer for rough paths*, arXiv:1205.2505, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[3] ———, *The Levy–Kintchine formula for rough paths*, arXiv:1212.5888, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[4] Ch. Bayer, B. Veliyev, *Utility maximization in a binomial model with transaction costs: A duality approach based on the shadow price process*, arXiv:1209.5175, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[5] E. Diederichs, A. Juditsky, A. Nemirovski, V. Spokoiny, *Spatially adaptive density estimation by localised Haar projections*, arXiv:1106.0321, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[6] St.W. Anzengruber, B. Hofmann, P. Mathé, *Regularization properties of the discrepancy principle for Tikhonov regularization in Banach spaces*, Preprint no. 12, Technische Universität Chemnitz, Fakultät für Mathematik, 2012.

[7] B. Hofmann, P. Mathé, *Parameter choice in Banach space regularization under variational inequalities*, Preprint no. 05, Technische Universität Chemnitz, Fakultät für Mathematik, 2012.

[8] H. Cornean, H. Neidhardt, L. Wilhelm, V. Zagrebnov, *Cayley transform applied to non-interacting quantum transport*, arXiv:1212.4965, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[9] S. Albeverio, A. Kostenko, M. Malamud, H. Neidhardt, *Schrödinger operators with concentric δ-shells*, arXiv:1211.4048, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[10] M.M. Malamud, H. Neidhardt, *Perturbation determinants and trace formulas for singular perturbations*, arXiv:1212.6887, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[11] I. Omelchenko, O. Omel'chenko, P. Hövel, E. Schöll, *Multi-chimera states in FitzHugh–Nagumo oscillators*, arXiv:1212.3190, Cornell University Library, Ithaca, USA, 2012.

[12] W.J. Menz, R.I. Patterson, W. Wagner, M. Kraft, *Application of stochastic weighted algorithms to a multidimensional silica particle model*, Preprint no. 120, University of Cambridge, Cambridge Center for Computational Chemical Engineering, UK, 2012.

[13] V. Spokoiny, *Parametric estimation. Finite sample theory*, arXiv:1111.3029, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[14] ———, *Roughness penalty, Wilks phenomenon, and Bernstein–von Mises theorem*, arXiv:1205.0498, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[15] V. Spokoiny, W. Wang, W.K. Härdle, *Local quantile regression*, arXiv:1208.5384, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[16] F. Gach, R. Nickl, V. Spokoiny, *Spatially adaptive density estimation by localised Haar projections*, arXiv:1111.2807, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

[17] P. Imkeller, N. Willrich, *Solutions of martingale problems for Lévy-type operators and stochastic differential equations driven by Lévy processes with discontinuous coefficients*, arXiv:1208.1665, Cornell University Library, arXiv.org, Ithaca, USA, 2012.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Main and Plenary Talks

1. P. Friz, *Rough paths and control*, Stochastic Systems Simulation and Control (SSSC2012), November 5–9, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, November 5.
2. R. Henrion, *On the coderivative of normal cone mappings to moving sets*, IV Alicante-Elche-Limoges Meeting on Optimization (ALEL 2012), July 2–4, Limoges, France, July 2.
3. V. Spokoiny, *Some methods of modern statistics*, Information Technology and Systems 2, August 19–25, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Petrozavodsk, August 20.
4. ———, *Sparse non-Gaussian component analysis*, 55th Scientific Conference of Moscow Physical and Technical Institute, November 23–25, Dolgoprudny, Russia, November 24.

A.8.2 Scientific Talks (Invited)

1. P. Friz, *Volatility expansions based on Laplace's method*, The 19th Annual Global Derivatives Trading & Risk Management, April 16–20, Barcelona, Spain, April 18.
2. ———, *Generalized sub-Riemannian cut loci and implied/local volatility smiles*, Probability Seminar, University of Cambridge, Faculty of Mathematics, UK, April 24.
3. ———, *Generalized sub-Riemannian cut loci and volatility smiles*, 6th European Congress of Mathematics, July 2–7, Jagiellonian University, Institute of Mathematics, Cracow, Poland, July 5.
4. ———, *Marginal density expansion with applications to Levy area and the Stein–Stein model*, Stochastic Analysis Seminar, University of Warwick, Mathematics Institute, Coventry, UK, November 28.
5. G. Hu, *Some inverse problems arising from elastic scattering by rigid obstacles*, International Conference on Inverse Problems and Related Topics 2012 (ICIP12), October 21–26, Southeast University, Nanjing, China, October 23.
6. ———, *Direct and inverse elastic scattering problems for diffraction gratings*, Chinese Academy of Sciences, Institute of Computational Mathematics and Scientific/Engineering Computing (ICMSEC), Beijing, China, November 7.
7. G. Aki, *An incompressible diffuse flow with phase transition*, 7th DFG-CNRS Workshop "Two-Phase Fluid Flows. Modeling and Computational Methods", February 14–16, Université Pierre et Marie Curie, Paris, France, February 15.
8. S. Amiranashvili, *A modeling framework for short pulses in optical fibers*, 5th Annual Meeting "Photonic Devices", Zuse-Institut Berlin (ZIB), Berlin, February 24.
9. ———, *Tiny waves we should never ignore*, OSA – The Optical Society, Topical Meeting "Nonlinear Photonics", June 17–21, Colorado Springs, USA, June 18.
10. R. Arkhipov, *Emission of the new frequencies in the resonant medium under the conditions of excitation by an object propagating at superluminal velocity*, XIV All-Russian Scientific School-Seminar "Wave Phenomena in Inhomogeneous Media" (Waves-2012), May 21–28, Zvenigorod, Russia, May 24.
11. I. Babushkin, *Emission and control of coherent broad-band THz radiation using plasma-generating femtosecond light pulses*, IPHT-Kolloquium, Institut für Photonische Technologien (IPHT), Jena, November 20.
12. U. Bandelow, *Mathematical modeling and simulation of semiconductor lasers*, Block Seminar of SFB 787 School of Nanophotonics, May 13–16, Technische Universität Berlin, Graal-Müritz, May 15.

13. ———, *Spatio-temporal pulse propagation in nonlinear dispersive optical media*, 12th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD12), August 26 – September 4, Shanghai, China, August 30.

14. ———, *Rogue waves in the Sasa–Satsuma equation*, International Symposium "Advances in Nonlinear Photonics", September 24–28, Belarusian State University, Minsk, September 25.

15. ———, *Rogue waves in extended nonlinear Schrödinger equations: Integrable Sasa–Satsuma case*, The Optical Society's (OSA) Annual Meeting Frontiers in Optics 2012, October 13–19, Rochester Section of the Optical Society of America, Rochester, USA, October 18.

16. CH. BAYER, *Some applications of the Ninomiya–Victoir scheme in the context of financial engineering*, Talks in Financial and Insurance Mathematics, Eidgenössische Technische Hochschule Zürich, Switzerland, April 26.

17. ———, *Some applications of the Ninomiya–Victoir scheme in the context of financial engineering*, Stochastic Analysis Seminar Series, Oxford University, Oxford-Man Institute of Quantitative Finance, UK, May 21.

18. ———, *Existence, uniqueness and stability of invariant distributions in continuous-time stochastic models*, 12th Conference of the Society for the Advancement of Economic Theory (SAET 2012), June 30 – July 3, University of Queensland, School of Economics, Australia, July 1.

19. ———, *Asymptotics beats Monte Carlo: The case of correlated local vol baskets*, Applied Mathematics and Computational Science Seminar, King Abdullah University of Science and Technology, Saudia Arabia, December 5.

20. S. BECKER, *Image processing via orientation scores*, Workshop "Computational Inverse Problems", October 23–26, Mathematisches Forschungsinstitut Oberwolfach, October 25.

21. ———, *Diffusion weighted imaging: Modeling and analysis beyond the diffusion tensor*, Methodological Workshop: Structural Brain Connectivity: Diffusion Imaging—State of the Art and Beyond, October 30 – November 2, Humboldt-Universität zu Berlin, November 2.

22. C. BRÉE, *Generalization of all-optical Kerr effect in gases and wide bandgap solids*, International Symposium "Advances in Nonlinear Photonics", September 24–28, Belarusian State University, Minsk, September 25.

23. A. CAIAZZO, *Model reduction approaches for simulation of pulmonary artery and pulmonary valve*, Seminar Lehrstuhl für Numerische Mechanik, Technische Universität München, August 29.

24. E. DIEDERICHS, *Adaptive weights clustering*, 2. SAW Workshop: Strukturelle Analyseverfahren für hochdimensionale Gentranskriptdaten, November 12–16, Deutsches Diabetes-Zentrum, Düsseldorf, November 13.

25. W. DREYER, *Thermodynamics of the diffuse interface setting and its sharp limits*, Projektseminar "Geometrische Analysis" (Prof. Kröner), Universität Freiburg, January 10.

26. ———, *The incompressible two-phase flow in the diffuse interface setting*, International Research Training Group 1529 "Mathematical Fluid Dynamics", Technische Universität Darmstadt, January 17.

27. ———, *Modeling, analysis and simulations of a many-particle cathode of a lithium-ion battery*, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, January 31.

28. ———, *A case study on reaction diffusion flows and entropy inequalities*, Seminar "Mathematik von Oberflächenphänomenen" (Prof. G. Grün), Universität Erlangen-Nürnberg, Erlangen, May 24.

29. ———, *Mathematical modelling of lithium-ion batteries*, 12th International Conference on Free Boundary Problems: Theory and Applications, June 11–15, Frauenchiemsee, June 11.

30. ———, *Rational thermodynamics of electrolytes*, Workshop "Solid State Electrochemistry for Energy Storage and Conversion" (SSEC2012), July 16–18, Universität Heidelberg, July 17.

31. ———, *On the 2nd law of thermodynamics*, Mechanics – New Challenges, The 2012 ISIMM Symposium – STAMM XVIII, September 3–6, Technion – Israel Institute of Technology, Haifa, September 5.

32. ———, *Sharp limits of diffuse interface models in the context of energy storage problems*, PDEs for Multiphase Advanced Materials (ADMAT2012), September 17–21, Cortona, Italy, September 18.

33. ———, *Mathematical models of rechargeable batteries*, Symposium "Mathematische Modellierung von Zwei-Phasen-Systemen", Martin-Luther-Universität Halle Wittenberg, Institut für Mathematik, November 22.

34. ———, *Mathematical modelling of Li-ion batteries*, Innovation Days – Partnering Research and Business, November 26–27, München, November 27.

35. ———, *Sharp limits of diffuse interface problems and thermodynamic consistency*, SFB TRR 75-Simtech-SPP 1506 Workshop "Numerical Methods for Two-phase Flow", November 28–30, Universität Stuttgart, November 30.

36. J. Elschner, *Inverse scattering of elastic waves by diffraction gratings*, Workshop "Inverse Problems for Partial Differential Equations", February 19–25, Mathematisches Forschungsinstitut Oberwolfach, February 22.

37. ———, *Direct and inverse scattering of elastic waves by diffraction gratings*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, February 29.

38. ———, *Elastic scattering by diffraction gratings and rough surfaces*, Academy of Mathematics and Systems Science, Institute of Applied Mathematics, Beijing, China, October 15.

39. ———, *An optimization method in inverse elastic scattering*, International Conference on Inverse Problems and Related Topics 2012 (ICIP 2012), October 21–26, Southeast University, Nanjing, China, October 23.

40. J. Fuhrmann, *Mathematical and numerical modeling of coupled flow, transport and reactions in electrochemical devices*, Workshop on Evolution Equations, Related Topics and Applications, March 19–23, Waseda University Tokio, Faculty of Science and Engineering, Japan, March 19.

41. K. Götze, *Some results for the motion of a rigid body with a liquid-filled cavity*, Seminar on Partial Differential Equations, Czech Academy of Sciences, Mathematical Institute, Prague, Czech Republic, November 6.

42. C. Guhlke, *Sharp limit of the viscous Cahn–Hilliard equation in the context of the 2nd law of thermodynamics*, 12th International Conference on Free Boundary Problems: Theory and Applications, June 11–15, Frauenchiemsee, June 13.

43. ———, *Thermodynamics of electrolytes*, Battery Day 2012 – Modelling, Analysis and Numerics of Battery Systems, Universität Konstanz, Fachbereich Mathematik und Statistik, November 28.

44. O. Gün, *Multilevel trap models and aging for spin glasses*, Seminar Wahrscheinlichkeitstheorie, Universität Wien, Fakultät für Mathematik, Austria, May 21.

45. ———, *Moment asymptotics for branching random walks in random environment*, Probability Laboratory at Bath, Prob-L@b Seminar, University of Bath, Department of Mathematical Sciences, UK, August 20.

46. H. Hanke, *Derivation of an effective damage evolution model*, "A Matheon Multiscale Workshop", Technische Universität Berlin, Institut für Mathematik, April 20.

47. ———, *Derivation of an effective damage evolution model using two-scale convergence techniques*, International Workshop on Evolution Problems in Damage, Plasticity, and Fracture: Mathematical Models and Numerical Analysis, September 19–21, University of Udine, Department of Mathematics, Italy, September 19.

48. R. Henrion, *Stability of chance constrained optimization problems*, 4 talks, Spring School in Variational Analysis, April 23–27, Paseky, Czech Republik, April 23–27.

49. ———, *On the coderivative of normal cone mappings to moving sets*, 58th Course "Variational Analysis and Applications", May 14–22, International School of Mathematics "Guido Stampacchia", Erice, Italy, May 18.

50. ———, *On (co-)derivatives of the solution map to a class of generalized equations*, 21st International Symposium on Mathematical Programming (ISMP), August 19–24, Technische Universität Berlin, August 23.

51. ———, *Numerical aspects of optimization problems with probabilistic constraints under Gaussian distribution*, The 2nd Sino-German Workshop on Optimization, Modeling, Methods and Applications in Industry and Management, September 22–27, Beijing, China, September 23.

52. ———, *Régularité métrique des contraintes en probabilité*, Journée sur la régularité métrique, Université de Limoges, Département Mathématiques – Informatique, France, October 26.

53. D. HÖMBERG, *On the phase field approach to shape and topology optimization*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 6.

54. ———, *Optimal control of multiphase induction hardening*, 83rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2012), Session on Optimization of Differential Equations, March 26–30, Technische Universität Darmstadt, Fachbereich Mathematik, March 29.

55. ———, *Modern multiphase steels: Modelling, simulation and control (part I)*, Universidad de Cádiz, Departamento de Matemáticas, Spain, April 18.

56. ———, *On a phasefield approach towards distortion compensation*, Universidad de Cádiz, Departamento de Matemáticas, Spain, April 18.

57. ———, *Modern multiphase steels: Modelling, simulation and control (part II)*, Universidad de Cádiz, Departamento de Matemáticas, Spain, April 19.

58. ———, *Optimal control of multiphase steel production*, 21st International Symposium on Mathematical Programming (ISMP), August 19–24, Technische Universität Berlin, August 23.

59. ———, *Optimal control of multifrequency induction hardening*, INDAM Workshop PDEs for Multiphase Advanced Materials (ADMAT2012), September 17–21, Cortona, Italy, September 18.

60. ———, *From dilatometer experiments to distortion compensation — Optimal control problems related to solid-solid phase transitions*, University of Bath, Department of Mathematical Sciences, UK, October 9.

61. ———, *Changing shapes and measuring phase transitions — Optimal control problems in thermomechanics*, University of Warwick, Mathematics Institute, UK, October 12.

62. ———, *On a phase field approach to topology optimization*, Mini-Workshop "Geometries, Shapes and Topologies in PDE-based Applications", November 25 – December 1, Mathematisches Forschungsinstitut Oberwolfach, November 27.

63. G. HU, *Elastic scattering by unbounded rough surfaces*, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, March 14.

64. ———, *Direct and inverse scattering of elastic waves by diffraction gratings*, 6th International Conference "Inverse Problems, Control and Shape Optimization" (PICOF '12), April 2–4, Palaiseau, France, April 4.

65. S. JANSEN, *Random partitions and heavy-tailed variables in statistical mechanics*, Probability Seminar, University of Alabama, Department of Mathematics, Birmingham, USA, February 9.

66. ———, *Fermionic and bosonic Laughlin state on thick cylinders*, Mathematical Physics Seminar, University of Alabama, Department of Mathematics, Birmingham, USA, February 17.

67. V. JOHN, *Finite element methods for the simulation of incompressible flows*, 10 talks, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, February 27 – March 2.

68. ———, *Numerical methods for the Stokes equations*, 2 talks, GEOSIM Summer School 2012 “Mathematical Modeling and Numerics for Geophysical Flows and Applications”, April 2–5, Gülpe, April 2–5.

69. ———, *On the analysis and numerical analysis of some turbulence models*, Workshop “Connections Between Regularized and Large-Eddy Simulation Methods for Turbulence”, May 14–17, Banff International Research Station for Mathematical Innovation and Discovery, Canada, May 15.

70. ———, *Some recent developments in numerical methods for convection-diffusion equations*, Annual Spring Festival of 3TU.AMI, University of Twente, The Netherlands, May 31.

71. ———, *On the error analysis for stabilized finite element methods*, Humboldt-Universität zu Berlin, Institut für Mathematik, June 14.

72. ———, *Numerical methods for the simulation of population balance systems*, Workshop “Modeling, Optimization and Simulation of Complex Fluid Flow”, June 20–22, Technische Universität Darmstadt, June 21.

73. ———, *On reduced order modeling methods for incompressible flows based proper orthogonal decomposition*, 6th Variational Multiscale Methods Workshop (VMS 2012), June 27–29, Christian-Albrechts-Universität zu Kiel, June 28.

74. ———, *On proper orthogonal decomposition methods for incompressible flows*, Kolloquium Angewandte Mathematik, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik/Technische Universität München, Zentrum Mathematik, December 5.

75. O. Klein, *A representation result for hysteresis operators acting on vector-valued continuous, piecewise monotaffine input functions*, 6th International Workshop on Multi-Rate Processes and Hysteresis (MURPHYS 2012), May 21–24, Stefan cel Mare University, Suceava, Romania, May 22.

76. D. Knees, *Modeling and mathematical analysis of elasto-plastic phenomena*, 8 talks, Winter School on Modeling Complex Physical Systems with Nonlinear (S)PDE (DoM ^{2} oS), February 27 – March 2, Technische Universität Dortmund, Fakultät für Mathematik, February 27 – March 2.

77. ———, *On a vanishing viscosity approach in damage mechanics*, Kolloquium der AG Modellierung, Numerik, Differentialgleichungen, Technische Universität Berlin, Institut für Mathematik, August 21.

78. ———, *A vanishing viscosity approach in fracture mechanics*, Nonlocal Models and Peridynamics, November 5–7, Technische Universität Berlin, Institut für Mathematik, November 5.

79. ———, *A vanishing viscosity approach in fracture mechanics*, Oberseminar zur Analysis, Universität Duisburg-Essen, Fakultät für Mathematik, November 13.

80. ———, *A vanishing viscosity approach to a rate-independent damage model*, Oberseminar zur Analysis, Universität Duisburg-Essen, Fakultät für Mathematik, November 20.

81. W. König, *Large deviations for cluster size distributions in a classical many-body system*, Oberseminar Stochastik, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, January 12.

82. ———, *The universality classes of the parabolic Anderson model*, AG Stochastik und Dynamische Systeme, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, January 19.

83. ———, *Large deviations for the local times of random walk among random conductances*, EPSRC Symposium Workshop – Large Scale Behaviour of Random Spatial Models, May 28 – June 1, University of Warwick, Mathematical Institute, Coventry, UK, June 1.

84. ———, *Ordered random walks*, Stochastisches Kolloquium, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, June 6.

85. ———, *Large deviations for the cluster size distribution in a classical interacting many-particle system*, Warwick Mathematics Institute Seminars, University of Warwick, Mathematics Institute, Coventry, UK, August 1.

86. ———, *Large deviations for cluster size distributions in a classical many-body system*, Probability Laboratory at Bath, Prob-L@b Seminar, University of Bath, Department of Mathematical Sciences, UK, August 20.

87. ———, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, 2 talks, SFB/TR12 Workshop, November 4–8, Universität zu Köln, SFB TR12 “Symmetries and Universality in Mesoscopic Systems”, Langeoog, November 7.

88. ———, *Large deviations for the cluster size distributions in a classical interacting many-particle system with Lennard–Jones potential*, Mark Kac Seminar, Eindhoven University of Technology, The Netherlands, November 9.

89. ———, *Moment asymptotics for branching random walks in random environment*, Stochastik-Oberseminar, Westfälische Wilhelms-Universität Münster, Institut für Mathematische Statistik, December 6.

90. CH. KRAUS, *Phasenfeldsysteme für Entmischungs- und Schädigungsprozesse*, Mathematisches Kolloquium, Universität Stuttgart, Fachbereich Mathematik, May 15.

91. ———, *Phase field systems for phase separation and damage processes*, 12th International Conference on Free Boundary Problems: Theory and Applications, June 11–15, Frauenchiemsee, June 12.

92. ———, *The Stefan problem with inhomogeneous and anisotropic Gibbs–Thomson law*, 6th European Congress of Mathematics, July 2–6, Cracow, Poland, July 5.

93. ———, *A nonlinear PDE system for phase separation and damage*, Universität Freiburg, Abteilung Angewandte Mathematik, November 13.

94. ———, *Cahn–Larché systems coupled with damage*, Università degli Studi di Milano, Dipartimento di Matematica, Italy, November 28.

95. CH. LANDRY, *Collision-free path planning of welding robots*, The 17th European Conference on Mathematics for Industry 2012 (ECMI 2012), July 23–27, Lund, Sweden, July 24.

96. ———, *Modeling of the optimal trajectory of industrial robots in the presence of obstacles*, 21st International Symposium on Mathematical Programming (ISMP), August 19–24, Technische Universität Berlin, August 22.

97. ———, *An optimal control problem for the collision-free motion planning of industrial robots*, École Polytechnique Fédérale de Lausanne, Mathematics Institute of Computational Science and Engineering (MATHICSE), Switzerland, November 28.

98. M. LIERO, *Interfaces in reaction-diffusion systems*, Seminar “Dünne Schichten”, Technische Universität Berlin, Institut für Mathematik, February 9.

99. ———, *Variational methods for evolution*, “A MATHEON Multiscale Workshop”, Technische Universität Berlin, Institut für Mathematik, April 20.

100. H. MAI, *Jump filtering in volatility estimation and connections to trend identification*, European University Institute, Department of Economics, Florence, Italy, October 25.

101. P. MATHÉ, *Regularization of statistical inverse problems in Hilbert space*, Journées Statistiques du Sud 2012, June 20–22, Université Toulouse, Institut National des Sciences Appliquées, France, June 20.

102. ———, *Diskrepanz-basierte Parameterwahl in statistischen inversen Problemen*, Technische Universität Chemnitz, Fakultät für Mathematik, September 19.

103. ———, *Statistical inverse problems*, Algorithms and Complexity for Continuous Problems, September 24–28, Schloss Dagstuhl, Leibniz-Zentrum für Informatik, September 25.

104. ———, *Using the discrepancy principle in statistical inverse problems*, Regularisation symposium, Australian National University, Mathematical Sciences Institute, Canberra, November 22.

105. ———, *An oracle-type bound for a statistical RG-rule*, Nonparametric and High-dimensional Statistics, December 17–21, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 20.

106. A. Mielke, *Dissipative quantum mechanics: Geometry meets thermodynamics*, Symposium "Recent Trends in Dynamical Systems", dedicated to Jürgen Scheurle's 60th birthday, January 11–14, Technische Universität München, Zentrum Mathematik, January 11.

107. ———, *Gamma convergence and evolution*, International Conference "Trends in Mathematical Analysis", March 1–3, Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Italy, March 1.

108. ———, *On geodesic convexity for reaction-diffusion systems*, Seminar on Applied Mathematics, Università di Pavia, Dipartimento di Matematica, Italy, March 6.

109. ———, *Linearized elastoplasticity is the evolutionary Gamma limit of finite elastoplasticity*, 83th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2012), Session on Applied Analysis, March 26–30, Technische Universität Darmstadt, Fachbereich Mathematik, March 27.

110. ———, *Gradienten-Strukturen und geodätische Konvexität für Markov-Ketten und Reaktions-Diffusions-Systeme*, Augsburger Kolloquium, Universität Augsburg, Institut für Mathematik, May 8.

111. ———, *On gradient structures for Markov chains and reaction-diffusion systems*, Applied & Computational Analysis (ACA) Seminar, University of Cambridge, Department of Applied Mathematics and Theoretical Physics (DAMTP), UK, June 14.

112. ———, *Multiscale modeling for evolutionary systems via Gamma convergence*, 5 talks, NDNS$^+$ Summer School in Applied Analysis, June 18–20, University of Twente, Applied Analysis & Mathematical Physics, Enschede, The Netherlands, June 18–20.

113. ———, *Small-strain elastoplasticity is the evolutionary Gamma limit of finite-strain elastoplasticity*, International Symposium on Trends in Applications of Mathematics to Mechanics (STAMM 2012), September 3–6, Israel Institute of Technology (Technion), Faculty of Aerospace Engineering, Haifa, September 4.

114. ———, *From small-strain to finite-strain elastoplasticity via evolutionary Gamma convergence*, Variational Models and Methods for Evolution, September 10–12, Centro Internazionale per la Ricerca Matematica (CIRM) and Istituto di Matematica Applicata e Tecnologie Informatiche/Consiglio Nazionale delle Ricerche (IMATI-CNR), Levico, Italy, September 11.

115. ———, *On consistent couplings of quantum mechanical and dissipative systems*, Jahrestagung der Deutschen Mathematiker-Vereinigung (DMV) 2012, Minisymposium "Dynamical Systems", September 17–20, Universität des Saarlandes, Fakultät für Mathematik und Informatik, Saarbrücken, September 19.

116. ———, *On gradient structures and geodesic convexity for energy-reaction-diffusion systems and Markov chains*, ERC Workshop on Optimal Transportation and Applications, November 5–9, Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy, November 8.

117. ———, *On gradient flows and reaction-diffusion systems*, Institutskolloquium, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, December 3.

118. ———, *Finite-strain viscoelasticity as a gradient flow*, Analysis and Applications of PDEs: An 80th Birthday Meeting for Robin Knops, December 10–11, International Center for Mathematical Sciences, Edinburgh, UK, December 11.

119. ———, *Multiscale gradient systems and their amplitude equations*, Workshop "Dynamics of Patterns", December 17–21, Mathematisches Forschungsinstitut Oberwolfach, December 18.

120. A. Möller, *Probabilistic programming in power production planning*, 21st International Symposium on Mathematical Programming (ISMP), August 19–24, Technische Universität Berlin, August 22.

121. H.-J. Mucha, *Clustering and visualisation based on dual scaling*, 4th Japanese-German Symposium on Classification (JGSC2012), March 8–10, Doshisha University, Kyoto, Japan, March 9.

122. ———, *Measures of incomparability and of inequality and their application*, 10th Workshop on Partial Order, Theory and Application: Multi-Indicator Systems and Modelling in Partial Order, September 27–28, Hochschule für Technik und Wirtschaft Berlin, September 28.

123. ———, *Visualisation and cluster analysis*, Herbsttagung der AG Datenanalyse und numerische Klassifikation, October 5–6, Landschaftsverband Rheinland, LVR-Amt für Bodendenkmalpflege im Rheinland, Bonn, October 6.

124. R. Müller, *Parallelisierung von Methoden für PDEs (compact course)*, 4 talks, Universität Bonn, Institut für Numerische Simulation, January 16–20.

125. ———, *Finite element method for a coupled damage model*, Forschungsseminar Numerik, Humboldt-Universität zu Berlin, April 25.

126. H. Neidhardt, *Jaynes–Cummings model coupled to leads: A model for LEDs?*, Quantum Circle Seminar, Czech Technical University, Faculty of Nuclear Sciences and Physical Engineering, Doppler Institute for Mathematical Physics and Applied Mathematics, Prague, Czech Republic, March 13.

127. ———, *Landauer–Büttiker formula applied to photon emitting and absorbing systems*, Kolloquium "Mathematische Physik", December 13–14, Technische Universität Clausthal/Technische Universität Braunschweig, Clausthal-Zellerfeld, December 14.

128. O. Omel'chenko, *Synchronization transition in the Sakaguchi–Kuramoto model*, 7th Crimean School and Workshop "Emergent Dynamics of Oscillatory Networks", May 20–27, Mellas, Crimea, Ukraine, May 22.

129. ———, *Coherence-incoherence patterns in systems of non-locally coupled phase oscillators*, Statistical Physics and Nonlinear Dynamics & Stochastic Processes, Humboldt-Universität zu Berlin, Institut für Physik, Berlin, June 18.

130. ———, *Coherence-incoherence patterns in systems of non-locally coupled phase oscillators*, XXXII Dynamics Days Europe, September 2–7, University of Gothenburg, Sweden, September 4.

131. ———, *Nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, Seminar Applied Analysis, Humboldt-Universität zu Berlin, October 29.

132. ———, *What are chimera states*, Westfälische Wilhelms-Universität Münster, Center for Nonlinear Science, November 6.

133. ———, *Chimera states: Spatiotemporal patterns of synchrony and disorder*, Universität Hamburg, Department of Mathematics, November 12.

134. ———, *Nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, Colloquium on Complex and Biological Systems, Universität Potsdam, November 26.

135. R.I.A. Patterson, *Soot as a boundary value problem*, University of Cambridge, Department of Chemical Engineering, UK, May 8.

136. D. Peschka, *Liquid/liquid dewetting – Theory and experiments*, Workshop "Thin Liquid Films and Fluid Interfaces: Models, Experiments and Applications", December 9–14, Banff International Research Station for Mathematical Innovation and Discovery, Canada, December 10.

137. Th. Petzold, *Finite element simulations of induction hardening of steel parts*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 6.

138. J. Polzehl, *Medical image analysis in R (tutorial)*, 2 talks, The 8th International R User Conference (Use R!2012), June 11–15, Vanderbilt University, Department of Biostatics, Nashville, TN, USA, June 12.

139. ———, *Adaptive methods for noise reduction in diffusion weighted MR*, BRIC Seminar Series, University of North Carolina, School of Medicine, Chapel Hill, NC, USA, July 10.

140. ———, *Modeling dMRI data: An introduction from a statistical viewpoint*, Workshop on Neurogeometry, November 15–17, Masaryk University, Department of Mathematics and Statistics, Brno, Czech Republic, November 16.

141. ———, *Statistical problems in diffusion weighted MR (dMRI)*, 5th International Conference of the ERCIM Working Group on Computing & Statistics (ERCIM 2012), December 1–3, Universidad de Oviedo, Departamento de Estadística e Investigación Operativa y Didáctica de la Matemática, Spain, December 1.

142. P.N. Racec, *Fano regime of transport through open quantum dots*, Seminar "Quanteneffekte in Festkörpern", Leibniz Universität Hannover, Institut für Festkörperphysik, June 13.

143. ———, *Quantum transport and the R-matrix formalism for cylindrical nanowire heterostructures*, Technische Universität Graz, Institut für Theoretische Physik, Austria, September 13.

144. M. Radziunas, *Spatial rocking for improving the spatial quality of the beam of broad area semiconductor lasers*, SPIE Photonics Europe Conference, April 16–19, Brussels, Belgium, April 17.

145. ———, *Theoretical study of beam quality improvement in broad area semiconductor devices*, International Symposium "Advances in Nonlinear Photonics", September 23–27, Belarusian State University, Minsk, September 24.

146. A. Rathsfeld, *Inverse problems for the scatterometric measurement of grating structures*, 6th International Conference "Inverse Problems: Modeling and Simulation", May 21–26, Antalya, Turkey, May 23.

147. J. Rehberg, *Hölderstetigkeit für Lösungen elliptischer Gleichungen*, Seminar der Arbeitsgruppe "Analysis", Martin-Luther-Universität Halle-Wittenberg, Institut für Mathematik, December 12.

148. J.G.M. Schoenmakers, *Multilevel dual approach for pricing American options*, Mini-workshop CWI-EUR Backward Stochastic Differential Equations (BSDE's), January 17–18, Eindhoven University of Technology, European Institute for Statistics, Probability, Stochastic Operations Research and its Applications (EURANDOM), January 18.

149. ———, *Multilevel primal and dual approaches for pricing American options*, 21st International Symposium on Mathematical Programming (ISMP), August 20–24, Technische Universität Berlin, August 24.

150. ———, *Libor model with expiry-wise stochastic volatility and displacement*, Jahrestagung der Deutschen Mathematiker-Vereinigung (DMV) 2012, Minisymposium "Applied Mathematical Finance", September 17–19, Universität des Saarlandes, Fakultät für Mathematik und Informatik, Saarbrücken, September 17.

151. ———, *Multilevel primal and dual approaches for pricing American options*, Stochastic Optimization and Optimal Stopping, September 24–28, Russian Academy of Sciences and Moscow Institute of Physics and Technology, Moscow, September 26.

152. ———, *Multilevel primal and dual approaches for pricing American options*, 2012 Winter Simulation Conference, December 10–12, WSC Foundation, Berlin, December 11.

153. H. Si, *TetGen, a Delaunay tetrahedral mesh generator*, Visual Computing Lab (VCL) Lunch Talk, University of California at Berkeley, USA, October 12.

154. ———, *Tetrahedral mesh generation: An introduction and the state of the art*, Symposium on Mesh Generation, December 27–28, Chinese Academy of Sciences, Institute of Computational Mathematics, Beijing, December 27.

155. V. Spokoiny, *Basics of modern parametric statistics*, 6 talks, Independent University of Moscow, Center for Continuous Mathematical Education, Russia, February 13–28.

156. ———, *Regularization and model choice in linear inverse problems*, 2 talks, Tagung des SFB 649 "Ökonomisches Risiko" in Motzen, February 16–18, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, February 16.

157. ———, *Parametric estimation: Modern view*, PreMoDay I, February 24, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, February 24.

158. ———, *Bernstein–von Mises theorem for quasi posteriors*, Workshop “Frontiers in Nonparametric Statistics”, March 11–17, Mathematisches Forschungsinstitut Oberwolfach, March 12.

159. ———, *Bernstein–von Mises theorem for quasi posteriors*, PreMoLab Seminar, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, March 15.

160. ———, *Bernstein–von Mises theorem for quasi posteriors*, International Workshop on Recent Advances in Time Series Analysis (RATS 2012), June 8–12, University of Cyprus, Department of Mathematics and Statistics, Protaras, June 9.

161. ———, *Bernstein–von Mises theorem for quasi posteriors*, Workshop II on Financial Time Series Analysis: High-dimensionality, Non-stationarity and the Financial Crisis, June 19–22, National University of Singapore, Institute for Mathematical Sciences, June 21.

162. ———, *Bernstein–von Mises theorem for quasi posteriors*, Workshop on Recent Developments in Statistical Multiscale Methods, July 16–18, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, July 17.

163. ———, *Bernstein–von Mises theorem for quasi-posterior*, Forschungsseminar Stochastische Geometrie und räumliche Statistik, Universität Ulm, Institut für Stochastik, October 23.

164. ———, *Sparse non-Gaussian component analysis*, Research Seminar, University of Geneva, Research Center for Statistics, Switzerland, November 2.

165. ———, *Critical dimension in the Bernstein–von Mises theorem*, Rencontres de Statistique Mathématique, December 19–21, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 19.

166. J. Sprekels, *Mathematical challenges in the industrial growth of semiconductor bulk single crystals*, Kick-off Symposium Mathematics: Official Opening of the Felix Klein Building, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, January 13.

167. ———, *Optimal control problems arising in the industrial growth of bulk semiconductor single crystals*, 21st International Symposium on Mathematical Programming (ISMP), Invited Session “Optimization Applications in Industry I”, August 19–24, Technische Universität Berlin, August 21.

168. ———, *Karl Weierstrass and optimization*, 21st International Symposium on Mathematical Programming (ISMP), August 19–24, Technische Universität Berlin, August 23.

169. ———, *Optimal control problems arising in the industrial growth of bulk single semiconductor crystals*, Applied Mathematics Seminar, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, September 11.

170. ———, *A time discretization for a nonstandard viscous Cahn–Hilliard system*, INDAM Workshop PDEs for Multiphase Advanced Materials (ADMAT2012), September 17–21, Cortona, Italy, September 19.

171. H. Stephan, *Linear evolution equations with positive solutions and connections to majorization theory and statistical physics*, International Conference “Spectral Theory and Differential Equations ” (STDE-2012), August 20–24, Karazin Kharkiv National University, Ukraine, August 21.

172. K. Sturm, *Shape optimization for an interface problem in linear elasticity for distortion compensation*, 21st International Symposium on Mathematical Programming (ISMP), August 19–24, Technische Universität Berlin, August 20.

173. K. Tabelow, *Adaptive methods for noise reduction in diffusion weighted MRI – Position orientation adaptive smoothing (POAS)*, University College London, Wellcome Trust Centre for Neuroimaging, UK, November 1.

174. ———, *Position-orientation adaptive smoothing (POAS) diffusion weighted imaging data*, Workshop on Neurogeometry, November 15–17, Masaryk University, Department of Mathematics and Statistics, Brno, Czech Republic, November 16.

175. M. Thomas, *Thermomechanical modeling via energy and entropy*, Seminar on Applied Mathematics, University of Pavia, Department of Mathematics, Italy, February 14.

176. ———, *Delamination in viscoelastic materials with thermal effects*, Seminar on Applied Mathematics, Università di Brescia, Dipartimento di Matematica, Italy, March 14.

177. ———, *Thermomechanical modeling via energy and entropy using GENERIC*, Workshop "Mechanics of Materials", March 19–23, Mathematisches Forschungsinstitut Oberwolfach, March 22.

178. ———, *A model for rate-independent, brittle delamination in thermo-visco-elasticity*, INDAM Workshop PDEs for Multiphase Advanced Materials (ADMAT2012), September 17–21, Cortona, Italy, September 17.

179. ———, *Mathematical methods in continuum mechanics of solids*, 3 talks, COMMAS (Computational Mechanics of Materials and Structures) Summer School, October 8–12, Universität Stuttgart, Institut für Mechanik (Bauwesen), October 11–12.

180. ———, *Analytical aspects of rate-independent damage models with spatial BV-regularization*, Seminar, SISSA – International School for Advanced Studies, Functional Analysis and Applications, Trieste, Italy, November 28.

181. A.G. Vladimirov, *Nonlinear dynamics in lasers*, FP7 Marie Curie Initial Training Network PROPHET Workshop: Theory and Modelling in Photonics, April 11–13, Pavia, Italy, April 11.

182. ———, *Theoretical modeling of mode-locked quantum dot lasers*, SPIE Photonics Europe Conference, April 16–19, Brussels, Belgium, April 18.

183. A.G. Vladimirov, *Asymptotic analysis of weak interaction of nonlinear localized structures*, Yaroslavl Demidov State University, Department of Mathematical Modeling, Russia, June 13.

184. B. Wagner, *Organic solar cell fabrication*, Workshop "Organic Solar Cells", Oxford, UK, April 2.

185. ———, *Effective slip for an upper convected Maxwell fluid*, 12th International Conference on Free Boundary Problems: Theory and Applications, June 11–15, Frauenchiemsee, June 12.

186. ———, *Effective slip for an upper convected Maxwell fluid*, SIAM Annual Meeting 2012, Minisymposium 49 "Dynamics and Applications of Thin Liquid Films – Part II", July 9–11, Minneapolis, USA, July 11.

187. W. Wagner, *Stochastic particle methods for coagulation problems*, 28th International Symposium on Rarefied Gas Dynamics, July 9–13, University of Zaragoza, Spain, July 9.

188. G. Witterstein, *The existence of transition profiles for compressible flows*, 12th International Conference on Free Boundary Problems: Theory and Applications, June 11–15, Frauenchiemsee, June 13.

189. T. Wolff, *Annealed asymptotics for occupation time measures of a random walk among random conductances*, University of California at Los Angeles, Mathematics Department, USA, October 24.

190. M. Wolfrum, *Collective and localized Turing patterns on irregular networks*, Seminar Complex Nonlinear Processes in Chemistry and Biology, Fritz-Haber-Institut, Berlin, June 15.

191. ———, *The Turing instability in irregular network systems*, Jahrestagung der Deutschen Mathematiker-Vereinigung (DMV) 2012, Minisymposium "Dynamical Systems", September 18–20, Universität des Saarlandes, Fakultät für Mathematik und Informatik, Saarbrücken, September 20.

192. ———, *Chimera states: Patterns of coherence and incoherence in coupled oscillator systems*, Workshop "Dynamics of Patterns", December 16–21, Mathematisches Forschungsinstitut Oberwolfach, December 21.

193. J. Zhang, *Dual representations for general multiple stopping problems*, Young Researchers Meeting on BSDEs, July 2–4, Oxford University, Man Institute, UK, July 2.

194. ———, *Dual representations for general multiple stopping problems*, Oberseminar Finanz- und Versicherungsmathematik, Ludwig-Maximilians-Universität München, Mathematisches Institut, July 17.

A.8.3 Talks for a More General Public

1. S. Amiranashvili, *Monsterwellen*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2012, WIAS, June 2.
2. J. Fuhrmann, *Rotierende Scheiben, Elektrolyte und Mathematik*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2012, WIAS, June 2.
3. K. Götze, *Mathematik für Fallschirmspringer und Tischtennisspieler*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2012, WIAS, June 2.
4. C. Guhlke, *Ein Fall für die Mathematik!*, Matheon Rent the Center, Technische Universität Berlin, September 26.
5. D. Hömberg, *Angewandte Mathematik — Beispiele aus der Praxis*, talk for students of the Katholische Schule Salvator, Weidmannslust, in the framework of Matheon school activities, Technische Universität Berlin, January 11.
6. D. Knees, *Auch Material ermüdet mal*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2012, WIAS, June 2.
7. W. König, *Die Anfänge der Wahrscheinlichkeitsrechnung als Wissenschaft*, 2 talks, Tag der Wissenschaften 2012, Carl-Zeiss-Oberschule, Lichtenrade, January 18.
8. ———, *Erfolgsgeschichte eines stochastischen Prozesses: Die Brown'sche Bewegung*, Tag der Wissenschaften 2012, Carl-Zeiss-Oberschule, Lichtenrade, January 18.
9. ———, *Die Anfänge der Wahrscheinlichkeitsrechnung als Wissenschaft*, Tag der Wissenschaften 2012, Weinberg-Gymnasium Kleinmachnow, November 15.
10. ———, *Erfolgsgeschichte eines stochastischen Prozesses: Die Brown'sche Bewegung*, Tag der Wissenschaften 2012, Weinberg-Gymnasium Kleinmachnow, November 15.
11. Ch. Landry, *Zeit ist Geld: Optimale Bewegung von Industrierobotern*, 17. Berliner Tag der Mathematik (17th Berlin Day of Mathematics), Freie Universität Berlin, May 5.
12. ———, *Zeit ist Geld: Optimale Bewegung von Industrierobotern*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2012, WIAS, June 2.
13. G. Reinhardt, A. Lehmann, J. Wittke, *Geometrische Betrachtungen zum Satz des Ptolemäus*, 17. Berliner Tag der Mathematik (17th Berlin Day of Mathematics), Freie Universität Berlin, May 5.
14. H. Stephan, *Dualität in der Elementaren Geometrie*, 17. Berliner Tag der Mathematik (17th Berlin Day of Mathematics), Freie Universität Berlin, May 5.
15. J. Zhang, *Das Black-Scholes-Merton-Modell zur Bewertung einfacher Finanzprodukte*, Role Models an die Schulen, Anne-Frank-Oberschule, Berlin, February 8.

A.8.4 Posters

1. R. Arkhipov, *Numerical analysis of hybrid mode-locking in edge-emitting quantum dot semiconductor lasers*, SPIE Photonics Europe Conference, Brussels, Belgium, April 16–19.

2. ———, *Numerical analysis of hybrid mode-locking in semiconductor quantum dot lasers*, XIV All-Russian Scientific School-Seminar "Wave Phenomena in Inhomogeneous Media" (Waves-2012), Zvenigorod, Russia, May 21–26.

3. R. Arkhipov, M.V. Arkhipov, S.A. Pulkin, *Numerical simulations of lasing without population inversion in two-level optically dense medium*, International Conference "Laser Optics 2012", St. Petersburg, Russia, June 25–29.

4. R. Arkhipov, M. Radziunas, A. Vladimirov, *Theoretical analysis of hybrid mode-locked quantum dot semiconductor lasers*, International Conference "Laser Optics 2012", St. Petersburg, Russia, June 25–29.

5. Th. Arnold, A. Rathsfeld, *On Born approximation for the scattering by rough surfaces*, Leibniz-Doktoranden-Forum der Sektion D, Berlin, June 7–8.

6. S. Becker, K. Tabelow, H.U. Voss, A. Anwander, R.M. Heidemann, J. Polzehl, *Position-orientation adaptive smoothing (POAS) at 7T dMRI*, Ultra-Highfield MRI Scientific Symposium, Max Delbrück Communication Center, Berlin, June 8.

7. A. Fiebach, A. Glitzky, A. Linke, *Voronoi finite-volume methods for reaction-diffusion-systems*, 33. Norddeutsches Kolloquium über Angewandte Analysis und Numerische Mathematik (NoKo 2012), Universität Rostock, Institut für Mathematik, May 4–5.

8. K. Gärtner, A. Glitzky, *Mathematics and simulation of the charge transport in semiconductor sensors*, Fachtagung Leibniz-Nano (1. Nanotechnologie-Workshop der Leibniz-Gemeinschaft), Berlin, January 30–31.

9. K. Götze, *Free fall of a rigid body in a viscoelastic fluid*, International Summer School on Evolution Equations (EVEQ 2012), Prague, Czech Republic, July 9–13.

10. Ch. Heinemann, *Kopplung von Phasenseparation und Schädigung in elastischen Materialien*, Leibniz-Doktoranden-Forum der Sektion D, Berlin, June 7–8.

11. ———, *Complete damage in linear elastic materials*, Variational Models and Methods for Evolution, Levico, Italy, September 10–12.

12. S. Heinz, *Regularization and relaxation of time-continuous problems in plasticity*, 11th GAMM Seminar on Microstructures, Universität Duisburg-Essen, January 20–21.

13. S. Jachalski, M. Korzec, D. Peschka, B. Wagner, *Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructure*, Fachtagung Leibniz-Nano (1. Nanotechnologie-Workshop der Leibniz-Gemeinschaft), Berlin, January 30–31.

14. V. John, E. Schmeyer, R. Bordás, D. Thévenin, *Reference experiments in a multiphase wind tunnel — Numerical simulation and validation*, MetStröm Jahrestreffen, Berlin, February 28–29.

15. Th. Koprucki, K. Gärtner, A. Wilms, U. Bandelow, A. Mielke, *Multidimensional modeling and simulation of quantum-dot lasers*, Fachtagung Leibniz-Nano (1. Nanotechnologie-Workshop der Leibniz-Gemeinschaft), Berlin, January 30–31.

16. H. Mai, *Maximum likelihood estimation for Lévy-driven SDEs*, Workshop on Statistics of Lévy-driven Models, Ulm, March 15–16.

17. ———, *Jump filtering and high-frequency data*, Statistical Methods for Dynamical Stochastic Models (DynStoch2012), Paris, France, June 7–9.

18. J. Dolata, H.-J. Mucha, H.-G. Bartel, *Eine neue Referenzgruppe für die römische Ziegelproduktion der I. Thrakerkohorte am Mittelrhein*, Archäometrie und Denkmalpflege 2012, Tübingen, March 27–31.

19. C. Morales-Merino, H.-J. Mucha, H.-G. Bartel, *Multivariate statistical analysis of clay and ceramic-data for provenance of Bronze age pottery from Troia*, Archäometrie und Denkmalpflege 2012, Tübingen, March 27–31.

20. P.N. Racec, H. Neidhardt, H.-Chr. Kaiser, R. Racec, *Electronic quantum transport in semiconductor nano-structures*, Fachtagung Leibniz-Nano (1. Nanotechnologie-Workshop der Leibniz-Gemeinschaft), Berlin, January 30–31.
21. G. Hu, A. Rathsfeld, *Numerical solution for scattering by biperiodic gratings using FEM coupled by Fourier-mode expansions*, Scientific Computing in Electrical Engineering (SCEE 2012), Zurich, Switzerland, September 11.
22. O.C. Suciu, *A numerical method for the simulation of uni- and bi-variate population balance systems*, 25th Chemnitz FEM Symposium, Chemnitz, September 24–25.
23. M. Thomas, *Coupling of reaction-diffusion processes with thermomechanics using GENERIC*, Winter School "Calculus of Variations in Physics and Materials Science", Würzburg, January 8–13.
24. ———, *Rate-independent evolution of sets*, Variational Models and Methods for Evolution, Levico, Italy, September 10–12.

A.9 Visits to other Institutions[6]

1. G. Hu, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, November 5–9.
2. R. Arkhipov, CNRS Laboratory for Photonics and Nanostructures and III-IV Lab, Marcoussis, Paris, France, October 11 – November 9.
3. Ch. Bayer, Eidgenössische Technische Hochschule Zürich, Departement Mathematik, Switzerland, April 23–27.
4. ———, King Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences and Engineering Division, Thuwal, Saudia Arabia, November 29 – December 11.
5. I. Bremer, Rücker EKS GmbH, Weingarten, April 16–27.
6. A. Caiazzo, Universitá di Trento, Dipartimento di Ingegneria Civile e Ambientale, Italy, May 14, 2012 – February 15, 2013.
7. E. Diederichs, University of California, Department of Statistics, Berkeley, CA, USA, June 16 – September 14.
8. J. Elschner, University of Tokyo, Graduate School of Mathematical Sciences, Japan, February 27 – March 9.
9. ———, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, October 8–21.
10. G. Faraud, Università Ca' Foscari Venezia, Dipartimento di Management, Italy, March 5–9.
11. ———, Université Paris 6 and 7, Laboratoire de Probabilités et Modèles Aléatoires, France, March 10–18.
12. ———, Università Ca' Foscari Venezia, Dipartimento di Management, Italy, August 30 – September 14.
13. J. Fuhrmann, Université des Sciences et Technologies de Lille, Laboratoire Paul Painlevé, INRIA SIMPAF Team, France, December 17–21.
14. K. Gärtner, Università della Svizzera italiana, Institute of Computational Science, Lugano, Switzerland, December 1–14.
15. K. Götze, Eidgenössische Technische Hochschule Zürich, Institut für Theoretische Informatik, Switzerland, February 27 – March 2.
16. ———, Eidgenössische Technische Hochschule Zürich, Institut für Theoretische Informatik, Switzerland, April 23–27.
17. ———, Eidgenössische Technische Hochschule Zürich, Institut für Theoretische Informatik, Switzerland, June 17–24.
18. ———, Czech Academy of Sciences, Mathematical Institute, Prague, November 5–9.
19. O. Gün, Universität Wien, Fakultät für Mathematik, Austria, May 20 – June 26.
20. ———, University of Bath, Department of Mathematical Sciences, UK, August 19–26.
21. Ch. Heinemann, Università di Milano, Dipartimento di Matematica, Italy, November 26 – December 1.
22. S. Heinz, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, April 10–13.
23. ———, Universität Bonn, Hausdorff Research Institute for Mathematics, July 9 – August 5.
24. ———, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, October 8–12.

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

25. R. Henrion, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, October 6–11.
26. D. Hömberg, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 5–9.
27. ———, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, April 17–20.
28. ———, University of Bath, Department of Mathematical Sciences, UK, September 24 – December 21.
29. G. Hu, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, March 12–16.
30. S. Jansen, University of Alabama, Department of Mathematics, Birmingham, USA, February 6–17.
31. V. John, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, February 27 – March 2.
32. ———, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, December 4–7.
33. W. König, University of Warwick, Mathematics Institute, Coventry, UK, July 23–27.
34. ———, University of Warwick, Mathematics Institute, Coventry, UK, July 29 – August 2.
35. ———, University of Bath, Department of Mathematical Sciences, UK, August 19–26.
36. Ch. Kraus, Universität Freiburg, Abteilung Angewandte Mathematik, November 12–16.
37. ———, Università di Milano, Dipartimento di Matematica, Italy, November 26 – December 1.
38. P. Mathé, Technische Universität Chemnitz, Fakultät für Mathematik, September 17–21.
39. ———, Australian National University, Mathematical Sciences Institute, Canberra, November 18 – December 12.
40. A. Mielke, Università di Pavia, Dipartimento di Matematica, Italy, February 27 – March 8.
41. ———, University of Cambridge, Department of Applied Mathematics and Theoretical Physics (DAMTP), UK, June 11–15.
42. ———, Charles University, Mathematical Institute, Prague, Czech Republic, July 23–26.
43. R. Müller, Universität Bonn, Institut für Numerische Simulation, January 16–20.
44. H. Neidhardt, Czech Technical University, Faculty of Nuclear Sciences and Physical Engineering, Doppler Institute for Mathematical Physics and Applied Mathematics, Prague, Czech Republic, March 12–17.
45. O. Omel'chenko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, February 2–6.
46. Th. Petzold, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 5–9.
47. J. Polzehl, University of Minnesota, School of Statistics, Minneapolis, MN, USA, June 6–10.
48. ———, University of Minnesota, School of Statistics, Minneapolis, MN, USA, June 16 – July 8.
49. ———, University of North Carolina, Department of Biostatistics, Chapel Hill, NC, USA, July 9–13.
50. P.N. Racec, National Institute of Materials Physics, Laboratory 30 “Nanoscale Condensed Matter Laboratory”, Bucharest, Romania, October 8–12.
51. V. Spokoiny, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, May 23–30.
52. ———, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, July 20–31.
53. ———, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, October 2–10.
54. J. Sprekels, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, September 10–16.

55. ———, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, October 9–14.
56. K. Sturm, University of Bath, Department of Mathematical Sciences, UK, November 12–16.
57. M. Thomas, Istituto di Matematica Applicata e Tecnologie Informatiche, Pavia, Italy, February 10–15.
58. ———, Università di Brescia, Dipartimento di Matematica, Italy, March 11–16.
59. ———, Istituto di Matematica Applicata e Tecnologie Informatiche, Pavia, Italy, September 12–16.
60. ———, Università di Roma "La Sapienza", Dipartimento di Matematica, Italy, November 19–23.
61. ———, SISSA – International School for Advanced Studies, Functional Analysis and Applications, Trieste, Italy, November 26–30.
62. A.G. Vladimirov, Yaroslavl Demidov State University, Department of Mathematical Modeling, Russia, June 10–17.
63. G. Witterstein, Technische Universität München, Fachbereich Mathematik, Garching, April 10–13.
64. ———, Technische Universität München, Fachbereich Mathematik, Garching, September 10–15.
65. ———, Technische Universität München, Fachbereich Mathematik, Garching, September 24–28.
66. ———, Technische Universität München, Fachbereich Mathematik, Garching, October 23–26.
67. T. Wolff, University of California at Los Angeles, Mathematics Department, ESF Exchange Grant within the framework "Random Geometry of Large Interacting Systems and Statistical Physics", USA, March 28 – June 5.
68. ———, University of California at Los Angeles, Mathematics Department, USA, October 20 – November 5.

A.10 Academic Teaching[7]

Winter Semester 2011/2012

1. P. Friz, *Differential Equations for Probabilists* (seminar), Technische Universität Berlin, 4 SWS.
2. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 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* (lecture), 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.

[7] SWS = semester periods per week

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.

Summer Semester 2012

1. P. Friz, *Differential Equations for Probabilists II* (seminar), Technische Universität Berlin, 2 SWS.
2. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
3. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
4. M. Becker, *Wahrscheinlichkeitstheorie für Lehramt* (practice), Universität Leipzig, 2 SWS.
5. A. Caiazzo, *Lineare Algebra I* (lecture), Freie Universität Berlin, 2 SWS.
6. P.-É. Druet, *Partielle Differentialgleichungen der klassischen Physik* (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, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
9. V. John, *Numerik I* (lecture), Freie Universität Berlin, 4 SWS.
10. 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.
11. D. Knees, M. Thomas, *Höhere Analysis II: Partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
12. ———, *Höhere Analysis II: Partielle Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
13. W. König, *Wahrscheinlichkeitstheorie I* (lecture), Technische Universität Berlin, 4 SWS.
14. J.-D. Deuschel, P. Friz, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS.
15. Ch. Landry, *Nichtlineare Optimierung* (practice), Technische Universität Berlin, 2 SWS.
16. P. Mathé, *Computerorientierte Statistik (CoSta)* (lecture), Freie Universität Berlin, 2 SWS.
17. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
18. R. Müller, *Parallele Algorithmen für Partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
19. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. V. Spokoiny, Th. Dickhaus, *Mathematische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

21. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
22. J. Sprekels, *Analysis II* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
23. H. Stephan, *Ungleichungen und Anfänge der Analysis* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
24. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
25. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

Winter Semester 2012/2013

1. P. Friz, *Introduction to rough path analysis with applications to stochastics* (lecture), Technische Universität Berlin, 4 SWS.
2. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
3. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
4. M. Becker, *Grundwissen Schulmathematik* (seminar), Universität Leipzig, 2 SWS.
5. A. Glitzky, *Einführung in die Kontrolltheorie und optimale Steuerung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
6. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
7. D. Hömberg, *PDE-constrained optimal control* (lecture), Mathematics Taught Course Centre/University of Bath, 2 SWS.
8. V. John, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
9. 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.
10. D. Knees, *Gewöhnliche Differentialgleichungen* (lecture), Universität Duisburg-Essen, 4 SWS.
11. ———, *Gewöhnliche Differentialgleichungen* (practice), Universität Duisburg-Essen, 2 SWS.
12. W. König, *Wahrscheinlichkeitstheorie II* (lecture), Technische Universität Berlin, 4 SWS.
13. J.-D. Deuschel, P. Friz, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
14. A. Mielke, *Mehrdimensionale Variationsrechnung/BMS Advanced Course on Multidimensional Calculus of Variations* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
15. ———, *Mehrdimensionale Variationsrechnung* (practice), Humboldt-Universität zu Berlin, 2 SWS.
16. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
17. R. Müller, *Numerische Verfahren für Erhaltungsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
18. R.I.A. Patterson, *Lineare Algebra I für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
19. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.

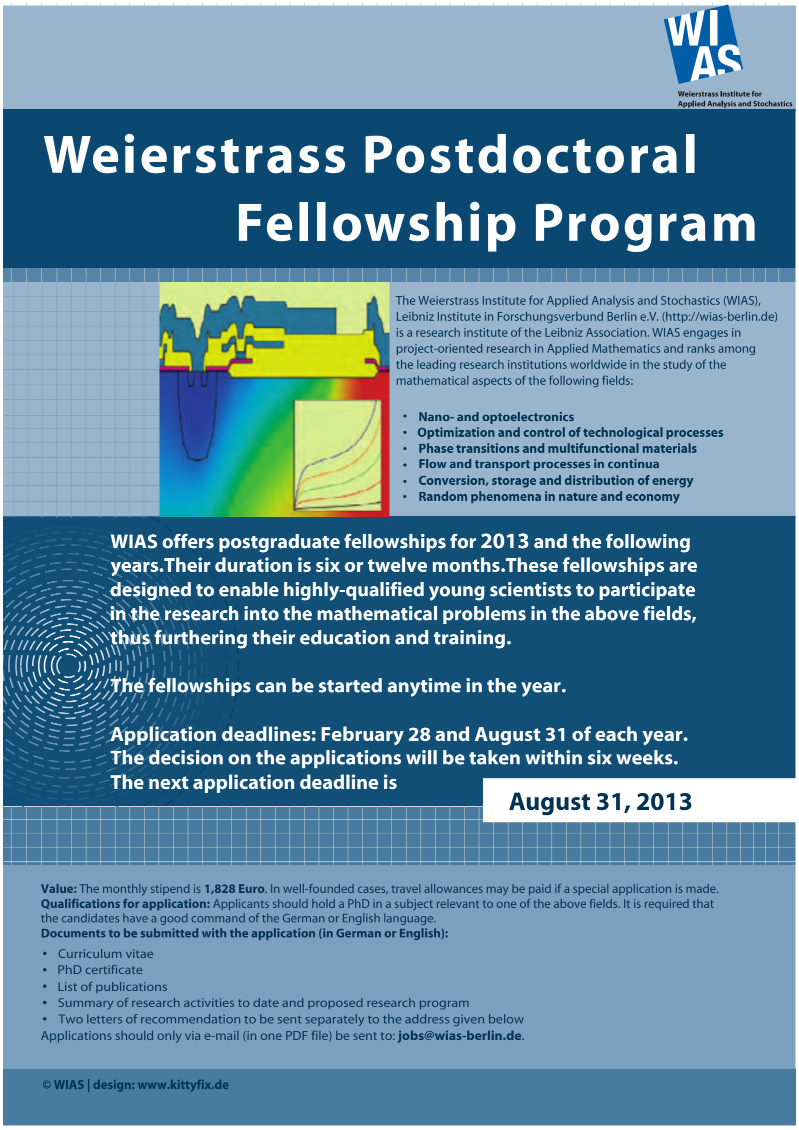
21. H. Stephan, *Additive Zahlentheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
22. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
23. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

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 2012, Dr. Karoline Götze (Technische Universität Darmstadt), Dr. Emmanuel Boissard (Université Paul Sabatier, Institut de Mathématiques de Toulouse, France), and Dr. Santiago Fortes (California Institute of Technology, Computational and Mathematical Sciences, Pasadena, USA) worked as fellowship holders at WIAS.



A.12 Visiting Scientists[8]

A.12.1 Guests

1. H.W. Alt, Technische Universität München, Fakultät für Mathematik, Garching, April 1 – December 31.
2. N. Baldin, Moscow Institute of Physics and Technology, Russia, May 6–13.
3. ———, September 1–30.
4. J. Behrndt, Technische Universität Graz, Institut für Numerische Mathematik, Austria, April 30 – May 4.
5. N. Bochkina, University of Edinburgh, The School of Mathematics, UK, September 1–8.
6. V. Bordo, University of Southern Denmark, Mads Clausen Institute, Sønderborg, May 10–13.
7. O. Boyarkin, Universität Augsburg, Institut für Mathematik, May 8–12.
8. A.B. Cibik, Gazi University, Faculty of Science, Teknikokullar, Ankara, Turkey, June 11, 2012 – June 10, 2013.
9. R. Ciegis, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, November 26 – December 7.
10. A. Collevecchio, Università Ca' Foscari Venezia, Dipartimento di Management, Italy, February 6–10.
11. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, May 16–25.
12. R. Dahlhaus, Ruprecht-Karls-Universität Heidelberg, Institut für Angewandte Mathematik, November 4–7.
13. C. Duval, Centre de Recherche en Économie et Statistique (CREST), Malakoff, France, May 8–11.
14. M.H. Farshbaf Shaker, Universität Regensburg, Fakultät für Mathematik, May 20–23.
15. K. Fellner, University of Graz, Institute for Mathematics and Scientific Computing, Austria, September 23–28.
16. M. Friedrich, Technische Universität München, Fakultät für Mathematik, Garching, April 24–27.
17. M. Friedrich, Technische Universität München, TopMath, April 24–27.
18. R. Fukushima, Tokyo Institute of Technology, Department of Mathematics, Japan, August 27 – September 9.
19. M. Gerdts, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, September 10–21.
20. J. Giesselmann, Archimedes Center for Modeling, Analysis & Computation, Heraklion, Greece, February 6–9.
21. W. Gong, Chinese Academy of Sciences, Institute of Computational Mathematics, Beijing, China, May 6–12.
22. L.I. Goray, Saint Petersburg Academic University, Russia, November 25 – December 1.
23. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, February 21–24.
24. ———, March 12–20.
25. M. Helmers, Universität Bonn, Institute for Applied Mathematics, August 13–17.
26. M. Herrmann, Universität des Saarlandes, Fachrichtung Mathematik, Saarbrücken, August 13–17.
27. U. Herzog, Rücker EKS GmbH, Weingarten, May 21–24.

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

28. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, February 13–17.
29. J. Horowitz, Northwestern University, Department of Economics, Evanston, Illinois, USA, May 13–19.
30. T. Ichinose, Kanazawa University, Faculty of Science, Department of Mathematics, Japan, June 17 – July 15.
31. T. Iliescu, Virginia Tech, Department of Mathematics, Blacksburg, USA, May 20–26.
32. Q. Jin, Australian National University, Mathematical Sciences Institute, Canberra, January 4 – February 3.
33. ———, June 4–15.
34. I. Kashchenko, Yaroslavl Demidov State University, Department of Mathematics, Russia, August 13–19.
35. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, July 23 – August 31.
36. K.U. Kristiansen, Technical University of Denmark, Department of Applied Mathematics and Computer Science, October 30 – November 2.
37. M. Kružik, Institute of Information Theory and Automation, Academy of Sciences, Prague, Czech Republic, October 15–19.
38. C. Laing, Massey University, Institute of Information and Mathematical Sciences, Auckland, New Zealand, August 26 – September 1.
39. M. Landstorfer, Universität Ulm, Institut für Numerische Mathematik, April 16 – May 18.
40. ———, August 20–24.
41. M. Liertzer, Technische Universität Wien, Institut für Theoretische Physik, Austria, September 10–14.
42. Q. Liu, Universität Bremen, Institut für Technomathematik, March 26–30.
43. Y. Liu, University of Tokyo, Graduate School of Mathematical Sciences, Japan, February 26 – March 5.
44. J. Maas, Universität Bonn, Institut für Angewandte Mathematik, June 4–8.
45. V.L. Maistrenko, National Academy of Sciences of Ukraine, Scientific Centre for Medical and Biotechnical Research, Kiev, February 6–17.
46. C. Marteau, Université de Toulouse, Institut National des Sciences Appliquées de Toulouse, France, October 28 – November 2.
47. N. McCullen, University of Bath, Department of Architecture and Civil Engineering, UK, November 18–23.
48. W. Menz, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, September 19–22.
49. R. Metzler, University of Texas at San Antonio, Multimedia and Mobile Signal Processing Laboratory, USA, January 4–14.
50. G. Milshteyn, Ural Federal University, Institute of Physics and Applied Mathematics, Ekaterinburg, Russia, August 2 – October 30.
51. K. Mischaikow, Rutgers University, Department of Mathematics, Piscataway, USA, July 10–15.
52. V. Moldoveanu, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, May 14–25.
53. ———, October 21 – November 3.
54. Th. Müller, Universität Freiburg, Abteilung für Angewandte Mathematik, November 19–22.
55. J. Mura, Pontificia Universidad Católica de Valparaíso, Civil Engineering, Santiago, Chile, June 5–25.
56. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, July 31 – August 9.

57. H. Nguyen, King Abdullah University of Science and Technology (KAUST), Division of Mathematics, Computer Sciences, and Engineering, Saudi Arabia, September 16–22.
58. F. Nier, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, September 9–29.
59. J. Novo, Universidad Autonoma de Madrid, Instituto de Ciencias Matemáticas, Spain, November 5–9.
60. F. Ortegón Gallego, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, August 15–19.
61. M. Panov, Russian Academy of Sciences, Institute for Information Transmission Problems, Russia, November 7–18.
62. V. Panov, Universität Duisburg-Essen, Fachbereich Mathematik, January 2–6.
63. ———, February 1–10.
64. V. Patilea, Institut des Sciences Appliquées de Rennes (INSA), Centre des Mathématiques, France, September 12–17.
65. C. Patz, Robert Bosch GmbH, Stuttgart, November 14–23.
66. T. Pryer, University of Kent, School of Mathematics, Statistics and Actuarial Science, Canterbury, UK, December 17–21.
67. D. Rachinskii, University College Cork, Department of Applied Mathematics, Ireland, July 8–14.
68. L. Rebholz, Clemson University, Department of Mathematical Sciences, USA, October 15–20.
69. P. Reynaud-Bouret, Université de Nice Sophia-Antipolis, Laboratoire J. A. Dieudonné, France, April 22–26.
70. F. Rindler, University of Cambridge, Cambridge Centre for Analysis, UK, October 16–27.
71. M. Roberts, McGill University, Department of Mathematics and Statistics, Montreal, Canada, May 20–26.
72. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, May 14–23.
73. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, January 26 – February 25.
74. ———, October 22 – November 21.
75. K. Sakamoto, Nippon Steel Corporation, Tokyo, Japan, August 20–24.
76. F. Schilder, Technical University of Denmark, Department of Mathematics, Lyngby, December 17–22.
77. A. Schmidt, Universität Bremen, Institut für Technomathematik, March 26–30.
78. B. Schmidt, Universität Augsburg, Institut für Mathematik, May 15–18.
79. Y. Şengül, Ozyegin University, Faculty of Arts and Sciences, Istambul, Turkey, July 9–13.
80. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, July 14–31.
81. M. Sini, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, June 17–22.
82. R. Sun, National University of Singapore, Department of Mathematics, July 11–15.
83. A. Suvorikova, Russian Academy of Sciences, Institute for Information Transmission Problems, Russia, November 7–18.
84. F. Theil, University of Warwick, Mathematics Institute, UK, May 2–25.
85. M. Tlidi, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, July 29 – August 5.
86. M. Tretyakov, University of Nottingham, School of Mathematical Sciences, UK, August 26 – September 7.
87. D. Turaev, Imperial College London, Department of Mathematics, UK, February 12–18.

88. ———, July 21 – August 8.

89. ———, July 24–31.

90. W. van Ackooij, Electricité de France R&D, Clamart, France, April 16–20.

91. W. Wang, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, January 1 – August 31.

92. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, April 12 – May 1.

93. ———, September 9 – October 3.

94. V. Zagrebnov, Université Aix-Marseille 2, Centre de Physique Théorique, Marseille, France, June 18 – July 15.

95. Ch. Zanini, Politecnico di Torino, Dipartimento di Scienze Matematiche (DISMA), Italy, September 2–7.

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 – August 31, 2013.

2. E. Boissard, Université Paul Sabatier, Institut de Mathématiques de Toulouse, France, Weierstrass Postdoctoral Fellowship Program, September 1, 2012 – August 31, 2013.

3. S. Fortes, California Institute of Technology, Computational and Mathematical Sciences, Pasadena, USA, Weierstrass Postdoctoral Fellowship Program, January 9 – December 31.

4. P. Friz, Technische Universität Berlin, Institut für Mathematik, WIAS, June 12, 2009 – June 11, 2014.

5. K. Götze, Technische Universität Darmstadt, Fachbereich Mathematik, Weierstrass Postdoctoral Fellowship Program, September 1, 2011 – January 31, 2012.

6. S. Lu, Fudan University, School of Mathematical Sciences, Shanghai, China, Humboldt Research Fellowship, September 12, 2011 – August 17, 2012.

7. 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, January 15–20.

8. 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, April 15–20.

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, May 13–28.

A.12.3 External Ph.D. Candidates and Post-docs supervised by WIAS Collaborators

1. W. Ackooij, Electricitè de France R&D, Clamart, Gaspard Monge Program for Optimization and Operations Research, launched by Electricité de France (EDF) and the Jacques Hadamard Mathematical Foundation, doctoral candidate, February 1, 2012 – December 31, 2013.

2. F. Almnoufi, Technische Universität Berlin, governmental grant of Syria, doctoral candidate, December 1, 2011 – October 31, 2014.

3. B. Bugert, Berlin Mathematical School, doctoral candidate, December 1, 2010 – December 31, 2013.

4. C. Patz, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, March 1, 2009 – September 11, 2013.
5. M. Salvi, Technische Universität Berlin, International Research Training Group GRK 1339: "Stochastic Models of Complex Systems and Their Applications" and Einstein Foundation, doctoral candidate, April 1, 2010 – March 31, 2013.
6. O. Sekulovic, Freie Universität Berlin, ERASMUS, doctoral candidate, January 1 – October 31.
7. O. Sekulovic, Berlin Mathematical School, Einstein Foundation, doctoral candidate, November 1, 2012 – August 24, 2013.
8. W. Wang, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, doctoral candidate, October 1, 2009 – March 31, 2012.
9. U. Wilbrandt, Freie Universität Berlin, Institut für Mathematik, Helmholtz-Kolleg GEOSIM, doctoral candidate, October 1, 2011 – September 30, 2013.
10. L. Wilhelm, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, Institut für Mathematik, doctoral candidate, October 1, 2012 – February 28, 2013.

A.13 Guest Talks

1. H.W. Alt, Technische Universität München, Zentrum Mathematik, *Free energy inequality in the limit of phase transitions*, October 9.
2. I. Bailleul, University of Cambridge, Statistical Laboratory, UK, *Flows driven by rough paths*, June 26.
3. G. Bao, Zhejiang University/Michigan State University, Hangzhou/East Lansing, China/USA, *Near field imaging via inverse scattering*, November 6.
4. G. Bauer, Technische Universität München, Lehrstuhl für Numerische Mechanik, *A variational multiscale finite element method for the numerical simulation of electrochemical systems*, January 12.
5. M. Bause, Helmut-Schmidt-Universität/Universität der Bundeswehr Hamburg, *Efficient and reliable numerical approximation of transport equations with small diffusion*, January 19.
6. J. Behrndt, Technische Universität Graz, Institut für Numerische Mathematik, Austria, *Spectral theory of Schrödinger operators with delta-potentials*, May 2.
7. P. Berg, Norwegian University of Science and Technology, Department of Physics, Trondheim, *Dynamics and formation of nanopores in polymer electrolyte membranes*, November 15.
8. J. Blath, Technische Universität Berlin, Institut für Mathematik, *On some challenges and recent progress in mathematical population genetics*, October 31.
9. D. Bothe, Technische Universität Darmstadt, Center of Smart Interfaces, *Transportprozesse an fluiden Grenzflächen*, May 3.
10. Ch. Breunig, Universität Mannheim, Abteilung Volkswirtschaftslehre, *Specification testing in nonparametric instrumental quantile regression*, November 28.
11. M. Burger, Westfälische Wilhelms-Universität Münster, Institut für Numerische und Angewandte Mathematik, *Variationsmethoden in der biomedizinischen Bildgebung*, May 2.
12. V. Capasso, University of Milan, Department of Mathematics, Italy, *The role of geometric randomness in the mathematical modeling of angiogenesis*, May 21.
13. J.M. Castelo, Hochschule RheinMain, Fachbereich Ingenieurwissenschaften, Rüsselsheim, *Numerical analysis of few-electron transport in multi-gate nanowire field-effect transistors: A multi-configurational approach*, November 7.
14. J. Cheng, Fudan University, School of Mathematical Sciences, Shanghai, China, *Reconstruction of the Stefan–Boltzmann coefficients in the heat transfer process*, May 8.
15. R. Ciegis, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, *Efficient numerical approximations of multidimensional Schrödinger problems*, November 26.
16. A. Collevecchio, Università Ca' Foscari Venezia, Dipartimento di Management, Italy, *On a preferential attachment model*, February 6.
17. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, *Existence of solutions for a hydrogen storage model*, May 23.
18. R. Dahlhaus, Ruprecht-Karls-Universität Heidelberg, Institut für Angewandte Mathematik, *Cointegration and phase synchronization: Bridging two theories*, November 6.
19. I. Dattner, Eindhoven University of Technology, European Institute for Statistics, Probability, Stochastic Operations Research and their Applications (EURANDOM), The Netherlands, *On deconvolution of distribution functions*, January 11.
20. E. De Vito, Università di Genova, Dipartimento di Matematica, Italy, *Kernel methods for support estimation*, November 21.

21. R. Denk, Universität Konstanz, Fachbereich Mathematik und Stochastik, *Pseudodifferential operators and maximal L^p -regularity*, September 13.
22. St. Dereich, Philipps-Universität Marburg, Fachbereich Mathematik und Informatik, *Condensation effects in preferential attachment models with fitness*, May 30.
23. H. Dette, Ruhr-Universität Bochum, Fakultät für Mathematik, *Of copulas, quantiles, ranks, and spectra. An L1-approach to spectral analysis*, October 31.
24. J. Diehl, Technische Universität Berlin, Institut für Mathematik, *Robust filtering: Correlated noise and multidimensional observation*, June 12.
25. G. Dumont, Université Bordeaux 1, Institut de Mathématiques, France, *Population dynamics of neural network*, September 12.
26. J. Dunlop, Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Abteilung Biomaterialien, Potsdam, *Geometric control tissue growth*, April 23.
27. C. Duval, Centre de Recherche en Économie et Statistique (CREST), Malakoff, France, *Adaptive wavelet estimation of a renewal reward process*, May 9.
28. P. Eberspächer, Universität Stuttgart, Institut für Steuerungstechnik der Werkzeugmaschinen und Fertigungseinrichtungen (ISW), *ECOMATION — Zustandsmodell-basierte Energieverbrauchsoptimierung von Werkzeugmaschinen durch Steuerungstechnik*, April 24.
29. R. Eymard, Université Paris Est, Département de Mathématiques, Marne-la-Vallée, France, *Finite volume schemes for flows in anisotropic heterogeneous porous medium*, April 19.
30. M.H. Farshbaf Shaker, Universität Regensburg, Fakultät für Mathematik, *Phase-field approaches to structural topology optimization*, May 22.
31. ———, *Optimization problems governed by Allen–Cahn and Cahn–Hillard inequalities*, September 12.
32. K. Fellner, University of Graz, Institute for Mathematics and Scientific Computing, Austria, *Drift-diffusion-recombination models for excitonic organic photovoltaic devices*, September 27.
33. M.A. Fernández, Institut National de Recherche en Informatique et en Automatique (INRIA), REO project, France, *Time-splitting schemes for incompressible fluid-structure interaction*, April 19.
34. K. Flasskamp, Universität Paderborn, Institut für Mathematik, *Motion planning for mechanical systems by exploiting inherent dynamical system structures*, November 20.
35. S. Fortes, California Institute of Technology, Computational and Mathematical Sciences, Pasadena, USA, *Power series expansions for waves in high-contrast periodic media*, February 14.
36. ———, *Pertubation methods for waves in high-contrast plasmonic crystal*, June 4.
37. M. Friedrich, Technische Universität München, TopMath, *From atomistic to continuum theory for brittle materials: A two-dimensional model problem*, April 25.
38. P. Friz, Technische Universität Berlin, Institut für Mathematik, *Rough stochastic PDEs, a primer*, May 22.
39. P. Gassiat, Université Paris Diderot (LPMA), France, *Optimal investment and consumption in a mixed liquid/illiquid market*, January 17.
40. P. Gassiat, Technische Universität Berlin, Institut für Mathematik, *Solving the KPZ equation (part II)*, November 13.
41. M. Gerdts, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, *Sensitivity analysis and realtime optimization*, September 11.
42. W. Gong, Chinese Academy of Sciences, Institute of Computational Mathematics, Beijing, *Finite element method for Dirichlet boundary control problems governed by parabolic PDEs*, May 8.

43. L.I. Goray, Saint Petersburg Academic University, Russia, *Energy state calculus in complex structures comprising quantum dots*, November 28.
44. D. Götz, Technische Universität Darmstadt, Fachbereich Mathematik, L_p *theory for non-Newtonian fluids*, December 5.
45. M. Hantke, Universität Magdeburg, Institut für Analysis und Numerik, *Exact solutions to the Riemann problem for compressible isothermal Euler equations for two phase flows with and without phase transition*, November 20.
46. M. Helmers, Universität Bonn, Institut für Angewandte Mathematik, *Convergence of a surface phase field model for axisymmetric two-phase biological membranes*, August 14.
47. M.-A. Henn, Physikalisch-Technische Bundesanstalt, Berlin, *Statistical approaches to the inverse problem of scatterometry*, January 10.
48. M. Hieber, Technische Universität Darmstadt, Fachbereich Mathematik, *Nonlinear parabolic-hyperbolic systems*, October 26.
49. M. Hintermüller, Humboldt-Universität zu Berlin, Institut für Mathematik, *Nichtglatte Strukturen in der Optimierung mit partiellen Differentialgleichungen*, May 2.
50. M. Höhle, Ludwig-Maximilians-Universität München, Institut für Statistik, *Bayesian nowcasting during the large EHEC/HUS outbreak in Germany, 2011*, November 7.
51. T. Ichinose, Kanazawa University, Department of Mathematics, Japan, *On improved Sobolev embedding theorems for vector-valued functions*, June 27.
52. T. Iliescu, Virginia Tech, Department of Mathematics, Blacksburg, USA, *Reduced-order modeling of complex flows: Analysis and computation*, May 24.
53. M.R.S. Iqbal, Universität Konstanz, Fachbereich Mathematik und Statistik, *Modellierung von Schädigungsprozessen*, December 7.
54. Q. Jin, Australian National University, Mathematical Sciences Institute, Canberra, *Nonstationary iterated Tikhonov regularization in Banach spaces*, January 31.
55. J. Johannes, Université catholique de Louvain, Institut de statistique, biostatistique et sciences actuarielles, Belgium, *Adaptive estimation in function linear models*, May 16.
56. R. Joubaud, ANDRA & Université Paris-Est, CERMICS, École des Ponts ParisTech, Marne la Vallée, France, *Continuous model for equilibrium electrolytes: Non ideality and phase separation*, August 1.
57. A. Jüngel, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, *Entropy structure of cross-diffusion models in biology and physics*, May 22.
58. P. Kaczmarkiewicz, Wilhelms-Universität Münster, Institut für Festkörpertheorie, *Non-uniformly shaped quantum dashes: Electronic and optical properties*, June 27.
59. L. Kamenskii, University of Kansas, Department of Mathematics, Lawrence, USA, *Modellierung von Schädigungsprozessen*, December 7.
60. I. Kashchenko, Yaroslavl Demidov State University, Department of Mathematics, Russia, *Local analysis of a model for mode-locking in lasers*, August 14.
61. ———, *Dynamics of equations with large spatially distributed control*, August 16.
62. A. Klar, Technische Universität Kaiserslautern and Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, *Modellierung, Analysis und Anwendungen von Transportgleichungen*, May 4.
63. A. Kneip, Universität Bonn, Wirtschaftswissenschaftlicher Fachbereich, *Factor models and variable selection in high dimensional regression analysis*, April 25.

64. M. Köhne, Technische Universität Darmstadt, Center of Smart Interfaces, *On incompressible Newtonian flows – Artificial boundary conditions and free boundary problems*, May 8.

65. D. Kourounis, Università della Svizzera italiana, Faculty of Informatics, Italy, *The constrained pressure residual (CPR) preconditioning strategy in reservoir simulation*, August 27.

66. M. Kružik, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *Variational problems depending on the inverted gradient and applications to nonlinear hyperelasticity*, October 17.

67. A. Kucher, University of Graz, Institute for Mathematics and Scientific Computing, Austria, *Directive-based hardware accelerator frameworks for hybrid CPU/many-core platforms*, November 29.

68. C. Laing, Massey University, Institute of Information and Mathematical Sciences, Auckland, New Zealand, *Chimeras in random non-complete networks of phase oscillators*, August 28.

69. S. Le Borne, Technische Universität Hamburg-Harburg, Institut für Mathematik, *Hierarchical matrices: Some theory and some applications in preconditioning discretized fluid flow problems*, October 9.

70. G. Lecué, Université Paris-Est, Laboratoire d'Analyse et de Mathématiques Appliquées, Marne-la-Vallée, France, *General oracle inequalities for empirical risk minimization (ERM) procedures, penalized ERM and regularized ERM with applications to high dimensional data analysis*, January 18.

71. C. Leendertz, Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Silizium-Photovoltaik, *Effizienzlimitierende Rekombinationsprozesse in amorph/kristallinen und polykristallinen Siliziumsolarzellen*, March 7.

72. M. Liertzer, Technische Universität Wien, Institut für Theoretische Physik, Austria, *Introduction to the steady-state ab-initio laser theory and its applications*, September 11.

73. Y. Liu, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Forward and inverse problems for hyperbolic systems modelling generation of structures*, February 28.

74. S. Lu, Fudan University, School of Mathematical Sciences, Shanghai, China, *On the inverse problems for the coupled continuum pipe flow model for flows in karst aquifer*, May 29.

75. ———, *Growth rate identification in the crystallization of polymers*, June 11.

76. S. Ma, University of California, Statistics Department, Riverside, USA, *Simultaneous variable selection and estimation in semiparametric modeling of longitudinal/clustered data*, June 20.

77. J. Maas, Universität Bonn, Institut für Angewandte Mathematik, *Approximating rough stochastic PDEs*, June 6.

78. E. Mammen, Universität Mannheim, Abteilung Volkswirtschaftslehre, *Flexible generalized varying coefficient regression modes and locally additive interaction models*, January 25.

79. C. Mancini, Università delle Science di Firenze, Dipartimento di Matematica, Italy, *Spot volatility estimation using delta sequences*, July 4.

80. C. Marteau, Université de Toulouse, Institut National des Sciences Appliquées de Toulouse, France, *Nonparametric goodness-of-fit tests and inverse problems*, October 30.

81. W. Menz, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, *Stochastic modelling of silicon nanoparticle synthesis*, September 19.

82. R. Metzler, University of Texas at San Antonio, Multimedia and Mobile Signal Processing Laboratory, USA, *Online prediction for simultaneous compression & encryption*, January 4.

83. S.E. Mikhailov, Brunel University, London, Department of Mathematical Sciences, Uxbridge, UK, *Extensions of partial differential operators and generalised co-normal derivatives in Sobolev spaces on Lipschitz domains*, December 4.

84. K. Mischaikow, Rutgers University, Department of Mathematics, Piscataway, USA, *Discrete Morse theory as a preprocessor for homology computations*, July 13.

85. V. Moldoveanu, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, *Off-resonant transport in interacting quantum dots*, May 16.

86. ———, *On the steady-state regime of open interacting systems*, October 24.

87. Th. Müller, Universität Freiburg, Abteilung für Angewandte Mathematik, *Scalar conservation laws on constant and time-dependent Riemannian manifolds*, November 21.

88. A. Munk, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, *The multiresolution Dantzig selector: From ion channel recordings to biomolecular microscopy*, May 3.

89. J. Mura, Pontificia Universidad Católica de Valparaíso, Civil Engineering, Santiago, Chile, *On some applications of small amplitude homogenization in elasticity*, June 5.

90. A. Nemet, ALSTOM (Switzerland Ltd.), Baden, Switzerland, *Alstom Gasturbinenentwicklung mit dem Block-Orientierten Prozess-Simulator BOP*, September 6.

91. St. Neukamm, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Quantitative estimates in stochastic homogenization*, May 18.

92. H. Nguyen, King Abdullah University of Science and Technology (KAUST), Division of Mathematics, Computer Sciences, and Engineering, Saudi Arabia, *The physics of wind erosion: A fundamental topic in climate research*, September 20.

93. F. Nier, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, *Asymptotic analysis of a 1D KP system*, September 25.

94. J. Novo, Universidad Autonoma de Madrid, Instituto de Ciencias Matemáticas, Spain, *Postprocessing the Galerkin method for the Navier–Stokes equations: A review*, November 8.

95. F. Ortegón Gallego, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, *Steel heat treating: Industrial procedure and numerical simulation*, August 16.

96. P. Paulau, Technische Universität Berlin, Institut für Theoretische Physik, *Boundary-mediated stabilization of a scroll ring in a tubular reactor*, May 18.

97. A. Pérez Serrano, Universitat de les Illes Balears, Institute for Cross-Disciplinary Physics and Complex Systems, Mallorca, Spain, *Exploring laser dynamics using a travelling wave model*, April 12.

98. T. Pryer, University of Kent, School of Mathematics, Statistics and Actuarial Science, Canterbury, UK, *Some geometric properties of discontinuous Galerkin finite element methods with applications to imaging and fluid flow*, December 19.

99. D. Rachinskii, University College Cork, Department of Applied Mathematics, Ireland, *Mode-locking effect in slow-fast population dynamics models*, July 10.

100. L. Rebholz, Clemson University, Department of Mathematical Sciences, USA, *Efficient, unconditionally stable, and optimally accurate FE algorithms for approximate deconvolution models of fluid flow*, October 18.

101. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *Maximal regularity and smooth dependence for elliptic and hyperbolic PDEs*, January 11.

102. ———, *Hopf bifurcation for dissipative hyperbolic PDEs*, December 5.

103. S. Riedel, Technische Universität Berlin, Institut für Mathematik, *Gaussian rough paths and multilevel Monte Carlo*, June 26.

104. F. Rindler, University of Cambridge, Cambridge Centre for Analysis, UK, *Directional oscillations and concentrations via microlocal compactness forms*, October 17.

105. M. Roberts, McGill University, Department of Mathematics and Statistics, Montreal, Canada, *Consistent maximal displacements for branching Brownian motion*, May 20.

106. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, *Recent results on the evolution of liquid crystals flows*, May 15.

107. L. Rosasco, Massachusetts Institute of Technology, The Center for Biological & Computational Learning, Cambridge, MA, USA, *Learning sets with separating kernels and spectral regularization*, June 20.

108. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *A model of rupturing lithospheric faults with re-occurring earthquakes*, February 15.

109. Th. Royen, Fachhochschule Bingen, Fachbereich 1 – Life Sciences and Engineering, *Some exact distributions derived from gamma random variables including Greenwood's statistic*, June 27.

110. M. Rumpf, Universität Bonn, Institut für Numerische Simulation, *Geometrie und Statistik im Raum von Formen – Anwendungen in Medizin und Pflanzenzucht*, May 9.

111. S. Sager, Otto-von-Guericke-Universität Magdeburg, Institut für Mathematische Optimierung, *Mixed-integer optimal control – A biased overview*, May 25.

112. B. Schäfer-Bung, Freie Universität Berlin, Institut für Mathematik, *Dimension reduction by balanced truncation: Application to light-induced control of classical dynamics and open quantum systems*, March 21.

113. F. Schilder, Technical University of Denmark, Department of Mathematics, Lyngby, *Coupling computational bifurcation analysis to lab experiments*, December 18.

114. A. Schmidt, Universität Bremen, Institut für Technomathematik, *Numerical simulations of metallic microcomponents with statistically distributed anisotropies*, March 27.

115. K. Schmidt, Technische Universität Berlin, Institut für Mathematik, *Asymptotic modelling of acoustic wave-propagation in viscous gases*, June 12.

116. V. Schmidt, Universität Ulm, Institut für Stochastik, *Stochastic modeling of the 3D morphology of energy materials on various length scales*, December 10.

117. J. Schmidt-Hieber, Vrije Universiteit Amsterdam, Department of Mathematics, The Netherlands, *Confidence statements for qualitative features in deconvolution*, May 2.

118. R. Schneider, Technische Universität Dresden, Institut für Numerische Mathematik, *With edge based refinement towards anisotropic adaptive refinement in FEM*, February 9.

119. Y. Şengül, Ozyegin University, Faculty of Arts and Sciences, Istambul, Turkey, *Quasistatic nonlinear viscoelasticity and gradient flows*, July 11.

120. J.A. Sethian, University of California, Department of Mathematics, Berkeley, USA, *Tracking multiphase physics: Geometry, foams, thin films, and biological cells*, June 18.

121. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, *Weighted Delaunay triangulations and restricted Delaunay triangulations in guaranteed-quality mesh generation*, July 26.

122. V. Sidoravicius, Instituto Nacional de Matemática Pura e Aplicada, Rio de Janeiro, Brasil, *From self-repelling and greedy motions to the Coffman–Gilbert conjecture*, November 28.

123. M. Sini, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *Reconstruction of interfaces using elastic waves*, June 19.

124. St.V. Sobolev, Helmholtz-Zentrum Potsdam, Deutsches GeoForschungsZentrum, Sektion Geodynamische Modellierung, *Major challenges in computational geodynamics, Part I*, February 16.

125. U. Stefanelli, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, *The De Giorgi conjecture on elliptic regularization*, April 18.

126. ———, *Crystallization in carbon nanostructures*, May 18.

127. B. Steinberger, M. Mulyukova, Helmholtz-Zentrum Potsdam, Deutsches GeoForschungsZentrum, Sektion Geodynamische Modellierung, *Major challenges in computational geodynamics, Part II*, February 16.

128. I. Steinwart, Universität Stuttgart, Fachbereich Mathematik, *Statistical learning: Classification, density level estimation, and clustering*, May 30.

129. H.-W. Teng, National Central University, Graduate Institute of Statistics, Jhongli City, Taiwan, *Implied state price densties of weather derivatives*, July 11.

130. E.J.W. ter Maten, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands/Bergische Universität Wuppertal, Fachgruppe Mathematik und Informatik, *Low and high, slow and fast*, July 10.

131. F. Theil, University of Warwick, Mathematics Institute, UK, *Wasserstein-Kristalle*, May 14.

132. ———, *Gamma-limit for transition paths of maximal probability*, May 16.

133. D. Tjoestheim, University of Bergen, Department of Mathematics, Norway, *Using local Gaussian correlation to test for independence, copula structure and financial contagion*, December 5.

134. N.M. Tran, University of California, Department of Statistics, Berkeley, USA, *FPCA thoughts on random quantile curves*, July 11.

135. T.D. Tran, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *An introduction to the Wright–Fisher model of mathematical population genetics*, September 13.

136. M. Tretyakov, University of Nottingham, School of Mathematical Sciences, UK, *Layer methods for Navier–Stokes equations with additive noise*, September 4.

137. V.Z. Tronciu, Technical University of Moldova, Department of Physics, Chisinau, *Analysis of a multi-stripe laser array with external optical feedback*, May 31.

138. D. Turaev, Imperial College London, Department of Mathematics, UK, *Energy growth in a chaotic oscillator coupled to a standing wave*, July 24.

139. P. Turkedjiev, Humboldt-Universität zu Berlin, Institut für Mathematik, *Approximating discrete backwards stochastic differential equations using least squares regression*, January 24.

140. W. van Ackooij, Electricité de France R&D, Clamart, France, *Decomposition methods for unit-commitment with coupling joint chance constraints*, April 17.

141. J. Vecer, Frankfurt School of Finance & Management, *Reference asset invariant price processes*, November 14.

142. A. Vershik, St. Petersburg State University, Department of Mathematics and Mechanics, Russia, *Classification of the functions via random matrices and related probabilistic problems*, December 12.

143. N. Verzelen, Institut Scientifique de Recherche Agronomique, Montpellier, France, *Minimax risks for sparse regression: A review*, June 13.

144. P. von Bülau, F. Kiraly, Technische Universität Berlin, Institut für Mathematik, *Stationary subspace analysis and ideal regression*, April 18.

145. M. Wakayama, Kyushu University, Institute of Mathematics for Industry, Japan, *Remarks on geodesics for multivariate normal models*, January 9.

146. A. Wakolbinger, Johann Wolfgang Goethe-Universität Frankfurt am Main, Institut für Mathematik, *Trickle-down processes and their boundaries*, November 14.

147. W. Wang, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *Tieing the straps: Uniform bootstrap confidence interval for generalized linear models*, May 15.

148. M. Weiser, Konrad-Zuse-Zentrum für Informationstechnik Berlin, *Goal-oriented error estimation for nonlinear optimal control problems*, July 3.

149. N. Willrich, Humboldt-Universität zu Berlin, Institut für Mathematik, *Solutions of martingale problems for Lévy-type operators with discontinuous parameters and existence of weak solutions for associated stochastic differential equations*, March 6.

150. J. Wohlgemuth, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Study of a model for reference-free plasticity*, December 12.

151. M.W. Wuttke, Leibniz-Institut für Angewandte Geophysik (LIAG), Hannover, *Unterirdische Kohlebrände in Nord-China: Lokales Problem mit globaler Wirkung und eine Herausforderung für die angewandte Geophysik*, December 10.

152. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Stability in determining shapes of subboundaries and quantitative unique continuation property for partial differential equations*, April 27.

153. ———, *Several inverse problems for fractional diffusion equations*, September 25.

154. V. Zagrebnov, Université Aix-Marseille 2, Centre de Physique Théorique, Marseille, France, *Non-equilibrium states of a leaky photon cavity*, June 20.

155. Ch. Zanini, Politecnico di Torino, Dipartimento di Scienze Matematiche (DISMA), Italy, *From finite to linear elastic fracture mechanics by scaling*, September 5.

156. D. Zeitz, Rolls-Royce Deutschland Ltd & Co KG, Blankenfelde, *Entwicklungsgeschichte und Anwendung von BOP*, September 6.

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/).

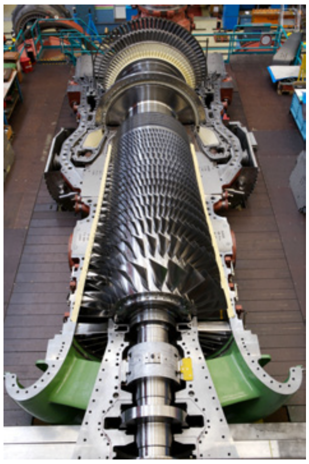
BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: juergen.borchardt@wias-berlin.de)

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 provides capabilities for, e.g., Monte Carlo simulation, correction curve computation, optimization, and script-directed simulation scenarios. 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



*©2009
Bryon Paul McCartney
www.image-engineers.com
all rights reserved*

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

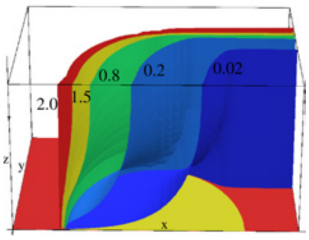
- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, non-conforming, discontinuous, higher-order, isoparametric, with bubbles)
- the use of implicit time-stepping schemes (θ-schemes, DIRK schemes, Rosenbrock–Wanner schemes)
- the application of a multiple-discretization 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.

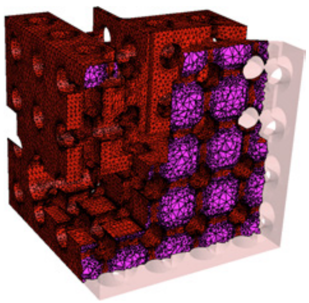


Concentration isosurfaces in a thin-layer flow cell

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`.