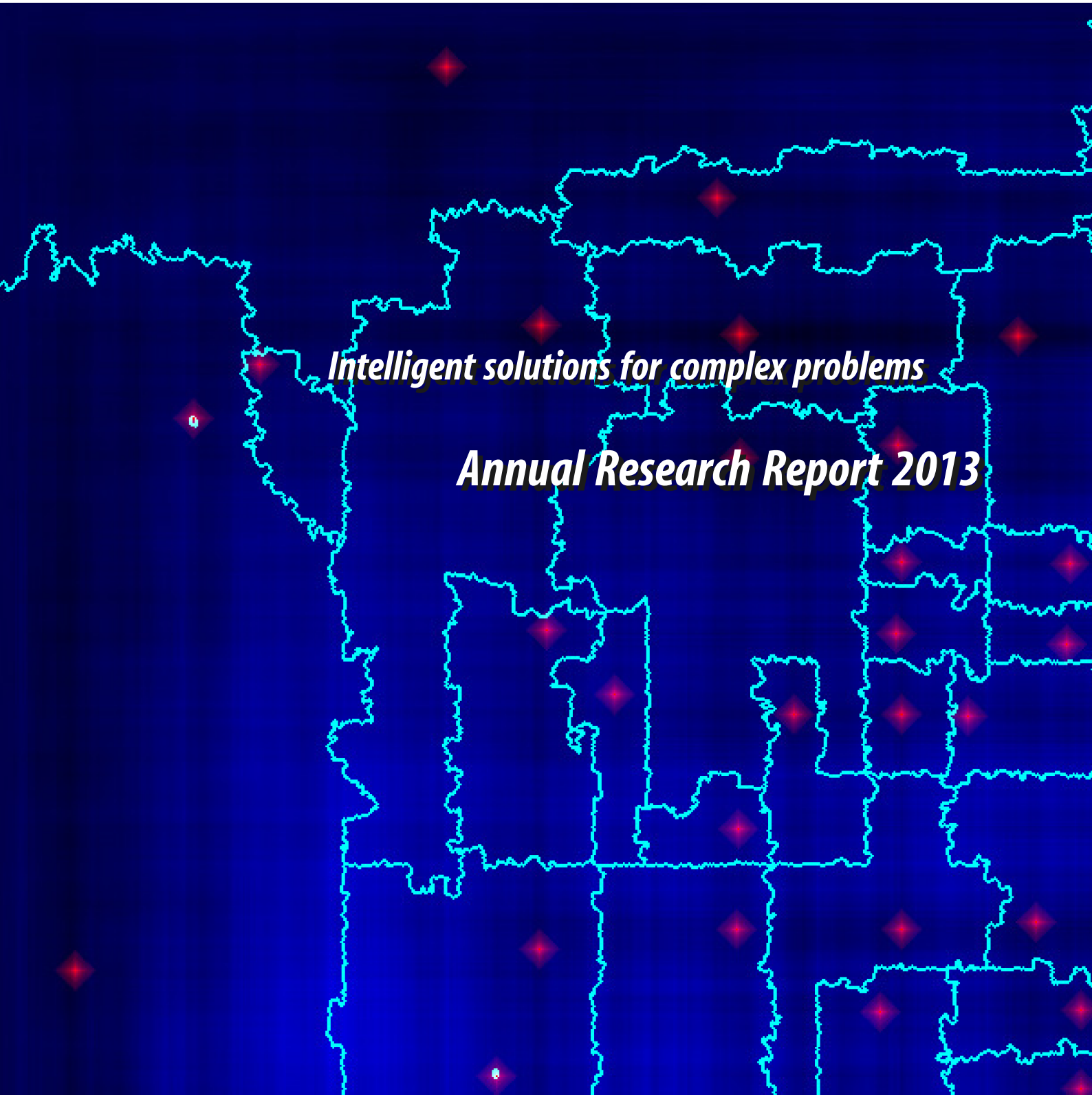
Leibniz Association

Weierstrass Institute for
Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2013

Cover figure: Partition induced by a random forest that is realized on a weighted oriented graph on the square lattice box. The components of the partition are the trees of the forest, the red points represent their roots.

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Prof. Dr. Jürgen Sprekels, Director

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 2013. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2013. Following a more general introduction in part one, in its second part seven selected scientific contributions, written for a broader public, highlight some results of outstanding importance. Finally, the third part presents the essential results of the research groups.

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 three 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. 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 year 2013 was a year of records for WIAS. Among other things, eleven doctoral theses were successfully defended, 135 research papers authored by WIAS members appeared in refereed scientific journals, and 151 preprints were written, both by far the largest numbers ever. Also the third-party funding reached a new all-time best, exceeding 3.2 million euros.

The main scientific highlight of the year 2013, which also led to a change in the institute's structure and is a strong indication of the importance and standing of WIAS in the international scientific community, was the fact that two Italian ERC grantees, Prof. Dr. Enrico Valdinoci and Prof. Dr. Elisabetta Rocca, chose in 2013 to move their ERC Starting Grants to WIAS and to become members of the WIAS staff. They now head the newly-founded ERC Groups *EPSILON – Elliptic PDEs and Symmetry of Interfaces and Layers for Odd Nonlinearities* and *EntroPhase – Entropy Formulation of Evolutionary Phase Transitions*, respectively. Altogether, WIAS is now hosting three ERC Starting Grants and one ERC Advanced Grant.

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*, is now fully operative. 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. Meanwhile it was decided by the Russian government to extend the grant for another two years.

Another highlight of 2013 was the fact that Prof. Dr. Wolfgang König, Second Deputy Director of WIAS and Head of the Research Group *Interacting Random Systems*, was successful in the competition of the Leibniz Association in the framework of the "Joint Initiative for Research and Innovation". As a result, a new Leibniz Group "Probabilistic Methods for Communication Networks with Mobile Relays" will take up its activities later this year.

The Young Scientists' Group *Modeling of Damage Processes* under the leadership of Dr. Dorothee

Knees and Dr. Christiane Kraus, which was founded in 2012 following a recommendation of the institute's Scientific Advisory Board, continued their work with great success. This 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" is active, and WIAS committed itself to implement the "Cascade Model" of the Leibniz Association and of the Joint Science Conference (GWK). Moreover, the institute is committed to improve the work-life balance of its members of staff. In this connection, the institute made important progress when it was awarded the "audit berufundfamilie" (audit job and family) quality seal in December 2013.

Besides these important events of the year 2013, WIAS continued the 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 large 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, 51 additional co-workers (+ 8 outside WIAS; Dec. 31, 2013) could be financed from grants.

The high rank of WIAS in the mathematical community was also witnessed by the fact that the long success story of transfer of knowledge via "brains" through the institute's members continued also in 2013: Dr. Dorothee Knees, head of the Young Scientists' Group *Modeling of Damage Processes*, received calls for a W2 professorship at the University of Kassel and for a W3 professorship at the University of Duisburg-Essen. Since the institute's foundation in 1992, a total of 48 calls were received by WIAS members, a truly remarkable output of which we are proud. In particular, since 2003 seven calls went to women, witnessing the intensive and successful promotion of female researchers at WIAS.

Eleven 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 2013, altogether six leading members of WIAS, including the director and his deputies, held WIAS-funded special chairs at the Berlin universities.

The highlight of cooperation with the mathematical institutions in Berlin was also in 2013 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, 2013, 15 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

Beginning with June 2014, after the funding of MATHEON by the DFG will have finished, a number of new MATHEON projects will be funded in the framework of the newly founded "Einstein Center for Mathematics (ECMath)". WIAS will be strongly involved in these projects, 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 more than 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 March 2014

J. Sprekels

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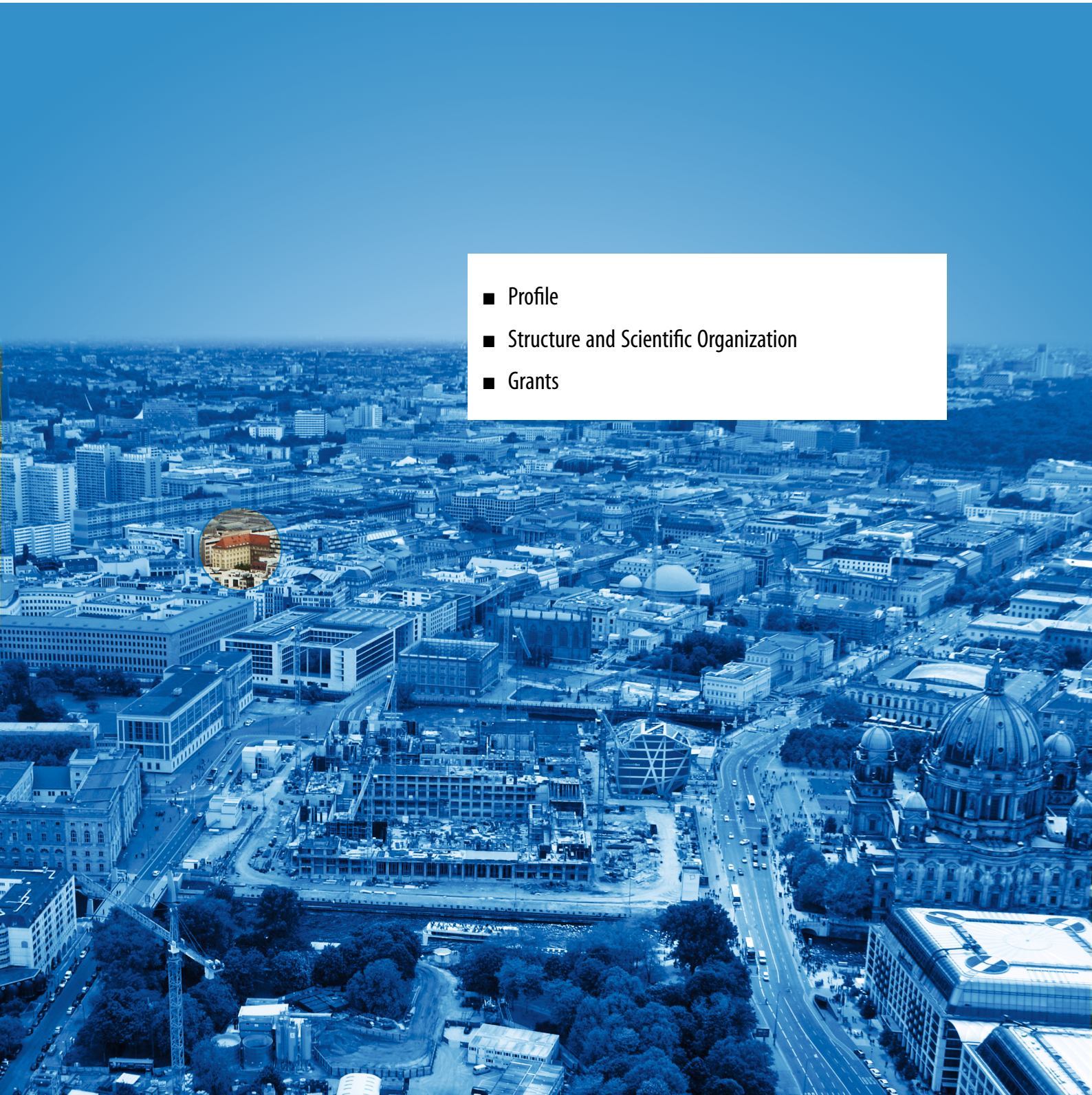
1 WIAS in 2013

- Profile
- Structure and Scientific Organization
- Grants



1.1 Profile

The *Weierstrass Institute for Applied Analysis and Stochastics* (Weierstraß-Institut für Angewandte Analysis und Stochastik, WIAS), *Leibniz Institute in Forschungsverbund Berlin e. V.* (Leibniz-Institut im Forschungsverbund Berlin e. V., FVB) is one of eight scientifically independent member institutes of the *Leibniz Association* forming the legal entity FVB. The *Director of WIAS* is responsible for the scientific work at WIAS, the *Manager* of the *Common Administration of FVB* is in charge of its administrative business.

The mission of WIAS is to carry out *project-oriented* research in applied mathematics. WIAS contributes to the solution of complex economic, scientific, and technological problems of supraregional interest. Its research is interdisciplinary and covers the entire process of problem solution, from mathematical modeling to the theoretical study of the models using analytical and stochastical methods, to the development and implementation of efficient and robust algorithms, and the simulation of technological processes. In its field of competence, WIAS plays a leading role in Germany and worldwide.

WIAS promotes the international cooperation in applied mathematics by organizing workshops and running guest and postdoc programs. Special emphasis is devoted to the extension of the institute's traditional contacts to the scientific institutions of Eastern Europe.

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

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

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.

In 2013, WIAS obtained the berufundfamilie audit certificate for a period of three years. A target agreement was signed to optimize the institute's family-friendly arrangements. With the certificate, WIAS aims to document its commitment towards the harmonization of work and family both internally and externally and implement central research policy objectives.

1.2 Structure and Scientific Organization

1.2.1 Structure

To fulfill its mission, WIAS was in 2013 organized into the departments for technical services, the Secretariat of the International Mathematical Union (IMU, see page 66), the seven scientific research groups, the Young Scientists' Group, one Leibniz group, and two ERC groups[1]:

RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing
RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase Transitions
YSG. Modeling of Damage Processes
LG 3. Mathematical Models for Lithium-Ion Batteries
ERC 1. EPSILON – Elliptic Partial Differential Equations and Symmetry of Interfaces and Layers for Odd Nonlinearities
ERC 2. EntroPhase – Entropy Formulation of Evolutionary Phase Transitions

The organization chart on the following page gives an overview of the organizational structure of WIAS in 2013.

1.2.2 Main Application Areas

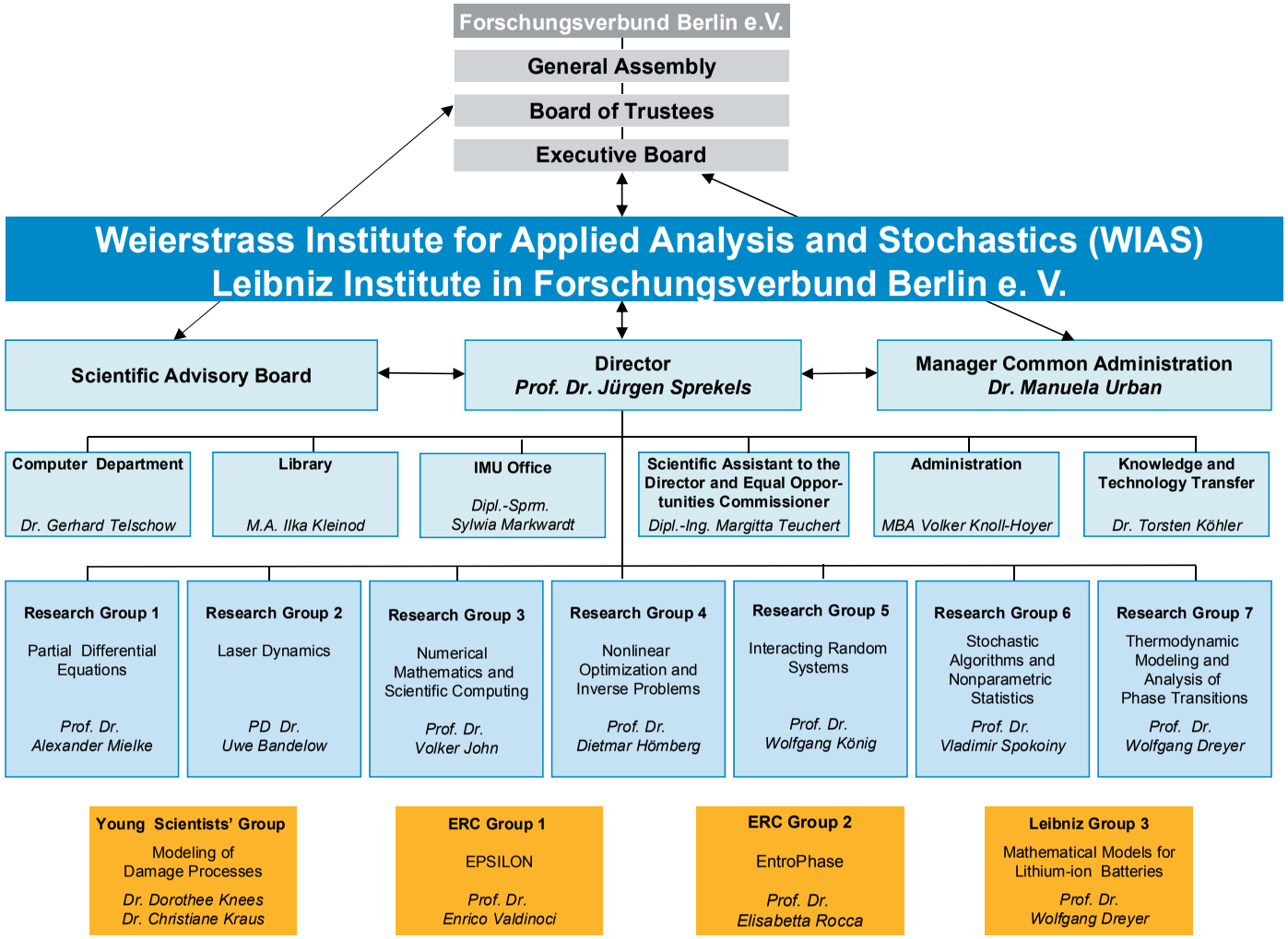
The research at WIAS focused in 2013 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

- **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] In the following, the terms "research group" will often be abbreviated by "RG", Young Scientists' Group by "YSG", and "Leibniz group" by "LG".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Research Group 6
Stochastic Algorithms and Nonparametric Statistics
Prof. Dr. Vladimir Spokoiny
Research Group 7
Thermodynamic Modeling and Analysis of Phase Transitions
Prof. Dr. Wolfgang Dreyer
Young Scientists' Group
Modeling of Damage Processes
Dr. Dorothee Knees
Dr. Christiane Kraus
ERC Group 1
EPSILON
Prof. Dr. Enrico Valdinoci
ERC Group 2
EntroPhase
Prof. Dr. Elisabetta Rocca
Leibniz Group 3
Mathematical Models for Lithium-ion Batteries
Prof. Dr. Wolfgang Dreyer

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

The seven research groups, the Young Scientists' group, the Leibniz group, and the two ERC groups form the institute's basis to fully bring to bear and develop the scope and depth of its expertise. The mathematical problems studied by the groups originate both from short-term requests arising during the solution process of real-world problems, and from the continuing necessity to acquire further mathematical competence as prerequisite to enter new fields of applications, 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 2013 in the interdisciplinary solution process described above.

Main application areas	RG 1	RG 2	RG 3	RG 4	RG 5	RG 6	RG 7	YS G	LG 3	EC 1	EC 2
Nano- and optoelectronics	X	X	X	X							
Optimization & control of technolog. processes	X		X	X		X	X				X
Phase transitions and multi-funct. materials	X			X	X		X	X	X	X	X
Flow and transport processes in continua	X		X		X		X	X	X		X
Conversion, storage and distribution of energy	X		X	X			X		X		
Random phenomena in nature and economy	X		X	X	X	X	X		X	X	

In the following, special research topics are listed that were addressed in 2013 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, 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)
- Transport in random media (in RG 3, RG 4, and 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 3, RG 7, and LG 3)
- Modeling and analysis of coupled electrochemical processes (fuel cells, 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, chemical reaction-diffusion processes, and gas flows; in RG 1, 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 3, 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 2013, having raised a total of 3.2 million euros, from which 51 additional researchers (+ 8 outside WIAS; Dec. 31, 2013) have been financed. In total in 2013, 25.3 per cent of the total budget of WIAS and 45.13 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].

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

ERC Starting Grant *Rough path theory, differential equations and stochastic analysis*

The project ERC-2010-StG no. 258237 takes part in RG 6 and is funded by the European Research Council since September 2010 and lasts for 5 years. The research is concerned with the analysis of finite- and infinite-dimensional stochastic systems with the aid of the recent rough path analysis. Concrete applications range from *non-Markovian Hörmander theory* to the analysis of (until recently) ill-posed *stochastic partial differential equations*, where we have pursued, in particular, Lions' *viscosity approach* adapted to this context. Applications to *statistics* and *nonlinear filtering* further illustrate the usefulness of this theory.

ERC Starting Grant *EPSILON – Elliptic partial differential equations and symmetry of interfaces and layers for odd nonlinearities*

The ERC-Stg 2011 Project no. 277749 is funded by the European Research Council since January 2012 and lasts for 5 years. The research topics include partial differential equations, nonlocal diffusion, fractional minimal surfaces, and phase transitions. The methods rely on variational techniques, geometric measure theory, asymptotic analysis, and nonlinear PDE tools.

ERC Starting Grant *EntroPhase – Entropy formulation of evolutionary phase transitions*

The ERC-Stg 2010 Project no. 256872 is funded by the European Council since April 1, 2011, and it will last 5 years. The project's aim is to obtain relevant mathematical results in order to get further insight into new models for phase transitions and the corresponding evolution PDE systems. The new approach presented here turns out to be particularly helpful within the investigation of issues like existence, uniqueness, control, and long-time behavior of the solutions to such evolutionary PDEs.

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.

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.

Research Initiative *Energy Storage Systems* of the German Federal Government

The Research Initiative *Energy Storage Systems* intends to accelerate the development of energy storage technologies in Germany. The Federal government funds the development of new energy storage technologies and concepts, as well as the improvement of existing techniques. This will create an important precondition for a successful extension of renewable energies. The initiative is supported by the Ministry of Education and Research (BMBF), the Ministry for the Environment, Nature Conservation and Nuclear Savety (BMU) and the Ministry of Economics and Technology (BMWi). In this framework, WIAS (RG 3) runs from 2013 to 2017 a subproject in the interdisciplinary research network "Perspectives for Rechargeable Magnesium-Air Batteries". Project partners are German experimental and theoretical groups in the field of electrochemistry.

ENERGIESPEICHER
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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 2013, 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, 2013, 15 scientists and several student assistants at WIAS were funded by MATHEON.

DFG Research Center MATHEON
Mathematics for key technologies

Graduate School *Berlin Mathematical School (BMS)*

One of the many great achievements of Berlin's mathematicians in recent years was the renewal of the success from 2006, when this graduate school was installed for the first time. In Summer 2012, the second funding period (2013–2017) was awarded to the BMS, underlining its success and the excellent work that it is carrying out since its inception. The BMS is jointly run by the three major Berlin universities within the framework of the German Initiative for Excellence. The BMS is funded with more than one million euros per year to attract excellent young Ph.D. students to the city. Many members of WIAS are contributing to the operations of the BMS, and the annual BMS Summer School in 2014 will entirely be taught by WIAS members.

Berlin Mathematical School

Research Training Group (RTG) 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.

International Research Training Group (IRTG) 1792 *High Dimensional Non Stationary Time Series Analysis* of the DFG

In October 2013, this new International Research Training Group took up its work. The faculty consists of internationally renowned scholars from Humboldt-Universität zu Berlin, WIAS (RG 6), Freie Universität Berlin, the German Institute for Economic Research (DIW), and Xiamen University in China. It will be funded by the DFG for 4.5 years.

Graduate Research School *GeoSim*

The graduate research school "GeoSim" is funded by the Helmholtz Association, GeoForschungsZentrum Potsdam, Freie Universität Berlin, and Universität Potsdam. Its goal is to train a new generation of outstanding young scientists based on a strong collaboration, systematically linking methodological expertise from the areas of Earth and Mathematical Sciences. Thanks to the connections to Freie Universität Berlin, WIAS can participate in the scientific expertise of this graduate school. Two students were supervised by Volker John (RG 3), working at the coupling of free flows and flows in porous media and at the simulation of mantle convection, respectively. For several other students from the Earth science, the supervision of the mathematical aspects of their work is performed.

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 the subproject "Structural adaptive data analysis" (RG 6). The SFB was again positively evaluated and prolonged for a third period until the end of 2016.

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

This Collaborative Research Center began its work on January 1, 2008, and is now in its second funding period (2012–2015). 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 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 (RG 4) 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. A number of numerical methods for turbulent two-phase flows were developed and studied. By comparison with experimental wind tunnel data, obtained from the collaborator in this project, accurate methods were identified.

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 (Oct. 2010 – Sept. 2013, principal investigators: Prof. B. Wagner and Dr. D. Peschka) and for the second funding period (Oct. 2013 – Sept. 2016, principal investigator: Prof. B. Wagner) with the subproject „Structure formation in thin liquid-liquid films” (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. W. König) with the subproject “Branching random walks in random environment” (in RG 5).

DFG Priority Program SPP 1679 *Dyn-Sim-FP – Dynamic simulation of interconnected solids processes*

This new priority program is planned for six years. In the first phase, started at the end of 2013, the project of RG 3 "Numerical methods for coupled population balance systems for the dynamic simulation of multivariate particulate processes using the example of shape-selective crystallization" aims at assessing and improving numerical methods for uni-variate population balance systems. The assessment of the methods will be based on data from experiments that are conducted by one of the project's partners. Numerical methods for solving the population balance equation, which is an integro-partial differential equation, will be developed together with two other collaborators.

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 terminated in June 2013, after organizing a closing workshop in Leipzig. Research was 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*

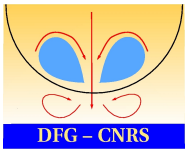
MICROPLAST

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

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

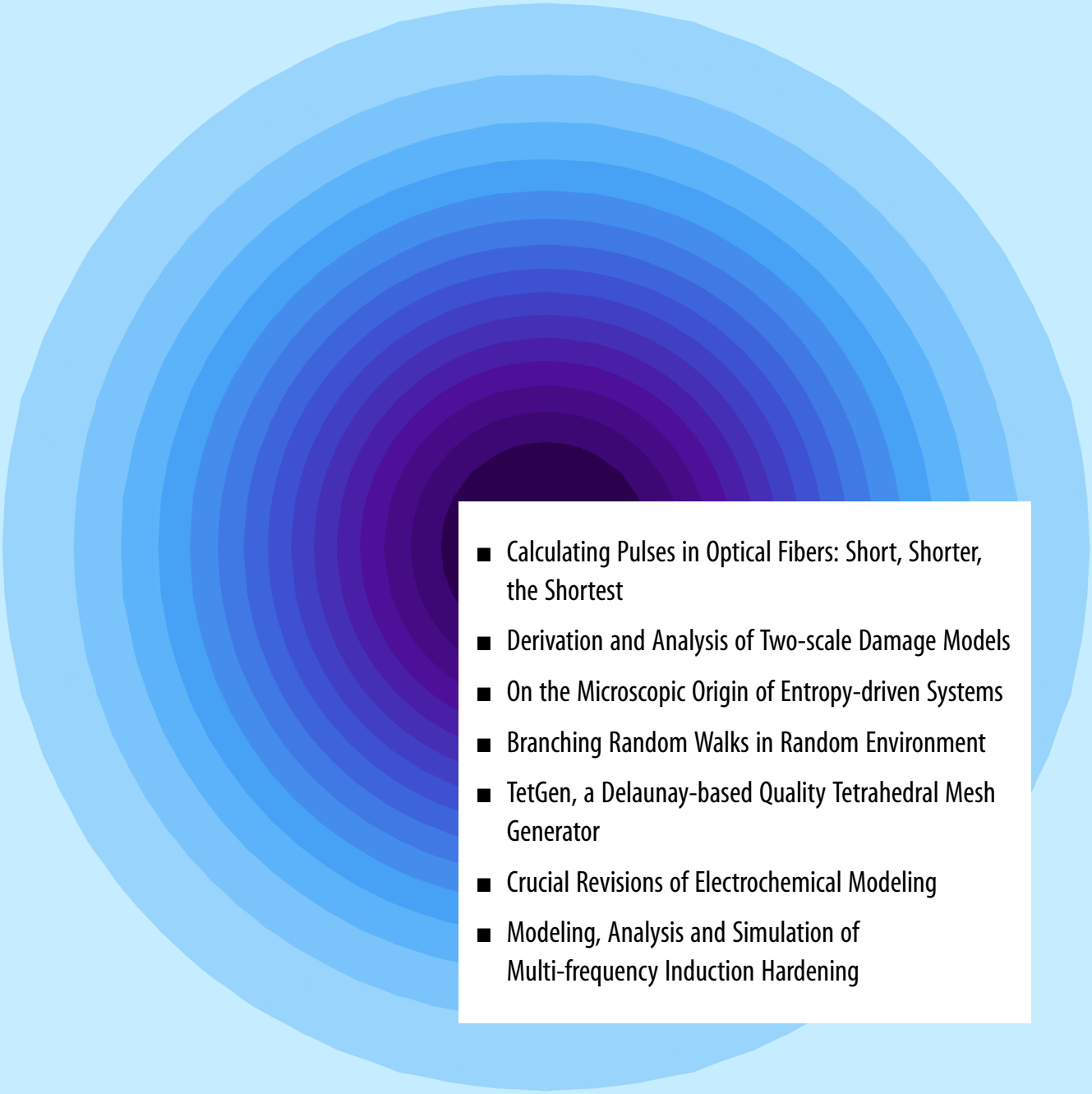
Complex data is often modeled using some structural assumptions. Structure adaptive methods attempt to recover this structure from the data and to use for estimation. The research group at WIAS is studying the convergence and efficiency of such algorithms (RG 6; first funding period: April 1, 2012 – 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".

2 Scientific Highlights



- Calculating Pulses in Optical Fibers: Short, Shorter, the Shortest
- Derivation and Analysis of Two-scale Damage Models
- On the Microscopic Origin of Entropy-driven Systems
- Branching Random Walks in Random Environment
- TetGen, a Delaunay-based Quality Tetrahedral Mesh Generator
- Crucial Revisions of Electrochemical Modeling
- Modeling, Analysis and Simulation of Multi-frequency Induction Hardening

2.1 Calculating Pulses in Optical Fibers: Short, Shorter, the Shortest

Shalva Amiranashvili

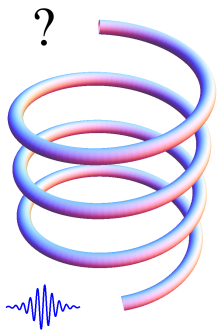


Fig. 1: *It is difficult to measure what happens with pulses in optical fibers. Instead, we just calculate how they evolve.*

An optical pulse that enters into a fiber cannot leave it unchanged. In most cases, the output pulse spreads out due to material dispersion. In nonlinear fibers, one can observe optical solitons that keep their shape but still experience slow changes of carrier frequency and pulse duration. An ultimate practical goal would be to control the propagating pulse, to change its properties in a predictable way, and eventually to make it even shorter than the input one. We report here on a new way to manipulate optical pulses in a simple, effective, and fairly reproducible manner, managing the output frequency, power, and pulse duration. Moreover, the output pulse can be made considerably steeper and shorter than the input one: It can be compressed up to the extreme limit of one and a half oscillations of the electric field. On the other hand, we found that similar compression processes naturally take place in optical supercontinuum, a highly chaotic, turbulent state of the optical field in fibers. The interaction in question contributes also to the rare appearance of extremely powerful optical waves, known as *champion solitons* or *optical rogue waves*. These findings resulted from mathematical models that were developed in WIAS and from parallel computations on the WIAS computer cluster. Later on, our collaborators started ongoing experiments in optical labs.

Introduction

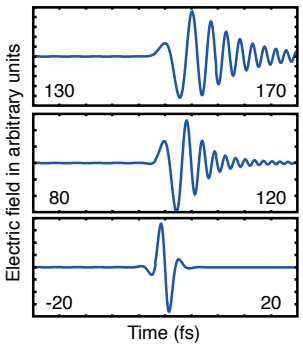


Fig. 2: *In a linear medium, the pulse just spreads out. This spreading can be stopped in nonlinear media.*

Modern photonics devices are capable to produce ultrashort optical pulses, which contain only a few oscillations of the electric field. Being extremely well localized in space and time, these pulses yield a high density of electromagnetic energy and have important applications in both applied and fundamental science. Unfortunately, they are difficult to control and quickly lose their extreme properties in the course of propagation. An ultrashort pulse contains many frequency components, which propagate with different velocities due to the unavoidable material dispersion. As a result, the pulse spreads out (see Figure 2) similar to marathon runners, which are well-localized at the start and scattered near the finish line. A possible strategy for localization is to use both dispersive and nonlinear materials. In terms of the marathon analogy, the nonlinearity can slow down the front runners and help the losers, keeping all runners together. Mathematically, we obtain a so-called *soliton*, a stable pulse where the spreading and focusing effects are in balance.

The task of pulse manipulation is more difficult. Designing the fiber dispersion once for all times, one can change all similar pulses in a prescribed way. Manipulating a given pulse is something different. Having in mind future all-optical technologies, we would like to control the optical pulses like electrons, which are manipulated *dynamically* by changing the applied electric field. In an optical setting, a signal pulse might be manipulated by a suitable control pulse; the latter should be chosen differently depending on the intended effect. Ideally, the control pulse should be taken as small as possible like in a common transistor, where a small electrical signal controls a considerably larger electrical signal.

By far, the all-optical control is difficult to achieve. Interaction between the propagating pulses is too weak; a small control pulse just passes through the signal pulse without inducing significant changes. The collision is fundamentally different for pulse interactions at the so-called *optical event horizons*. They appear due to the nontrivial dispersion (Figure 3), allowing pulses with very different carrier frequencies to have similar velocities. The common velocity gives rise to an extended and efficient interaction that may change both pulses.

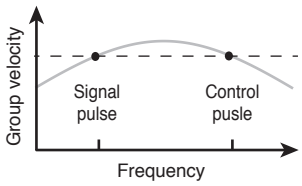


Fig. 3: *Pulses with very different frequencies can have very similar velocities*

Optical event horizons and all-optical switching

Event horizons are usually attributed to general relativity and to the singular character of the space-time metric near a black hole. Mathematically equivalent objects appear in many other systems and can be investigated in laboratory experiments [1]. The concept of an event horizon can be explained by analogy with a fish in a quickly moving water, say, near a waterfall. Assuming that the fish moves with the velocity V as a maximum, if the fish happens to come close to the waterfall upstream, where the water velocity is already larger than V, it is trapped and cannot return back. The line of no return in Figure 4 is mathematically equivalent to the event horizon of a black hole, where the light is trapped in a similar way. Downstream from the waterfall, the flux velocity decreases. The downstream fish experiences an opposite effect: It cannot approach the waterfall because it cannot overcome the second imaginary line of equal velocities, which corresponds to a white hole horizon.

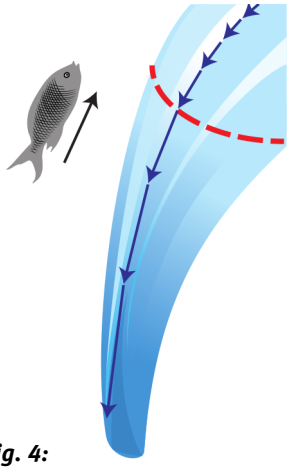


Fig. 4: *If a fish's velocity is smaller than that of the water, the fish will be trapped. The line of no return (red dashed) determines the event horizon.*

A similar situation was discovered recently in fiber optics. Assume that a weak control pulse approaches a co-propagating signal pulse that is much more powerful. The control pulse experiences a small deviation of the refractive index created by the signal pulse. Typically, the refractive index increases, and the control pulse is slowed down. Even a very small decrease in speed can equalize the velocities of the pulses, provided that initially these velocities have already been sufficiently close. A suitable dispersion profile (shown in Figure 3) can be found in optical materials in the vicinity of the so-called *zero dispersion frequency*.

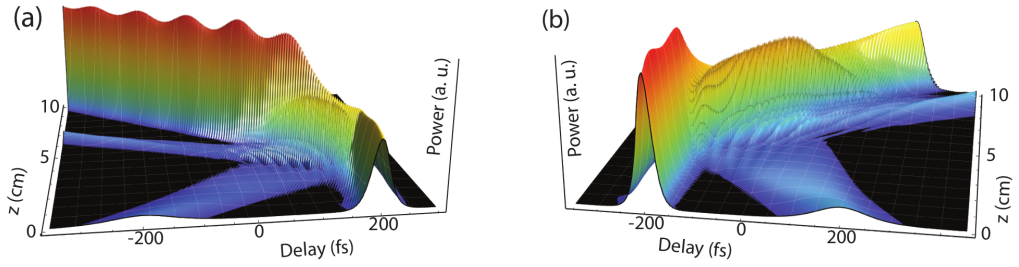


Fig. 5: *A large pulse is controlled by a small one. Left: switching on. Right: switching off. After [2], for further applications; see [3]. a.u. means arbitrary units.*

As a result, both pulses "stick" to each other and co-propagate while interacting and exchanging energy. The interaction affects primarily the weaker pulse, changing its carrier frequency and thus changing its velocity. The control pulse is either slowed down or accelerated, in any case it eventually leaves the stronger signal pulse. The signal pulse is affected less, but still it can experience

a considerable reshaping and frequency shift. Two typical collisions are shown in Figure 5. To the best of our knowledge, in spite of all efforts invested by previous researchers in the all-optical switching, it was for the first time that a stronger signal pulse was effectively switched on and off by a considerably weaker control one [2]. Beyond switching, such interactions have been found important in many optical settings. An interesting example is the spontaneous appearance of extremely short and powerful solitons in the optical supercontinuum.

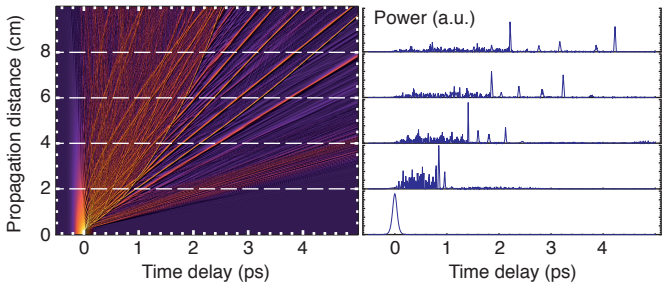


Fig. 6: *A typical calculation of the optical supercontinuum. Left: 2D representation of the power density. Solitons trajectories are clearly observed. Right: snapshots of the pulse power. Note that some solitons are considerably larger than the others.*

Extreme events in optical fibers

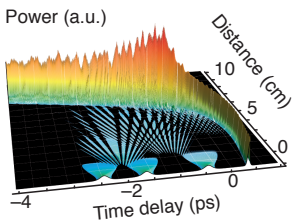


Fig. 7: *An optical rogue wave: a considerable increase of the soliton amplitude yielded by hidden interactions with tiny dispersive waves, [5].*

Recently, there has been much interest in so-called *extreme events* or *rogue waves*, referring to rare and short-living, but huge and dangerous water waves. They seem to “appear from nowhere and disappear without a trace” (Nail Akhmediev, Australian National University). Surprisingly similar objects exist in many other systems, including optical fibers [4]. To explain this behavior, let us consider the propagation of an optical pulse that is several times larger than the standard soliton for the given frequency and duration. Such a higher-order soliton quickly breaks down into a sequence of secondary pulses including stable ordinary solitons and spreading wave packets. The resulting complicated field possesses a wide spectrum and is called *optical supercontinuum* (Figure 6).

The process of supercontinuum generation is highly unpredictable. In experiments, the number of the secondary solitons, their frequencies and amplitudes dramatically vary from shot to shot. Spontaneously, extremely large secondary solitons, so-called *optical rogue waves*, may appear. According to our calculations, one of the mechanisms behind such extreme events is the feeding and the reshaping of the solitons by interactions with the co-propagating tiny dispersive waves at optical event horizons. A typical excitation of a rogue wave by almost invisible control pulses (i.e., from "nowhere") that was extracted from our supercontinuum calculations is shown in Figure 7. The reported mechanism is universal, the only essential precondition is a non-monotone dispersion profile as in Figure 3, yielding the propagation of different wave packets with the same velocity [5].

The mathematics behind the pulses

The physical models behind the presented calculations have a complicated mathematical structure and are demanding in terms of numerical solutions. First, they are nonlinear, e.g., both all-

optical switching and optical rogue waves are highly nonlinear effects. Second, we have to deal with the medium dispersion, i.e., with the delayed response of the fiber material to the pulse field. Moreover, the ultrashort pulses have a wide spectrum and, therefore, the dispersion function cannot be described in a standard way, i.e., by the leading terms of a Taylor expansion at the carrier frequency. Instead, one has to develop a more elaborated approach (Figure 8). Last but not least, we are dealing with a multi-scale problem. The shortest time scale, given by a single field oscillation, corresponds to several femtoseconds. The longest scale is determined by the slow evolution of the solitary waves (e.g., due to the Raman effect), and it may be 1,000,000 times larger. Under such conditions, a full solution of the field and material equations is impractical, and one has to look for approximations. They are derived using a suitable factorization of the fundamental equations. For instance, a weakly nonlinear and weakly dispersive wave equation for the wave field $E(z,t)$ in one spatial dimension can be written as

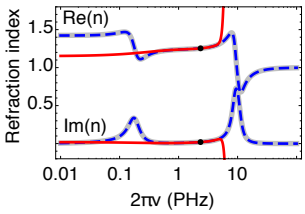


Fig. 8: *Rational functions (blue) are better suited to the real and imaginary parts of the refraction index (grey) than Taylor series (red)*

$$\partial_z^2 E - V^2 \partial_t^2 E = \text{r.h.s.}, \tag{1}$$

where both dispersion and nonlinearity are absorbed by the "small" right-hand side and V is the characteristic velocity. The operator on the left-hand side is factorized as $(\partial_z - V\partial_t)(\partial_z + V\partial_t)$, leading to the familiar picture of forward and backward waves. The important unidirectional approximation deals with a family of waves propagating mostly in one direction. The corresponding scaling law reads $E = E(z,\tau)$, where the retarded time or delay $\tau = t - z/V$ is the main variable, and the dependence of $E(\tau, z)$ on z is weak. A reduced propagation equation is then obtained by applying a standard perturbation technique.

In some cases, factorization becomes possible after an increase of the unknowns number. For instance, to deal with the nonlinear oscillator

$$\frac{d^2u}{dt^2} + u = u^3, \tag{2}$$

one can introduce a complex equation for the new complex variable $U(t) = u(t) + iv(t)$, where by construction

$$\frac{d^2U}{dt^2} + U = \frac{3}{4}|U|^2U + \frac{1}{4}U^3. \tag{3}$$

It is easy to check that each solution to (3) produces a solution to (2). Equation (3) might look more complicated, but the benefit is that with the complex numbers one can factorize its left-hand side. This approach leads to the famous slowly varying envelope approximation. It can be generalized to derive a numerically tractable pulse propagation equation for the complex electric field in a very general setting.

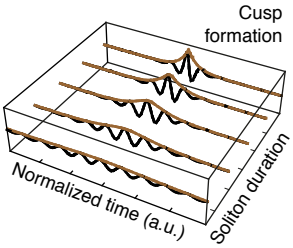


Fig. 9: *A family of solitary solutions to the generalized propagation equation: pulse envelope (brown) and electric field (black). Existence of too short solitons is prohibited because of the cusp formation. See [6] and references cited therein.*

In some special situations, even analytical solutions to the propagation equations are available. For instance, very short solitons are typically destroyed because, due to their large spectral width, they start to feel the "opposite" dispersion branch, i.e., the one with the control pulse in Figure 3. However, even for the most favorable dispersion law, there is an absolute limit for the soliton duration. The family of ultrashort solitons has a limiting member, showing an unphysical cusp; see Figure 9. This is the shortest possible soliton.

Outlook

The methods and concepts described above have already found interesting applications; in addition to all-optical switching, they open a new way for supercontinuum generation [3] and the possibility to destroy rogue waves by simply switching them off like in Figure 5. Another interesting problem is to develop an analytical approach to the pulse interactions at event horizons and to derive both the optimal pulse parameters and the most suitable dispersion law. We believe that these topics will play an important role in the future development of nonlinear fiber optics.

Acknowledgments. Performing the research work reported here, members of the Research Group *Laser Dynamics* at the Weierstrass Institute enjoyed a fruitful collaboration with Ayhan Demircan and Uwe Morgner (Institute of Quantum Optics, Hannover University), Christoph Mahnke and Fedor Mitschke (Institute of Physics, Rostock University), and Günter Steinmeyer (Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin). Financial support by the DFG Research Center Matheon (project D14) is gratefully acknowledged.

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2.2 Derivation and Analysis of Two-scale Damage Models

Hauke Hanke and Dorothee Knees

The performance of modern micromechanical or microelectronic devices relies to a large extent on the use of so-called *multifunctional materials*. These are materials that apart from basic structural stiffness or strength properties possess additional functionalities. Typical examples are piezoelectric materials, magnetostrictive materials, or materials showing the shape memory effect. In general, these additional effects result from changes in the microstructure of the materials and are induced, for instance, by the interplay of mechanical stresses with applied voltages, magnetic fields, or temperature changes. Apart from identifying the processes on the microscale that lead to specific desired macroscopic properties of the materials, it is of great importance to understand damage and degradation processes in these materials. Such processes not only affect the functionality of the material, but they also reduce the overall strength and life-time and may lead to the complete failure of the device. Detailed microscopic, as well as averaged, representative macroscopic models that describe these effects, are needed in order to finally optimize structures, for instance, with respect to their functionalities, shapes, costs, or life-time.

Different phenomenological damage phenomena. Clearly, the particular processes that cause the weakening and failure of devices depend strongly on the materials involved, on temperature, and the loading conditions. For instance, in brittle damage phenomena occurring in materials such as ceramics, rocks, or concrete under the action of external loadings, small cracks or micro-defects may develop at impurities in the material. If a certain critical load is reached, catastrophic failure in terms of macroscopic cracks occurs without showing large deformations before breaking.

In contrast to this behavior, in ductile materials under the action of applied forces large plastic deformations develop before microvoids appear, grow, and coalesce, leading finally to macroscopic rupture. Figure 2 shows the plastic deformation and distribution of voids occurring during the ductile damage of copper.

In rubber-like materials, small cavities can nucleate under large overall tensile hydrostatic stresses. Here, the bulk material is typically considered as hyperelastic, and the models describing the deformation and damage evolution are typically set up in the finite strain framework.

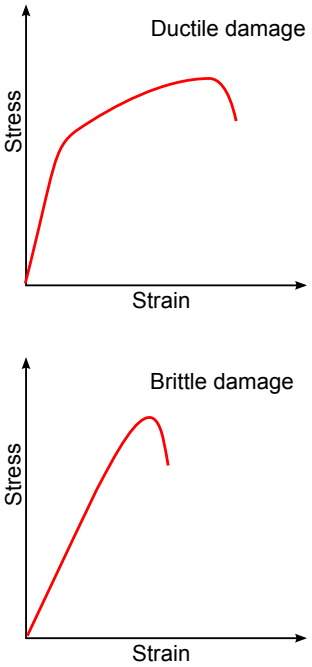

Fig. 1: *Typical stress-strain relations for ductile and brittle materials*

Continuum damage mechanics. Mechanical models describing damage processes in solids go back to the works by L.M. Kachanov (1958) and Yu.N. Rabotnov (1968) in the context of creep, providing the basis for the large branch of modern *Continuum Damage Mechanics*. The basic idea for these models can be summarized as follows: Every point of the solid has a certain stiffness, which serves as an indicator for the damage state of the respective point. High stiffness is interpreted as the presence of a small amount of damaged material, whereas low stiffness is associated with highly progressed damage. In Continuum Damage Mechanics, state variables are introduced that on the macroscopic level represent this local damage state. Moreover, constitutive relations are postulated that describe the dependence of the material constants (like, for instance, the elastic

moduli) on these damage variables. The full damage evolution model then consists of a macroscopic momentum balance that is coupled with a suitable evolution law for the damage variable. This approach leads to damage models of phase-field type with the damage variable as the phase field variable.

Although these models proved to be very useful in the prediction of damage and failure, it is lively debated how specific degradation processes that take place on the microscale can be reflected more realistically. In general, models describing processes on all length and time scales are too complex to allow for numerical simulations. Hence, analytical investigations are needed to provide averaged macroscopic models that reflect the relevant processes on the microscale suitably and that reduce numerical issues arising from the microscales involved in the original problem.

Here, we discuss a prototypical model that describes damage processes in elastic solids from a macroscopic, averaged point of view, but where the evolution of the macroscopic quantities, such as the variables characterizing damage states, results from elementary processes on the microscale.

Description of the model

We present a model for a solid undergoing deformations and a damage process caused by time-dependent external loadings. It is assumed that the relevant degradation process on the microscale is the formation of microvoids. Moreover, it is assumed that the damage process can be considered as rate independent. Rate-independence means that the damage response of the solid is independent of the velocities with which the loadings are applied, i.e., rescaling the forces in time leads to a response that is scaled accordingly. Ductile damage processes in copper can be considered as rate independent; see, for instance, [5]. In order to simplify the presentation, we neglect plasticity effects and are interested only in the interplay between time-dependent damage formation on the microscale and the effective behavior of the solid on the macroscale.

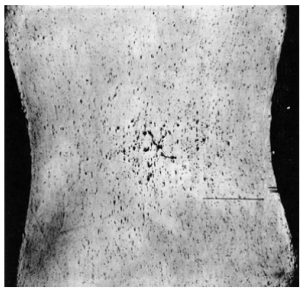

Fig. 2: *Ductile damage of copper, [1]*

We denote by $\Omega \subset \mathbb{R}^3$ the reference configuration of the solid. In the context of standard generalized materials providing a modeling framework for deformable solids with additional internal degrees of freedom, it is assumed that the actual state of the body is characterized completely by the (vector-valued) displacement field $u(t,x)$ and some internal variables that cover the actual inner structure of the material. For damage processes, the inner structure is captured by a damage variable $z(t,x)$ that might be scalar, vector, or tensor valued. Here, we focus on the scalar case. During damage processes, the strength of the solid will locally decrease due to the formation of micro-defects. Since self-healing is not possible for the materials considered here, a monotonicity constraint on the time evolution of the damage variable is imposed.

Energy and dissipation. The evolution model is set up on the basis of an energy functional $\mathcal{E}(t,u,z)$ that accounts for the elastic energy stored in the solid for given external loadings at time t, displacements u, and a damage state z, as well as a dissipation distance $\mathcal{D}(z_1,z_2)$ that quantifies the amount of energy needed to proceed from one damage state z_1 to another state z_2. Here, the unidirectionality of the damage process is taken into account by setting $\mathcal{D}(z_1,z_2)=\infty$

if the state z_2 is not admissible with respect to z_1, in the sense that z_2 does not comprise the damage characterized by z_1.

In the global energetic modeling framework for rate-independent processes, the damage evolution model is given by the conditions (S) and (E), which are explained in more detail in the following: Find functions $(u, z) : [0, T] \to \mathcal{U} \times \mathcal{Z}$ (suitable state spaces) such that for all $t \in [0, T]$:

$$\text{(S)} \qquad \mathcal{E}(t, u(t), z(t)) \le \mathcal{E}(t, \widetilde{u}, \widetilde{z}) + \mathcal{D}(z(t), \widetilde{z}) \qquad \text{for all } (\widetilde{u}, \widetilde{z}) \in \mathcal{U} \times \mathcal{Z},$$

$$\text{(E)} \qquad \mathcal{E}(t, u(t), z(t)) + \mathrm{Diss}_{\mathcal{D}}(z; [0, t]) = \mathcal{E}(0, u(0), z(0)) + \int_0^t \partial_t \mathcal{E}(s, u(s), z(s)) \mathrm{d}s.$$

The energetic formulation (S) and (E) is also used to model other rate-independent phenomena, like, for instance, plasticity, the shape memory effect, or ferroelectric effects. In the case of damage, the first condition (S) forces the temporarily stored energy $\mathcal{E}(t, u(t), z(t))$ to be less than or equal to the energy $\mathcal{E}(t, \widetilde{u}, \widetilde{z})$ of any other admissible state $(\widetilde{u}, \widetilde{z})$ plus the energy $\mathcal{D}(z(t), \widetilde{z})$ needed to transform the damaged area associated to $z(t)$ into that given by $\widetilde{z}$. The second condition (E) models the energy conservation: The actual stored energy $\mathcal{E}(t, u(t), z(t))$ plus the energy $\mathrm{Diss}_{\mathcal{D}}(z; [0, t])$ spent to damage the solid until the time t is equal to the energy $\mathcal{E}(0, u(0), z(0))$ initially stored in the solid plus the energy entering the system due to external forces.

To describe reasonable damage processes by these evolution laws, the structure of the underlying functionals $\mathcal{E}$ and $\mathcal{D}$ needs to be specified.

The micromechanical model. As already mentioned in the introduction, in many materials a damage process is initiated on the microscale, where small defects start to develop. These defects can be cracks, voids, or cavities, for instance. The model presented here allows for various different defect geometries; see Figure 5. Here, we concentrate on a micromechanical model that describes a solid consisting of homogeneous material where damage causes the creation of small spherical holes. We assume that the defects are periodically distributed, i.e., the centers of the defects are elements of the periodic lattice $\varepsilon\mathbb{Z}^3$ for some $\varepsilon > 0$. Moreover, we assume that the diameters of the holes cannot exceed the maximal value εD_0 for some fixed $D_0 \in (0, 1)$. The value $\varepsilon > 0$ denotes the intrinsic length scale of the solid undergoing the damage process. Note that the periodical distribution of the centers and the assumption $D_0 < 1$ prevent the holes from connecting with each other. We emphasize that the sizes of the holes can vary from one another.

The damage variable z_ε associated with a specific distribution of the holes is introduced as follows: At time t the damage variable $z_\varepsilon(t, x)$ takes the value 1 if the point x still belongs to the solid, while $z_\varepsilon(t, x) = 0$ if x is part of a small hole included in the solid. In Figure 3, for the respective time t and $\varepsilon > 0$, the damage variable $z_\varepsilon(t)$ is constantly 1 in the grey part of the solid and takes the value 0 on the union of all red balls. Note that according to the damage progression, the defects can only grow, so z_ε actually is a non-increasing function with respect to time.

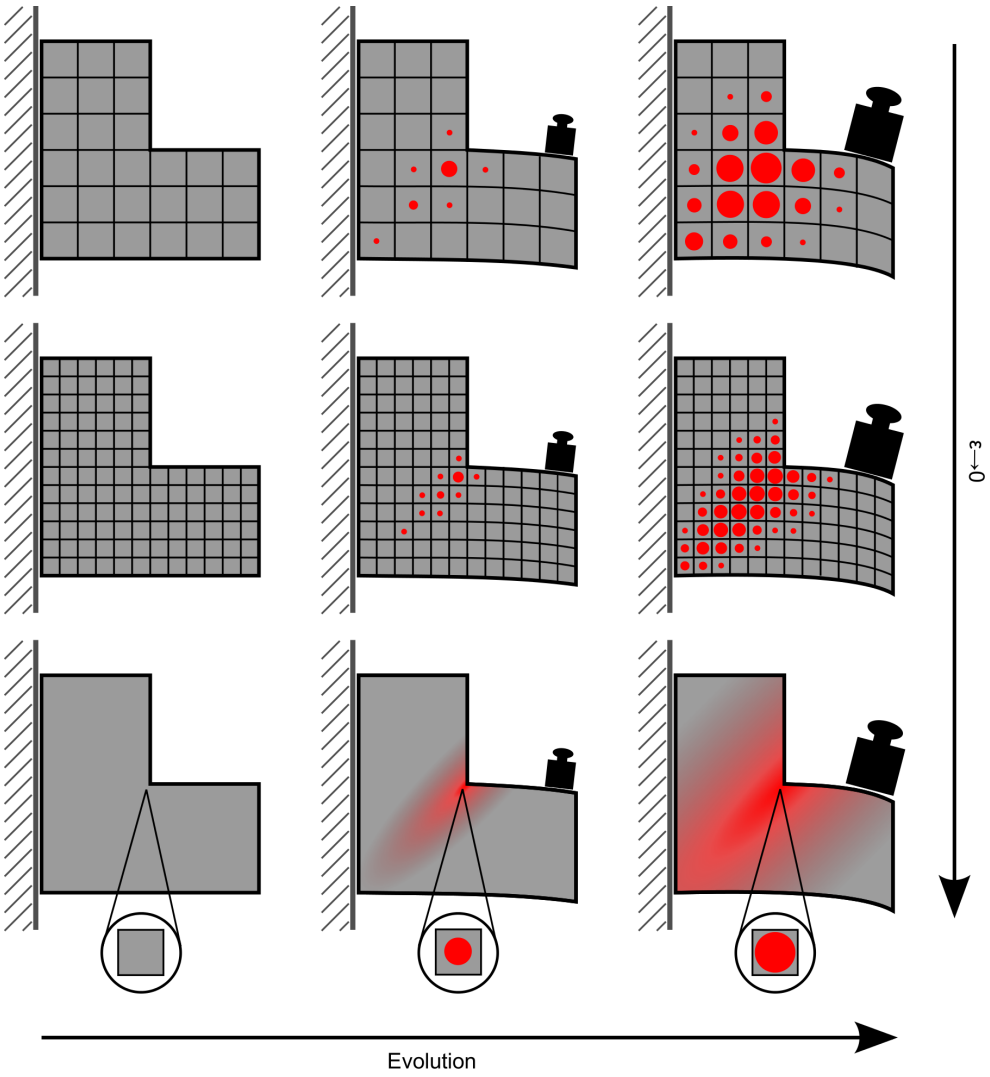

Fig. 3: *From left to right: damage progression in an L-shaped solid for different parameters $\varepsilon \geq 0$. From top to bottom: limit passage $\varepsilon \to 0$ to the effective damage model (homogenization).*

To model the evolution with the help of the energetic formulation, the energy $\mathcal{E}_\varepsilon$ and the dissipation distance $\mathcal{D}_\varepsilon$ have to be defined, and the defect distribution needs to be linked to the material description. For linear elastic, homogeneous solids with elasticity tensor $\mathbb{C}$, the functional $\mathcal{E}_\varepsilon$ is given as follows:

$$\mathcal{E}_\varepsilon(t, u_\varepsilon, z_\varepsilon) = \int_\Omega \tfrac{1}{2} \langle z_\varepsilon(x) \mathbb{C}\, \mathbf{e}(u_\varepsilon(x)), \mathbf{e}(u_\varepsilon(x)) \rangle_{3\times 3} \mathrm{d}x + \mathcal{G}_\varepsilon(z_\varepsilon) - \langle \ell(t), u_\varepsilon \rangle. \tag{1}$$

For fixed time t, the first term describes the stored elastic energy in the perforated solid characterized by z_ε, and $\mathbf{e}(u_\varepsilon)$ denotes the linearized strain tensor. $\mathcal{G}_\varepsilon(z_\varepsilon)$ is a penalty term. Roughly speaking, for large values of $\mathcal{G}_\varepsilon(z_\varepsilon)$ the damage variable z_ε describes a strongly alternating diameter distribution of the microvoids. Since (S^ε) forces $\mathcal{E}_\varepsilon(t, u_\varepsilon(t), z_\varepsilon(t))$ to be as small as possible, $\mathcal{G}_\varepsilon(\cdot)$ prefers the creation of defects in the vicinity of already damaged material and penalizes their generation in areas of intact material; see Figure 4. The last term $-\langle \ell(t), u_\varepsilon \rangle$ represents the work of external loadings $\ell(t)$ consisting of volume and surface forces.

The dissipation distance $\mathcal{D}_\varepsilon$ quantifies the energy needed to switch from one damage state z_1 to the new damage state z_2. Here, we assume that it is proportional to the volumetric change of the damaged region leading to

$$\mathcal{D}_\varepsilon(z_1, z_2) = \begin{cases} \int_\Omega \kappa(z_1(x) - z_2(x))\mathrm{d}x & \text{if } z_1(x') \geq z_2(x') \text{ for all } x' \in \Omega, \\ \infty & \text{otherwise,} \end{cases} \tag{2}$$

with a material-dependent constant $\kappa > 0$. Other choices are possible, as well. The total dissipation along an admissible (i.e., geometrically admissible and monotone) trajectory $t \mapsto z_\varepsilon(t)$ with $t \in (t_0, t_1)$ is then given by

$$\mathrm{Diss}_{\mathcal{D}_\varepsilon}(z_\varepsilon; [t_0, t_1]) = \sup_{\text{partitions of } (t_0,t_1)} \sum_k \mathcal{D}_\varepsilon(z_\varepsilon(t_{k-1}), z_\varepsilon(t_k)) = \mathcal{D}_\varepsilon(z_\varepsilon(t_0), z_\varepsilon(t_1)).$$

For every positive ε, the abstract theory on energetic solutions to rate-independent systems guarantees the existence of a solution $(u_\varepsilon, z_\varepsilon) : [0, T] \to \mathcal{U}_\varepsilon \times \mathcal{Z}_\varepsilon$ to (S^ε) and (E^ε) set up with the above introduced energy functional $\mathcal{E}_\varepsilon$ and dissipation distance $\mathcal{D}_\varepsilon$.

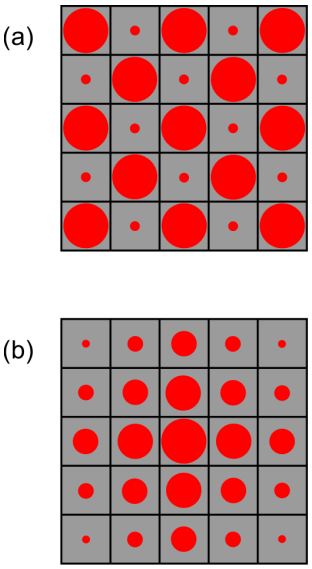

Fig. 4: *Different defect diameter distributions leading to (a) a large and (b) a small value of $\mathcal{G}_\varepsilon(\cdot)$*

Passage to the limit. Letting $\varepsilon \to 0$, the main task is to identify a macroscopic, averaged limit model defined by an energy $\mathcal{E}_0$ and a dissipation $\mathcal{D}_0$ such that the sequence (or subsequence) of solutions $(u_\varepsilon, z_\varepsilon)_{\varepsilon>0}$ converges to limit functions $(u_0, z_0) : [0, T] \to \mathcal{U}_0 \times \mathcal{Z}_0$ and to prove that (u_0, z_0) satisfies (S^0) and (E^0) as defined by $\mathcal{E}_0$ and $\mathcal{D}_0$.

For fixed $\varepsilon > 0$, during the damage progression a certain number of voids of individual sizes grow as a reaction to the influence of the external loadings. Since the length scale constrains the size of the defects, applying the same external loadings for a decreased length scale leads to the creation of a larger number of defects of smaller size to compensate the amount of formerly damaged material. For fixed time t, this structure is captured by the damage variables $z_\varepsilon(t)$ that, for ε tending to zero, alternate faster and faster between the values 0 and 1. Hence, the limit function $z_0(t)$ will no longer be restricted to these two values but is allowed to take values within the interval $[0, 1]$. The limit value $z_0(t, x)$ can be interpreted as the ratio of damaged and undamaged material in the point $x \in \Omega$ at time t, as will be visible from the structure of the limit functional $\mathcal{E}_0$. The main result is the following.

Theorem. For given ℓ and suitable initial conditions, consider (S^ε) and (E^ε) with $\mathcal{E}_\varepsilon$ from (1) and $\mathcal{D}_\varepsilon$ from (2). Then there exist limit functionals $\mathcal{E}_0$ and $\mathcal{D}_0$ (see below) such that the limit functions $(u_0, z_0) : [0, T] \to \mathcal{U}_0 \times \mathcal{Z}_0$ of the sequence $(u_\varepsilon, z_\varepsilon)_{\varepsilon>0}$ (or subsequence) of microscopic solutions $(u_\varepsilon, z_\varepsilon) : [0, T] \to \mathcal{U}_\varepsilon \times \mathcal{Z}_\varepsilon$ form a solution to (S^0) and (E^0) defined by $\mathcal{E}_0$ and $\mathcal{D}_0$.

The limit dissipation distance $\mathcal{D}_0$ is identical to the one for positive ε; see (2). Moreover, the limit functional $\mathcal{E}_0$ inherits the particular structure of the assumed damage geometries (balls in this case) and is given by

$$\mathcal{E}_0(t, u_0(t), z_0(t)) = \int_\Omega \tfrac{1}{2}\langle \mathbb{C}_{\mathrm{eff}}(z_0(t, x))\mathbf{e}(u_0(t, x)), \mathbf{e}(u_0(t, x))\rangle_{3\times 3}\mathrm{d}x + \mathcal{G}_0(z_0(t)) - \langle \ell(t), u_0(t)\rangle.$$

The effective material tensor $\mathbb{C}_{\mathrm{eff}}(z_0(t, x))$ for every $x \in \Omega$ and any t is given by the following unit

cell problem:

$$\langle \mathbb{C}_{\mathrm{eff}}(z_0(t,x))\xi,\xi\rangle_{3\times 3} = \min_{v} \int_{[0,1]^3\setminus B(z_0(t,x))} \langle \mathbb{C}(\xi+\mathbf{e}(v(y)),\xi+\mathbf{e}(v(y))\rangle_{3\times 3}\mathrm{d}y. \tag{3}$$

Here, $B(z_0(t,x))$ denotes the ball of volume $1-z_0(t,x)$ having the same center as the unit cube $[0,1]^3$. Since the ball $B(z_0(t,x))$ has to be contained in the cube $[0,1]^3$ of volume 1, and since its volume is given by $1-z_0(t,x)$, the limit damage variable $z_0(t)$ cannot fall below the positive value $1-\mathrm{vol}(B_{D_0})$, where D_0 is the diameter introduced above. This result corresponds to the fact that the effective model describes incomplete damage, i.e., damage of the solid is expressed in a decrease of the strength of the material, but no macroscopic holes are created. Despite this fundamental difference to the microscopic models, their structure is preserved in the following sense: As one can see in (3), the description of the effective material is based on the material tensor $\mathbb{C}$ and the defect's geometry (balls) chosen for the microscopic models. Moreover, the size of the defect responsible for the effective tensor $\mathbb{C}_{\mathrm{eff}}(z_0(t,x))$ is related to the limit $z_0(t,x)$ of the sequence $(z_\varepsilon(t,x))_{\varepsilon>0}$ of microscopic damage variables.

The mathematical methods applied rely on the abstract concept of evolutionary Γ-convergence for rate-independent systems. A major challenge was the construction of a so-called *mutual recovery sequence* that is admissible simultaneously for the functionals $\mathcal{E}_\varepsilon$ and $\mathcal{D}_\varepsilon$. A discrete gradient for piecewise constant functions was introduced to construct the regularizing term $\mathcal{G}_\varepsilon$, and convergence and embedding results for broken Sobolev spaces from literature had to be adapted. Without essential changes, more complex void geometries that are characterized by more than one geometrical parameter can be included, leading to vectorial damage variables; see Figure 5. In this way, anisotropic effects can be modeled explicitly. Future extensions of the model may cover additional plasticity effects or more complex delamination processes that take place on the microscale. The result presented here is a first step to provide a rigorous mathematical analysis for two-scale damage models described in the engineering literature; see, for instance, [4].

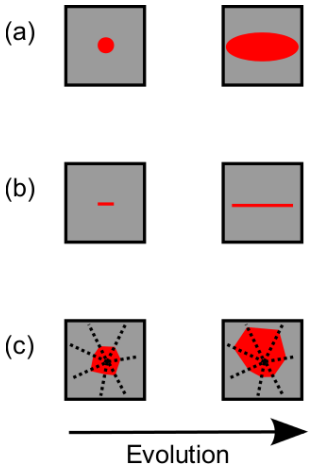

Fig. 5: *(a) Ellipsoidal defect shape. (b) Horizontal crack path. (c) Anisotropic defect.*

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2.3 On the Microscopic Origin of Entropy-driven Systems

Matthias Liero, Alexander Mielke, and D.R. Michiel Renger

Many fundamental ordinary or partial differential equations in mechanics, physics, and the natural sciences in general have an underlying geometric structure in the sense that the evolution of the system is driven towards its equilibrium by an energy or entropy functional. These so-called *gradient systems* are discussed in more detail in Subsection (a). In particular, we are interested in gradient systems that are driven by the "standard" entropy functional. This notion of entropy is inherently related to stochastic fluctuations of a microscopic particle system through its large deviations, as we explain in Subsection (b). This fact raises the question whether a similar connection exists between entropy-driven gradient systems and dynamical large deviations. The first ideas of this connection can be traced back to the work of Onsager in the early fifties [6]. We pursue this direction further, and, using the contemporary knowledge of gradient systems and large deviations, we aim to connect these concepts in a sound mathematical way. As such, our research program acts as a bridge between the fields of analysis and stochastics.

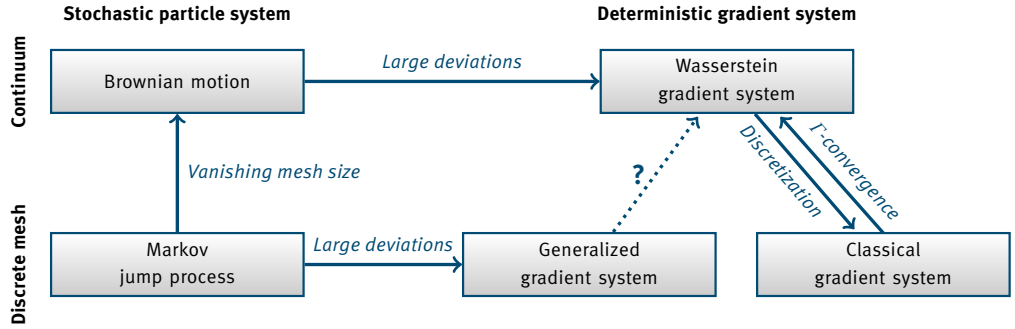

Fig. 1: *The research program*

Figure 1 depicts an overview of this program. There are essentially two types of transitions that we study: limits where the number of particles goes to infinity (see Figure 3), and limits where the number of lattice positions goes to infinity (see Figure 6). Regarding the many-particle limit, we describe in Subsection (c) how the fluctuations in a system of independent Brownian particles leads to the Wasserstein gradient system for the diffusion equation via its large deviations. Next, in Subsection (d), we will see that with a slight generalization the same principle can be used to derive a gradient system for Markov chains from independent Markovian particles on a discrete state space. Surprisingly (at first sight), the latter yields a gradient system that is different from the classical gradient system that was recently found in [3, 4]. At second sight, however, it becomes clear that the different stochastic fluctuations around an evolution give rise to different gradient structures for the same equation. Therefore, a given evolution equation can have a myriad of gradient structures.

Lastly, with gradient systems at hand for diffusion on continuous and discrete spaces, the question arises whether and how these structures are related. At the level of the particle systems, this transition can easily be made by shrinking the lattice width. In Subsection (e), we will see that the

same transition can be done rigorously at the level of the gradient systems, using the evolutionary Γ-convergence of the discrete structure.

(a) Gradient structures for evolution equations

We consider the evolution of a physical system, which is described by an ordinary or partial differential equation of the form $\dot{u}_t = -\mathcal{F}(u_t)$. Here, $\mathcal{F}$ is a given (nonlinear) vector field modeling the physical effects in the system (e.g., diffusion and/or reaction processes). We say that the equation has a *gradient structure* if it can be written in the form

$$\dot{u}_t = -\mathcal{F}(u_t) = -K(u_t)\mathrm{D}\mathcal{S}(u_t). \tag{1}$$

The functional $\mathcal{S}$ describes how much energy or entropy can be dissipated or produced while the system goes from one state to the other. The linear operator $K(u)$ is symmetric and positive semi-definite and gives the dissipation mechanism due to the physical effects. We call $\mathcal{S}$ and K the *gradient system* that induces the evolution equation as in (1). In the cases that we consider, $\mathcal{S}$ will be the relative entropy

$$\mathcal{S}(u) := \int u(\mathrm{d}x) \log \frac{\mathrm{d}u}{\mathrm{d}w}(x), \qquad \text{or} \qquad \mathcal{S}(u) := \sum_x u_x \log \frac{u_x}{w_x}, \tag{2}$$

on a continuous or a discrete space, respectively. Here, w is a reference measure, which is typically the invariant measure for the evolution equation. The relative entropy is then, up to the constant factor of temperature, equal to the free energy of the system.

In the most simple, finite-dimensional setting, the dissipation mechanism is inherited from the geometry of the Euclidean space $\mathbb{R}^d$. An evolution with a gradient system then can be written as the ordinary differential equation

$$\dot{u}_t = -\mathrm{grad}\,\mathcal{S}(u_t),$$

that is, the evolution follows the gradient, or the steepest descent of the entropy, towards the equilibrium state; see Figure 2. In that sense, the right-hand side in (1) can be interpreted as the Riemannian gradient of the functional $\mathcal{S}$ with respect to the metric tensor given by $K(u)^{-1}$.

Gradient systems received much attention after the important discovery by Otto and his coauthors in the late nineties that the Fokker–Planck equation

$$\dot{u}_t = \mathrm{div}(\nabla u_t + u_t \nabla V) \tag{3}$$

can be interpreted as the gradient flow of the relative entropy (2) (with reference measure $w(\mathrm{d}x) = \frac{1}{Z}\exp(-V(x))\mathrm{d}x$) in the space of probability measures equipped with the Wasserstein distance. Therefore, the Wasserstein distance gives rise to the dissipation mechanism:

$$K_{\mathrm{Wass}}(u)\xi = -\mathrm{div}(u\nabla\xi). \tag{4}$$

This reinterpretation connects partial differential equations to the theory of optimal transport and has opened the door for new treatments of more general diffusion equations.

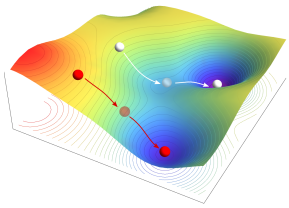

Fig. 2: *The evolution follows the steepest descent towards the equilibrium state*

We highlight that this gradient structure was generalized to reaction-diffusion systems with reversible mass-action kinetics by Mielke (2011).

The connection between gradient systems, the large-deviation principle, and the transitions that we prove lies in an alternative formulation of (1) in terms of the *dissipation potentials*

$$\Psi(u,s) := \frac{1}{2}\langle K(u)s, s\rangle \qquad \text{and} \qquad \Psi^*(u,\xi) = \sup_s \langle \xi, s\rangle - \Psi(u,s). \tag{5}$$

With these potentials, (1) can be rewritten as

$$\Psi(u_t, \dot{u}_t) + \Psi^*\big(u_t, -\mathrm{D}\mathcal{S}(u_t)\big) + \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(u_t) = 0. \tag{6}$$

This formulation is known as an *energy-dissipation balance*. In even more abstract settings, we allow for any nonnegative, convex dual potentials Ψ, Ψ^* in (6), yielding a so-called *generalized gradient system* if $\Psi^*(u,\cdot)$ is not quadratic.

(b) Entropy and the large-deviation principle

As briefly mentioned above, the notion of entropy in (2) is strongly related to stochastic fluctuations in an underlying particle system. To explain this idea, first consider a system with no dynamics involved, consisting of independent random particles that are identically distributed with given probability w. The corresponding empirical measure $\frac{1}{n}\sum_{k=1}^n \delta_{X_k}$, which is itself a random measure, then tells us how all particles are distributed over space. As a consequence of the law of large numbers, the empirical measure converges to w as the number of particles $n \to \infty$; see Figure 3. Although in the limit, any state different from w becomes impossible, we can say that for large n some states are more unlikely than others. These fluctuations are characterized by *Sanov's large-deviation principle* (1957):

$$\mathrm{Prob}\left(\frac{1}{n}\sum_{k=1}^n \delta_{X_k} \approx u\right) \sim \exp\big(-n\mathcal{S}(u)\big) \qquad \text{as } n \to \infty, \tag{7}$$

where $\mathcal{S}$ is the entropy (2). Since the probability to deviate from the state w is exponentially small with respect to n, these deviations are called *large deviations*.

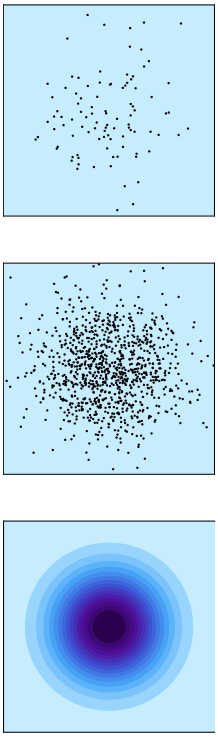

Fig. 3: *A limit as the number of particles goes to infinity*

(c) From Brownian motion to Wasserstein gradient structures

To mimic the ideas of Sanov's large-deviation principle (7) and to capture dynamic fluctuations, we consider a system of n particles with positions $X_k(t)$. Each particle moves independently according to a Brownian motion with a drift, i.e., their probabilities evolve according to the Fokker–Planck equation (3).

Again, as a consequence of the law of large numbers, the empirical process $t \mapsto \frac{1}{n}\sum_{k=1}^n \delta_{X_k(t)}$ converges to the solution to (3) as the number of particles goes to infinity. Under suitable initial conditions, a well-known result from large-deviations theory provides the equivalent of (7) for time-

dependent processes:

$$\mathrm{Prob}\Big(\Big(\frac{1}{n}\sum_{k=1}^{n}\delta_{X_k(t)}\Big)_{t=0}^{T}\approx u\Big)\sim\exp\Big(-n\int_0^T\mathcal{L}(u_t,\dot u_t)\,\mathrm{d}t\Big)\qquad\text{as } n\to\infty. \tag{8}$$

Here, all information about the stochastic fluctuations is encoded in $\mathcal{L}(u_t,\dot u_t)$, which is interpreted as a probabilistic cost to deviate from the limiting equation (3). Recent work, starting from [1], shows that this cost function can be directly linked to an energy-dissipation balance (6), in the following way:

$$\mathcal{L}(u_t,\dot u_t)=\frac{1}{4}\|\dot u_t-\Delta u_t\|^2_{H^{-1}(u_t)}=\frac{1}{4}\|\dot u_t\|^2_{H^{-1}(u_t)}+\|\tfrac{1}{2}\mathrm{D}\mathcal{S}\|^2_{H^1(u_t)}+\frac{\mathrm{d}}{\mathrm{d}t}\tfrac{1}{2}\mathcal{S}(u_t), \tag{9}$$

where $\mathcal{S}$ is again given by (2) with w being the Lebesgue measure. Formally, this relation means that the probabilistic cost of having stochastic fluctuations is exactly the entropy defect in the energy-dissipation balance (6). The resulting structure is the Wasserstein gradient structure in (4) driven by $\frac{1}{2}\mathcal{S}$.

(d) From Markov jump processes on discrete sets to generalized gradient systems

In our recent work [5], we move beyond this particular case of the Fokker–Planck equation and construct a general theory that connects large deviations of a very general class of systems to entropy-driven gradient systems, similar to (9). In particular, we use this theory to derive a previously unknown gradient structure for continuous-time, finite-state Markov chains.

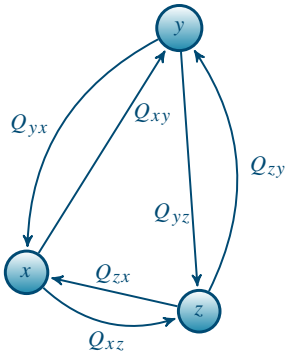

Fig. 4: *Markov chain on finite state space with transition rates Q_{xy}, etc.*

Markov chains are a fundamental tool in the modeling and simulation of certain processes in chemistry, physics, and biology. Prominent examples are the dynamical behavior of genes or molecules or the charge carrier transport in organic semiconductor devices. In the simplest case, one is interested in the time-continuous evolution of a stochastic particle on a finite state space satisfying the Markov property. Knowing the average waiting times at each state as well as the transition probabilities between each pair of states, we can write the evolution of the probabilities in the form of *Kolmogorov's forward equations*, i.e., a linear system of ordinary differential equations of the form

$$\dot u_t=Q^{\mathsf{T}}u_t. \tag{10}$$

Here, the vector u_t gives the probability of finding the particle in a certain state at time t if the initial probability distribution is u_0. Moreover, Q is a matrix whose components give the rates for a transition between states, i.e., Q_{xy} gives the rate for the transition from x to y; see Figure 4.

Analogously to the continuous case, we consider independent Markovian particles on the discrete state space with intensity matrix Q. By the law of large numbers, the empirical process $t\mapsto\frac{1}{n}\sum_{k=1}^{n}\delta_{X_k(t)}$ now converges in the many-particle limit to the system of the ordinary differential equations (10). For this transition we prove a large-deviation principle similar to (8), with some cost function $\mathcal{L}$.

Moreover, we show that in general, whenever the Markov chain satisfies detailed balance, then the large-deviation cost function $\mathcal{L}$ can be related to a generalized gradient system:

$$\mathcal{L}(u_t, \dot{u}_t) = \Psi_{\mathrm{gen}}(u_t, \dot{u}_t) + \Psi^*_{\mathrm{gen}}\big(u_t, -\mathrm{D}\tfrac{1}{2}\mathcal{S}(u_t)\big) + \frac{\mathrm{d}}{\mathrm{d}t}\tfrac{1}{2}\mathcal{S}(u_t), \tag{11}$$

where $\mathcal{S}$ is again the entropy (2) with respect to the invariant measure w, and the dual dissipation potential corresponding to the above large-deviation principle is given by

$$\Psi^*_{\mathrm{gen}}(u, \xi) = \frac{1}{2}\sum_{x,y}\sqrt{u_x u_y Q_{xy} Q_{yx}}\,\big(\cosh(\xi_x - \xi_y) - 1\big).$$

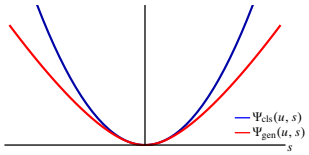

Fig. 5: *Comparison of Ψ_{gen} and Ψ_{cls} for a two-state Markov system at fixed u: large velocities s are penalized stronger by Ψ_{cls}*

Interestingly, the resulting potentials $\Psi_{\mathrm{gen}}, \Psi^*_{\mathrm{gen}}$ are not quadratic as opposed to the classical (i.e., non-generalized) gradient structure for Markov chains found in [3, 4]; see Figure 5 for a comparison. The latter gradient structure is again driven by the entropy $\mathcal{S}$, but the dual dissipation potential is of quadratic form, namely

$$\Psi^*_{\mathrm{cls}}(u, \xi) = \frac{1}{4}\sum_{\substack{x,y\\ Q_{xy}>0}} Q_{xy} w_x \frac{\frac{u_x}{w_x} - \frac{u_y}{w_y}}{\log\frac{u_x}{w_x} - \log\frac{u_y}{w_y}}(\xi_x - \xi_y)^2. \tag{12}$$

(e) From finite-dimensional to Wasserstein gradient systems

Using suitable discretization schemes for the Fokker–Planck equation in (3), we obtain a linear system of ordinary differential equations as in (10). Finite-volume methods for drift-diffusion, for example, provide numerical schemes with remarkable properties such as the exact conservation of mass and the local conservation of the numerical fluxes. This last feature makes the finite-volume method quite attractive for problems where the flux is of importance, such as in fluid mechanics, semiconductor device simulation, energy and mass transfer, etc.

It is known that finite-volume schemes can be interpreted as Markov chains on the discrete state space given by the spatial discretization. In particular, in this case similar gradient structures as in (12) can be stated, and it is natural to ask if the discrete-to-continuous passage can be established by using solely these structures; this is depicted as the right arrow in Figure 1. Recently, the limit passage was carried out by Maas and Gigli (2013) by proving the Gromov–Hausdorff convergence of the associated discrete dissipation distances. However, the proof relies on very strict conditions on the geometry of the discrete state space, namely equidistant meshes. In [2], we succeeded to establish the limit passage by using solely the involved gradient structures permitting more general discretizations. The key in this approach is to use the time-integrated version of the energy-dissipation balance (6). Using a notion of evolutionary Γ-convergence, we can pass to the limit and prove the integrated energy-dissipation formulation with respect to the Wasserstein structure in (4).

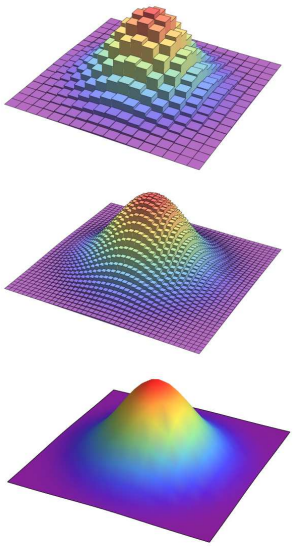

Fig. 6: *Equilibrium state in the limit of vanishing mesh size*

(f) Open questions

Although our recent work has shed some light upon the microscopic origin of entropy-driven systems, there are still many open questions that pose challenges for future research.

In particular, our general theory that connects gradient structures to large deviations is tailored to systems of independent particles, whereas little in this direction is known about interacting particles. This can be especially interesting for nonlinear reaction-diffusion equations, more general coagulation-fragmentation processes, as well as for diffusion processes with specific boundary conditions.

Another interesting question comes from the fact that there are now two different gradient structures available for Markov chains. The generalized structure is related to a system of independent particles; whether the classical structure is also related to some stochastic particle system remains an open question. The same question can be asked in greater generality: Given a gradient structure, can one always construct a suitable particle system whose large deviations relate to that structure?

With regard to our work on the vanishing mesh transition of the classical gradient structure, there still remain two important open questions. Firstly, it is not known whether, if one starts from the generalized gradient structure, the same transition can be made, and whether it yields the Wasserstein gradient structure in the limit. Secondly, how does the understanding of this limit passage in terms of gradient structures help to develop more efficient numerical schemes that respect the underlying geometric structure of the problem?

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2.4 Branching Random Walks in Random Environment

Onur Gün

Branching Random Walks in Random Environment (BRWRE) describe a system of particles diffusing in space, and at the same time randomly producing new particles (branching) according to space-dependent, time-independent rates that are themselves random. The space-dependent branching rates constitute a *random environment*, which is fixed throughout the evolution of the system. BRWRE is one of the fundamental models of reaction-diffusion systems in random media and has applications in various areas ranging from chemical engineering and biological evolution to population dynamics. Some important examples that can be modeled using BRWREs are chemical reactants diffusing in a medium with randomly scattered fixed catalysts, biological evolution on a rugged fitness landscape, and urban modeling with spatial randomness.

The Research Group *Interacting Random Systems* has started a program on BRWREs aiming at achieving new theoretical results and using them in biological applications, supported partially by the DFG Priority Program SPP 1590 *Probabilistic Structures in Evolution*.

A striking feature of these models is the competition between the diffusion part, forcing the particles to spread through the space, and the random environment of branching rates, creating regions of high production of particles. Our main goal is to achieve a complete understanding of this picture: For what kind of random environments are the particles, in the long run, concentrated in small islands of high branching rates, and how do the particles flow between these islands?

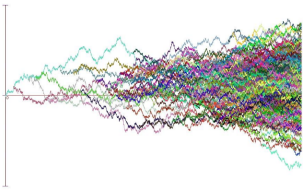

Fig. 1: *A 1-dimensional branching random walk*

A main aspect of our approach is to relate these questions to the first-order approximation in terms of the well-known *Parabolic Anderson Model (PAM)*, which has been intensively studied in the last 20 years. Recently, PAM and related phenomena of Anderson localization have found new applications in the theory of biological evolution. The two main driving forces of Darwinian evolution of living organisms are natural selection, which is given through a fitness function, and mutations, which are random errors in the copying of the genetic material upon reproduction. The PAM describes the evolution of asexually reproducing organisms (such as bacteria and viruses) in a space of either genotypes or phenotypes. The selection is directly related to the fitness of a given genotype or phenotype, which is proportional to its mean reproduction rate. Values of the fitness function for all the possible genetic variations form a fitness landscape. Since it is very difficult to evaluate fitness values, several models have been proposed. A rugged landscape, that is, a random uncorrelated fitness landscape, has received special attention. In this way, BRWRE is a model for Darwinian evolution: The rugged fitness landscape corresponds to the random environment of branching rates, and mutations to the diffusion of the particles. Localization is now related to the co-existence of several mutants of the fittest one, a phenomenon known as *quasispecies*.

BRWRE on $\mathbb{Z}^d$

We consider the BRWRE on the d-dimensional lattice $\mathbb{Z}^d$. The random environment is given by attaching independent, identically distributed (i.i.d.) positive numbers $\xi(x)$ to each lattice site x. The diffusion parameter is given by $\kappa > 0$. The evolution of the model is that of a continuous-time

Markov process and is described as follows. In a small time interval of length Δt, any particle at a site x

- produces a new particle at the same site with probability $\xi(x)\Delta t$ and
- moves to one of the neighboring sites with probability $\kappa\Delta t$.

For the interpretation of BRWRE on $\mathbb{Z}^d$ in terms of biological evolution we use [1]. $\mathbb{Z}^d$ represents the space of phenotypes: all the visible traits of a gene. We can think of each dimension of the lattice as a phenotypic property, e.g., height, weight, eye color. Naturally, the number of phenotypes needed to specify biological species is very large, ranging from 10^2 to 10^4. For the mutation process, we see that the errors happen as jumps to neighboring sites on $\mathbb{Z}^d$, e.g., the offspring of an individual can only be a little taller than its parent.

In order to analyze this model, we study the higher moments of the number of particles. Let $m_k(t,x)$ denote the expectation of the k-th power of the number of particles at space point x at time t, starting from one particle everywhere at time 0. The first-order approximation, i.e., the first moment m_1, satisfies the *heat equation with random potential*, also known as the *Parabolic Anderson Model (PAM)*,

$$\partial_t m_1(t,x) = \kappa\Delta m_1(t,x) + \xi(x)m_1(t,x), \quad t > 0, x \in \mathbb{Z}^d,$$

with the delocalized initial condition $m_1(0,x) \equiv 1$. Here, Δ is the discrete Laplacian, representing the diffusion. The key tool for studying the properties of m_1 is the *Feynman–Kac formula*, which expresses m_1 in terms of an expectation of the exponential integral of the simple random walk X on $\mathbb{Z}^d$ in the random potential:

$$m_1(t,x) = \mathbb{E}_x\left[\exp\left(\int_0^t \xi(X_s)\,\mathrm{d}s\right)\right],$$

where $\mathbb{E}_x$ denotes the expectation with respect to X that starts at x. In the terminology of branching processes, the Feynman–Kac formula is known as a *spine integral* of the branching system, namely, instead of taking the expectation over all the branching trees of the system, one distinguishes the trajectory of a certain particle, the spine, and carries out the integration over the spine. The Feynman–Kac formula is known as the *many-to-one lemma* in the branching processes community.

To evaluate the k-th moment, we use an extension of the spine techniques, namely, we use a multi-spine construction and a resulting many-to-few lemma. The multi-spine construction starts with a particle carrying k marks initially. This particle diffuses with a rate that depends on the potential at the location and on the number of marks it carries. It gives birth to a size-biased number of offspring, again depending on the potential at the splitting site. Upon a splitting event, marks are distributed among the offspring randomly.

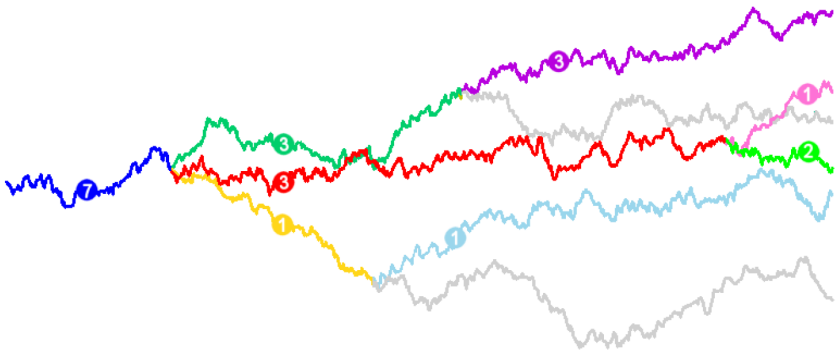

Fig. 2: *Multi-spine with 7 marks*

In [2], we carried out this analysis for potentials that are unbounded from above. We constructed the multi-spine system and obtained a Feynman–Kac-like formula for the k-th moment, m_k. For simplicity, we give the formula only for the second moment: $m_2(t,x) = m_1(t,x) + \widetilde{m}_2(t,x)$, where

$$\widetilde{m}_2(t,x) = \int_0^t \mathbb{E}_x\Big[\exp\Big\{\int_0^s \xi(X_r)\,\mathrm{d}r + \int_s^t \xi(X'_r)\,\mathrm{d}r + \int_s^t \xi(X''_r)\,\mathrm{d}r\Big\} 2\xi(X_s)\Big]\,\mathrm{d}s.$$

Here, s is the splitting time, and $(X_r)_{r\in[0,s]}$, $(X'_r)_{r\in[s,t]}$, and $(X''_r)_{r\in[s,t]}$ are independent simple random walks, with starting points $X_0 = x$, and $X'_s = X''_s = X_s$. This formula, although more involved than the original Feynman–Kac formula, is amenable to applying probabilistic tools. We used large deviations theory to obtain the large-time asymptotics of the k-th moments, revealing that they behave essentially like the k-th power of the first moment, the solution to the PAM. Together with a moment analysis, this result shows that the BRWRE exhibits the same localization properties as the PAM. Thus, this proves that even in the population models of evolutionary dynamics on the phenotype space described below, there is an extremal concentration of particles on the islands of high potentials.

Multi-type BRWRE

In a very recent work [3], we analyzed BRWRE with an additional structure of particles carrying types, the so-called *Multi-type Branching Random Walks in Random Environment*. In the context of biological applications, we think of different types as being different habitats, where the organisms live in. In this way, we add biological dispersion to the model.

The space of types is given by a finite, directed, connected graph $\mathcal{T}$. We assume that the space of genetic variations is the same for all types and is chosen as a finite, connected graph $\mathcal{X}$. To each type i and space point x, we attach a collection $\{F_x^{(i,j)} : j \in \mathcal{T}\}$ of i.i.d. random distributions on $\mathbb{N}$ and assume that these collections are i.i.d. in i and x. We describe the model as a discrete-time Markov chain whose dynamics is given by the following steps

- each particle of type i at site x produces a number of particles of type j at the same site x with distribution $F_x^{(i,j)}$, for all j,

- each particle at site x, independent of their types, moves to a neighboring site chosen uniformly at random.

The first part of the dynamics can be seen as the organisms moving between different habitats via reproduction, and the second part corresponds to mutations once again.

We study this model in an annealed sense, that is, averaged over the random environment. We denote by $\langle\rangle$ the corresponding expectation and by $\xi_x^{(i,j)}$ the first moment (mean) of $F_x^{(i,j)}$. The induced distribution of $F_x^{(i,j)}$ is assumed to be Weibull with parameter $1/\rho_{ij}$. For fixed environment, we denote by $m(n,i,x)$ the expectation of the number of particles of type i located at x at time n. We describe the annealed moments $\langle m(n,i,x)\rangle$ by a two-levels variational problem as follows

$$\langle m(n,i,x)\rangle = \exp\Big(\lambda(\rho)n\log n - n\chi(\rho) + o(n)\Big), \quad \text{as } n\to\infty.$$

Here, the leading term $\lambda(\rho)$ describes the main particle flow in type space, i.e., the trajectories of the types (neglecting their genetic evolution) of the branching particles that give the main contribution to the moments. The second-order term $\chi(\rho)$ gives a finer description of these trajectories, involving a balance criterion between the mutation (entropy) and fitness (energy).

BRWRE for molecular evolution on rugged fitness landscapes

Finally, we mention a current research project together with Luca Avena, a post-doc of the Research Group *Interacting Random Systems* supported by the above-mentioned SPP project. We study the BRWRE for the molecular evolution in the context of quasispecies theory on rugged fitness landscapes.

On the molecular level, the genotype of an organism is encoded as a finite sequence $\sigma = (\sigma_1, \dots, \sigma_N)$, where the entries σ_i belong to a finite alphabet. For example, for DNA this alphabet is that of nucleotides $\{A, C, G, T\}$, and for proteins, the list of 20 amino acids. It is always assumed that the sequence length N is fixed. For simplicity, we use an alphabet with two letters, 0 and 1. Hence, the genome, the set of all genotypes, is the N-dimensional hypercube $\mathcal{S}_N = \{0,1\}^N$. The size of $\mathcal{S}_N$ is $L = 2^N$, and we label genotypes by an integer $i = 1, \dots, L$.

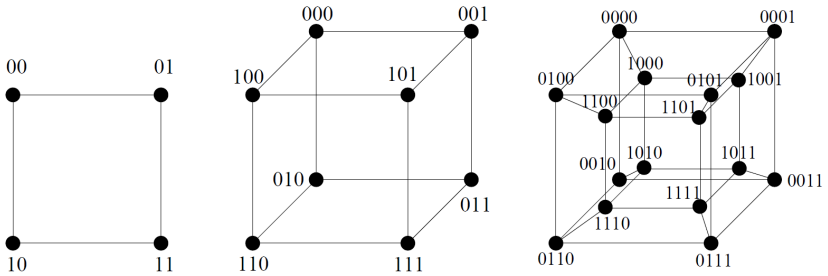

Fig. 3: *Hypercubes with dimension 2, 3, and 4*

The mutation chain is given by switching a uniformly chosen letter with rate κ. Usually, nothing is known about the values of a fitness landscape, and several models have been proposed in the biology literature. Recently, rugged landscapes, that is, a random fitness function, gained particular

attention, and we follow this approach. Our choice of the landscape is the *Random Energy Model (REM)*, which is borrowed from spin glass theory. We choose the fitness landscape $\{\xi(\sigma)\colon \sigma \in \mathcal{S}_N\}$ as an i.i.d. sequence of normal random variables with mean 0 and variance N. We denote by $x(t,i)$ the expectation of the number of particles with label i at time t. Spectral theory yields a limiting frequency of i-labeled particles, i.e., the limit $z(i) = \lim_{t\to\infty} x(t,i)/\sum_j x(t,j)$.

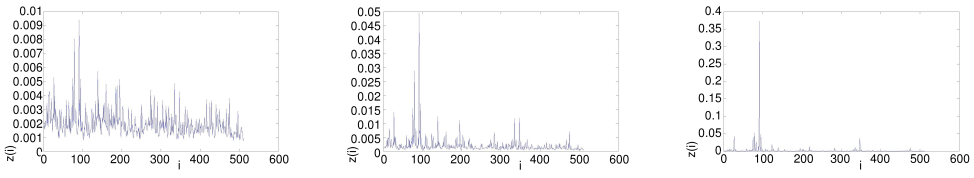

Fig. 4: *The frequencies $z(i)$ for genome length $N = 9$ for 3 different mutation rates κ. On the left: $\kappa = 1.2$, in the middle: $\kappa = 0.8$, and on the right: $\kappa = 0.4$.*

As seen in the numerical simulation in Figure 4, as the mutation rate decreases, the frequencies create peaks, similarly to the phase transition seen in the REM. Below a critical mutation rate, as the volume diverges, the best fit genome should dominate the population. On the other hand, above the critical rate, all possible genome sequences start to emerge. Our first goal is to prove and to quantify this phase transition using probabilistic tools via the Feynman–Kac formula and extreme value analysis.

Next, we will investigate intermediate time scales, in comparison to the mesoscopic time scales considered in the dynamics of disordered systems. We expect to find, depending on the time scale, a critical mutation rate below which there is a random hopping between local maximum fitness values. This behavior resembles very much the metastability phenomena seen in the dynamics of disordered systems.

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2.5 TetGen, a Delaunay-based Quality Tetrahedral Mesh Generator

Hang Si

Background and motivation

A mesh (or synonymously called *grid*) is a discrete representation of a continuous space. It is the form that can be automatically processed by computers. Therefore, it can be found in numerous applications, like visualization, image and geometry processing, numerical simulation, and so on. Mesh generation refers to the practice of generating a mesh that approximates a geometric domain. It is highly interdisciplinary, combining topics from mathematics, computer science, and engineering. The meshes should be created automatically, by algorithms and software, rather than by the end users of the meshes themselves.

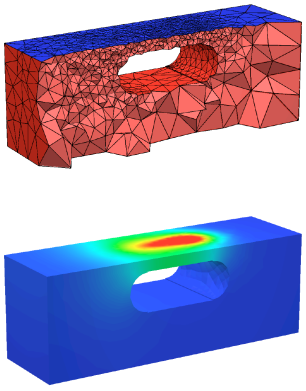

Fig. 1: *An adaptive tetrahedral mesh (top) and the calculated numerical solution (bottom) of a heat conduction problem*

A tetrahedral mesh is a three-dimensional unstructured grid that partitions a three-dimensional domain into simplices. This type of partition has many favorable properties. For example, it can be used for domains with arbitrarily complicated geometry, it can be easily locally refined and coarsened (with no hanging nodes), and it can be created fully automatically.

The development of TetGen is mainly motivated by the numerical solution of partial differential equations (PDEs) using, e.g., finite element and finite volume methods. An example is shown in Figure 1. The quality of the mesh tremendously affects the accuracy and convergence of the numerical solution. The generation of a tetrahedral mesh with the desired mesh quality is a complicated problem, both in theory and practice.

Technologies for mesh generation have been greatly advanced in the recent three decades. Early (before 2000) tetrahedral mesh generation methods are comprehensively surveyed in the book [5]. Some of these methods have been transferred into codes. However, a major problem in most of the early methods is the lack of theoretical background. As the 3D geometries that the users wish to process become more and more complicated, these methods may be either not suitable or can easily fail. In many engineering applications, the robustness of the codes is a crucial issue.

The problem of tetrahedral mesh generation has been explored in theoretical studies since about the mid-1990's. Since then, methods with theoretical guarantees have been developed; see [1]. However, these methods still suffer many theoretical limitations. They can only handle certain classes of three-dimensional geometries, and their robustness and speed do not meet the requirements of many engineering applications. Now it has been commonly acknowledged that the construction of robust and efficient mesh generation methods can only be achieved through algorithms that have a solid theoretical justification and practical heuristics. It is this principle that TetGen faithfully follows.

The original development of TetGen (from 2000 to 2001) was largely inspired by the program `Triangle` [2], which is a two-dimensional quality triangular mesh generator, and aimed to ex-

tend it into three dimensions. However, tetrahedral mesh generation is challenged by many theoretical and practical issues. The initial version of TetGen was neither reliable nor efficient.

Since 2002, TetGen has been supported by WIAS and has been continuously developed to date. The goal of TetGen is two-fold: First, it is a research project aimed to investigate the underlying mathematical problems and to develop innovative algorithms for mesh generation; second, it provides a robust, efficient, and easy-to-use software to generate quality tetrahedral meshes for various engineering applications. TetGen is available under the GNU Public License through http://www.tetgen.org.

The way of combining research and applications has proved its worth. The algorithms developed in the current version of TetGen are theoretically correct and practically efficient. The robustness of TetGen is very much improved. Today, TetGen is used worldwide by people from universities, research labs, and scientific institutions. It has been applied in various application areas and integrated in several commercial software packages.

The methodology of TetGen

The methodology of TetGen follows the classical boundary-constrained methods. This is the most efficient way to obtain a quality tetrahedral mesh. To overcome the main difficulty of boundary conformity and boundary recovery, new algorithms were developed. Moreover, TetGen provides more flexibility in handling domain boundary. The input domain boundary mesh can either be entirely preserved or subdivided into a refined boundary mesh.

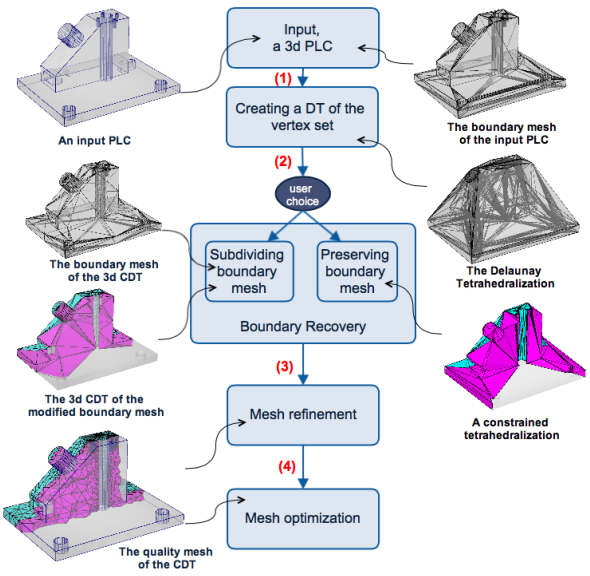

Fig. 2: *The pipeline of the mesh generation process of TetGen*

Figure 2 shows the pipeline of the mesh generation process in TetGen. A three-dimensional input domain is given, described by a piecewise linear complex (PLC), i.e., its boundary consists of a set of vertices, segments, and facets. A quality tetrahedral mesh of this PLC is generated in four steps:

(1) **Delaunay tetrahedralization**. In this step, only the input vertices of the PLC are considered. It constructs a Delaunay tetrahedralization (DT) of the set of vertices.

(2) **Boundary recovery**. In this step, the set of segments and facets of the PLC are considered. A domain boundary mesh is first constructed. It contains the set of segments and subfaces (which are triangles on facets of the PLC). Starting from the DT constructed in step (1), the segments and subfaces are recovered (incrementally). Depending on the user-specified choice, they are either entirely recovered or subdivided into smaller elements.

(3) **Mesh refinement**. In this step, the mesh quality is considered. New vertices are created and inserted into the tetrahedralization obtained in step (2) in order to create a quality mesh based on a set of user-specified mesh quality criteria. Depending on the user choice, the domain boundary mesh can either be further refined or remain unmodified.

(4) **Mesh optimization**. In this step, the mesh quality is further improved by using a set of local mesh operations.

Each of the above steps has its own problems and needs to be accomplished by corresponding algorithms. In the following, we give a brief description of the problems and solutions of TetGen.

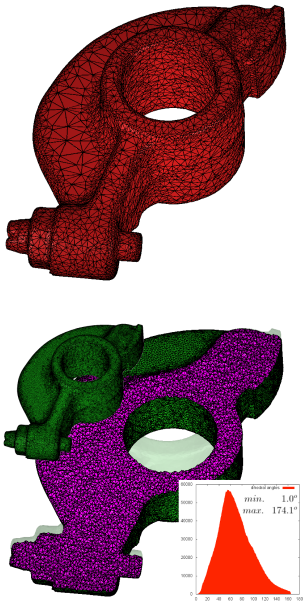

Fig. 3: *Top: the input* `rocker-arm` *(*10, 044 *vertices,* 20, 088 *triangles). Bottom: the generated tetrahedral mesh and the mesh quality plot (*136, 729 *vertices,* 622, 375 *tets,* 6.8 *sec.).*

Delaunay tetrahedralization. The structure of a Delaunay tetrahedralization is well studied. Optimal algorithms are proposed. The problem here is how to achieve a robust and efficient implementation.

TetGen implemented two incremental algorithms, the Bowyer–Watson and the randomized flip algorithms. Here, the key operations are point location and point insertion. TetGen implemented an efficient vertex insertion algorithm based on the Bowyer–Watson algorithm. For large data sets, the efficiency of incremental algorithms depends on the order of point insertion. TetGen first sorts the points through a spatial point sorting scheme. Inserting points based on this order, each point can be located efficiently (in nearly constant time). The robustness of the implementation is achieved by using filtered exact geometric predicates.

Boundary recovery. One of the fundamental difficulties in boundary recovery is to preserve an arbitrary constraint (an edge or a triangle) in a tetrahedral mesh. It is ubiquitously needed in tetrahedral meshing. Recall that in two space dimensions, an input edge can always be enforced into a triangulation by a sequence of edge flips. Moreover, it does not need extra points. But this is not always possible in three space dimensions. It is well known that some additional vertices, so-called *Steiner points*, may be needed. However, many questions, like the optimal locations and the minimum number of Steiner points, are unsolved. In practice, flips in 3D usually work efficiently in recovering a constraint, but there is no guarantee of success in 3D (a major open problem).

It turns out that a necessary key operation is to remove an edge from a tetrahedral mesh. Many other mesh operations, like edge recovery, face recovery, and vertex removal, can be accomplished by a sequence of edge removal operations. So far, no theoretical solution is available. A practical edge removal operation should be able to efficiently remove an edge if it can be removed without using extra points. In TetGen, a new edge removal algorithm was developed for this purpose.

Another difficulty is to generate a tetrahedral mesh that contains the domain boundary mesh. It is necessary to add interior Steiner points. The challenge is to design a robust and efficient algorithm that is able to process inputs of arbitrary complexity and to optimally place interior Steiner points when they are necessary. TetGen utilizes a flip-based algorithm to recover the constraints. It uses a new edge removal operation. Numerical studies show that this recovery algorithm introduces a relatively small number of Steiner points compared with those reported in the literature.

When the domain boundary mesh is allowed to be subdivided, a distinguished solution proposed by TetGen is to maintain a constrained Delaunay tetrahedralization (CDT), which is a variant of Delaunay tetrahedralization and is able to preserve constraints. Provable and efficient algorithms for constructing and refining CDTs are implemented. Robustness of the CDT generation is fully guaranteed [4].

Quality mesh generation.

A central question in quality mesh generation is how to efficiently place an appropriate number of Steiner points inside the mesh domain such that they form a good quality tetrahedral mesh. Various mesh refinement and mesh improvement techniques were proposed. However, there is no theory-based guarantee of some useful mesh quality measures, such as the minimum and maximum dihedral angles. In practice, it is extremely hard to completely remove some very badly shaped tetrahedra, so-called *slivers* (which contain nearly 0^o or 180^o dihedral angles), located near the preserved constraints.

TetGen uses the Delaunay refinement technique to generate quality tetrahedral meshes. It places Steiner points in locally optimal locations, and it guarantees that there are no small face angles (but not dihedral angles) in every resulting tetrahedron. However, Delaunay refinement is far from practical. It may produce slivers, and it may not terminate if there are *sharp features* that form acute angles or dihedral angles between constraints. TetGen maintains a CDT during the Delaunay refinement. The sharp features are protected, and the termination is guaranteed. The same guarantees of Delaunay refinement hold on the tetrahedra in the bulk of the mesh domain. Some badly shaped tetrahedra may remain. They are all located (within a bounded distance) near sharp features. The algorithm is described in detail in [3]. After the mesh refinement, TetGen uses a mesh improvement phase to remove slivers. Numerical studies show that these procedures of TetGen usually generate excellent quality meshes (with good dihedral angles) for inputs with no small angles. It is efficient in practice.

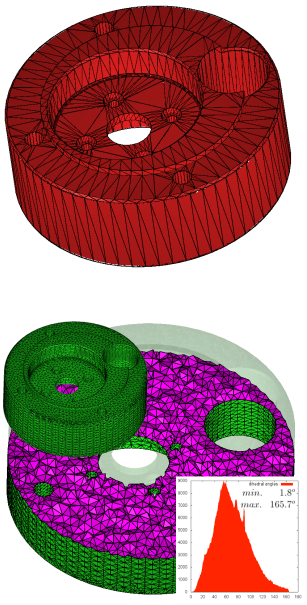

Fig. 4: *Top: the input* `couplingdown` *(*1, 841 *vertices,* 3714 *triangles). Bottom: the generated tetrahedral mesh and the mesh quality plot (*22, 952 *vertices,* 96, 796 *tets,* 1.0 *sec.).*

Examples

In this section, some examples regarding the behavior and efficiency of the implemented algorithms in TetGen are reported. These experiments were performed using TetGen version 1.5 (pre-release version, March 2013).

We selected three inputs. They are obtained from the AIM@SHAPE Repository. Two of them (Figures 3 and 4) are formed by relatively coarse surface meshes. The other example (Figure 5) has a relatively good quality surface mesh. For all of these examples, TetGen efficiently produced tetrahedral meshes with a good mesh quality.

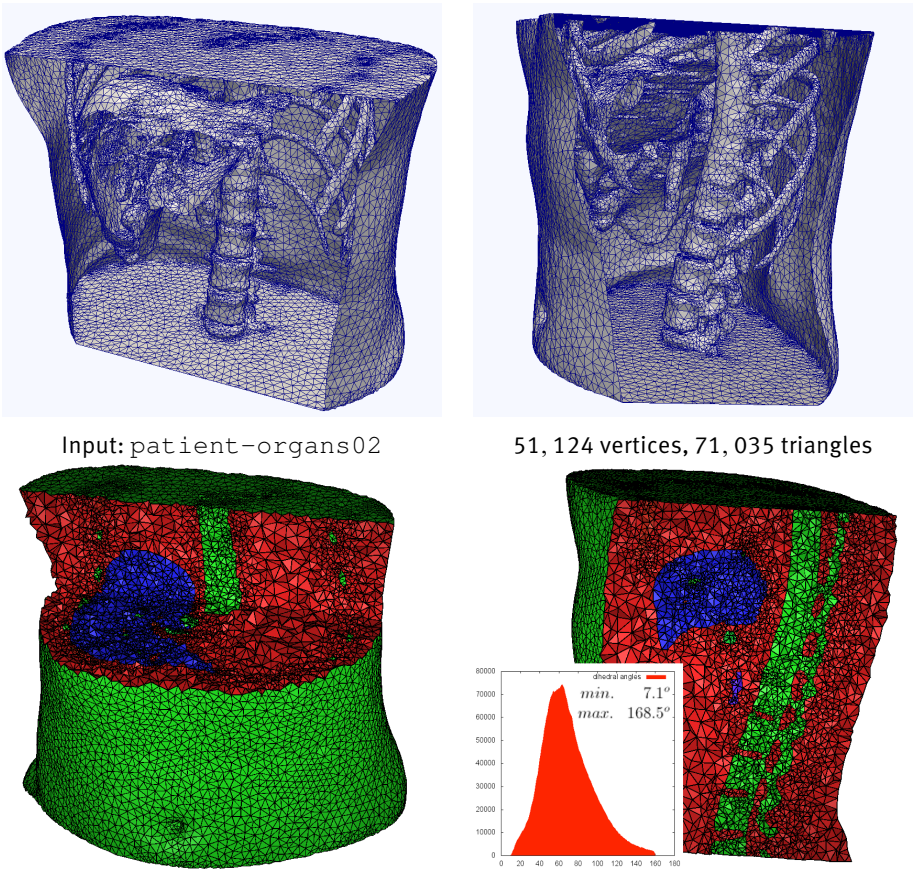

Fig. 5: *Top: the input surface mesh. Bottom: the output mesh of TetGen.*

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2.6 Crucial Revisions of Electrochemical Modeling

Wolfgang Dreyer, Clemens Guhlke, Manuel Landstorfer, and Rüdiger Müller

Historical background. The laws of nature are represented by universal *equations of balance* and by material-dependent *constitutive equations* describing the material at hand. Within thermodynamics, this rational approach was started in 1940 by Carl Eckart. In the following years, the theory was completed by Josef Meixner. In his seminal 1943 paper *"Zur Thermodynamik der irreversiblen Prozesse in Gasen mit chemisch reagierenden, dissoziierenden und anregbaren Komponenten"*, he studied the phenomenological coefficients and equipped them with Onsager–Casimir reciprocal relations [3]. Finally in 1963, Sybren Ruurds de Groot and Paul Mazur reached a certain completion when putting everything together in the fundamental monograph *"Non-equilibrium thermodynamics"*.

Fig. 1: *Carl Eckart (1902–1973)*

Fig. 2: *Josef Meixner (1908–1994)*

The mathematical modeling of electrochemical phenomena, particularly in electrolytes, started already fifty years earlier, namely within the last ten years of the nineteenth century. In that time, Walter Nernst and Max Planck laid down what nowadays is called the *Nernst–Planck model*. Due to the missing non-equilibrium thermodynamics, the Nernst–Planck model exhibits some serious inherent deficiencies. However, it is still often considered as the relevant theoretical basis and widely used.

For two years the Leibniz Group *Mathematical Models for Lithium-Ion Batteries* at WIAS has revisited the old Nernst–Planck model and has removed its deficiencies by a rational, thermodynamically consistent coupling between mechanics and diffusion. By the method of formal asymptotic expansion, results for practical applications of the theory are derived. To keep this representation simple, we do not consider temperature variations, polarization, viscosity, and chemical reactions in detail and refer to [4, 5, 6].

Thermodynamic state of electrolytes. A liquid electrolyte is a chemically reacting mixture consisting of N constituents. Their particles have atomic masses $(m_\alpha)_{\alpha=1,2,\dots,N}$ and may be carriers of charges $(z_\alpha e_0)_{\alpha=1,2,\dots,N}$. The constant e_0 is the elementary charge, and the z_α denote positive or negative integers including the value zero. The constituent with the index N is the neutral solvent, i.e., $z_N = 0$.

At any time $t \geq 0$, the thermodynamic state of a mixture in a region $\Omega \subset \mathbb{R}^3$ is described by N particle densities $(n_\alpha)_{\alpha=1,2,\dots,N}$, the barycentric velocity $\mathbf{v}$, and the temperature T of the mixture and by the electric field $\mathbf{E}$. These quantities may be functions of time $t \geq 0$ and space $\mathbf{x} = (x^i)_{i=1,2,3}$.

Equations of balance for mass and momentum. The evolution of the thermodynamic state is determined by a coupled system of partial differential equations. A part of this system are the equations of balance for the N partial mass densities and for the barycentric momentum:

$$\partial_t m_\alpha n_\alpha + \operatorname{div}(m_\alpha n_\alpha \mathbf{v}_\alpha) = r_\alpha, \qquad \alpha = 1, 2, \dots, N \tag{1}$$

$$\partial_t \rho \mathbf{v} + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v} - \sigma) = \mathbf{k}. \tag{2}$$

Besides the variables from the last paragraph, there occur new quantities here: $\mathbf{v}_\alpha$ – partial velocities, r_α – mass productions, σ – stress, and $\mathbf{k}$ – Lorentz force density. These quantities must be related to the variables by constitutive equations. However, their generality is restricted because there are some important constraints. (i) The local conservation of total mass requires $\sum_{\alpha=1}^{N} r_\alpha = 0$. (ii) The barycentric velocities follow from the partial velocities by $\rho\mathbf{v} = \sum_{\alpha=1}^{N} m_\alpha n_\alpha \mathbf{v}_\alpha$ so that the mass density of the mixture $\rho = \sum_{\alpha=1}^{N} m_\alpha n_\alpha$ satisfies the conservation law for the total mass $\partial_t \rho + \operatorname{div}(\rho\mathbf{v}) = 0$. (iii) The partial velocities are substituted by the diffusion fluxes, which are defined by $\mathbf{J}_\alpha = m_\alpha n_\alpha(\mathbf{v}_\alpha - \mathbf{v})$. Consequently, there are only $N-1$ independent diffusion fluxes, because we have the constraint $\sum_{\alpha=1}^{N} \mathbf{J}_\alpha = 0$. Thus, the N partial mass balances split into the mass balance for the mixture and $N-1$ so-called *diffusion equations*,

$$\partial_t \rho + \operatorname{div}(\rho\mathbf{v}) = 0, \qquad \partial_t m_\alpha n_\alpha + \operatorname{div}(m_\alpha n_\alpha \mathbf{v} + \mathbf{J}_\alpha) = r_\alpha, \quad \alpha = 1, 2, ..., N-1\,. \tag{3}$$

The quasi-static setting of Maxwell's equations. The full system of Maxwell's equations is considerably reduced if magnetic fields are ignored so that the electric field is given by a potential $\mathbf{E} = -\nabla\varphi$. Then the equation determining the electric field is $\varepsilon_0 \operatorname{div}(\mathbf{E}) = n^{\mathrm{e}}$, where n^{e} is the electric charge density that, for simplicity, is represented here only by the density of free charges $n^{\mathrm{e}} = n^{\mathrm{F}} = \sum_{\alpha=1}^{N} z_\alpha e_0 n_\alpha$. In this setting, the Lorentz force in the momentum balance is simply given by $\mathbf{k} = -n^{\mathrm{F}}\nabla\varphi$.

Deficiencies of the Nernst–Planck model and their removal

Fig. 3: *Walther Nernst (1864–1941)*

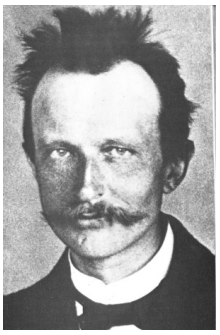

Fig. 4: *Max Planck (1858–1947)*

The essential flaws of the Nernst–Planck model are

- local electro-neutrality in the whole electrolyte
- the pressure due to the constituents of the electrolyte is ignored
- the diffusion fluxes do not reflect the interaction of anions and cations with the solvent

To fully recognize the content of these assumptions, let us consider more details.

Local electro-neutrality. Walther Nernst argues in his paper *"Die elektromotorische Wirksamkeit der Ionen"* from 1889 *"...da im Innern der Lösungen keine freie Elektrizität (...) bestehen kann, so muss die Bedingung* $n^{\mathrm{F}} = 0$ *erfüllt sein."* Max Planck agrees with Nernst. One year later in *"Über die Erregung von Electrizität und Wärme in Electrolyten"*, Planck gives an explanation by means of the Poisson equation that reads in dimensionless form

$$\lambda^2 \Delta\varphi = -n^{\mathrm{F}}. \tag{4}$$

Here, λ is a small dimensionless parameter that defines a characteristic length scale $\lambda L_0 = \sqrt{(kT\varepsilon_0/e_0^2 n_0)}$. L_0 may be the distance between two electrodes in the electrolyte, and n_0 is related to the overall density of the anions and cations. For $n_0 = 0.1$ mole per liter we have $\lambda L_0 = 1.5\ 10^{-10} m$, which leads Planck to argue that (4) cannot be used to determine the potential φ. Moreover, he concludes that the only information attained from (4) is $n^{\mathrm{F}} = 0$. However, both statements are only true if $\Delta\varphi$ is of order $\mathcal{O}(1)$. In fact, this property is met in the bulk region

of the electrolyte, but not in the vicinity of the electrode-electrolyte interfaces where boundary layers develop with $\Delta\varphi = \mathcal{O}(1/\lambda^2)$. The extension of the model by using (4) instead of $n^{\mathrm{F}} = 0$ is called *Poisson–Nernst–Planck model*.

Pressure. There is a further important law of nature that is ignored by Nernst and Planck, and it is usually ignored even nowadays. This is the conservation law of momentum. For simplicity of the illustration, let us consider the equilibrium case and exclusively electric forces. Then the momentum balance reads

$$\nabla p = -n^{\mathrm{F}} \nabla\varphi, \tag{5}$$

where p denotes the local material pressure of the electrolyte. In the elastic case, the pressure is given by a constitutive function of the form $p = \hat{p}(T, n_1, \ldots n_N, \mathbf{E})$. If the local charge neutrality (1) were satisfied everywhere, the pressure would be a constant in the whole electrolyte and equal to the outer pressure $p_0 \approx 1$ bar. However, in the vicinity of an electrode-electrolyte interface, we have $n^{\mathrm{F}} \neq 0$. Combining (4) and (5) then yields

$$\operatorname{div}(\Sigma) = 0 \quad \text{with} \quad \Sigma = -\big(p + \tfrac{1}{2}\lambda^2 |\nabla\varphi|^2\big)\mathbf{1} + \lambda^2 \nabla\varphi \otimes \nabla\varphi. \tag{6}$$

The quantity Σ is the total stress of the electrolyte. Near to the boundary, the gradients of the electric potential may become very large and must be counterbalanced by the material pressure because at the boundary with normal ν, we obviously have $\Sigma \cdot \nu = -p_0 \nu$.

Ion-solvent interaction. The third wrong ingredient of the Nernst–Planck model is the ignorance of the solvent, leading to a variety of subtle implications. These arise due to the special form of the $N-1$ diffusion fluxes for the $N-1$ dissolved constituents. The Nernst–Planck model proposes

$$\mathbf{J}_\alpha^{\mathrm{NP}} = -M_\alpha^{\mathrm{NP}} \Big(\nabla n_\alpha + \frac{z_\alpha e_0}{kT} n_\alpha \nabla\varphi \Big), \tag{7}$$

where $M_\alpha^{\mathrm{NP}} > 0$ are phenomenological coefficients. On the other hand, the general form of thermodynamically consistent diffusion fluxes is represented by

$$\mathbf{J}_\alpha = -\sum_{\beta=1}^{N-1} M_{\alpha\beta} \left(\nabla\Big(\frac{\mu_\beta - \mu_N}{T}\Big) + \frac{1}{T}\Big(\frac{z_\beta}{m_\beta} - \frac{z_N}{m_N}\Big)\nabla\varphi \right). \tag{8}$$

The $M_{\alpha\beta}$ are the phenomenological coefficients of the symmetric and positive definite mobility matrix. The quantities μ_α are the chemical potentials. They are derivatives of the free energy density $\rho\psi$, which is the central constitutive quantity of continuum thermodynamics. In the present case, we have $\psi = \hat{\psi}(T, n_1, \ldots, n_N, \mathbf{E})$. Then the chemical potentials are defined by $\mu_\alpha = \partial\rho\psi/\partial m_\alpha n_\alpha$. The appearance of the differences $\mu_\beta - \mu_N$ describes the interaction of the constituent β with the solvent indexed by N and with $z_N = 0$. These differences appear in the diffusion fluxes due to the constraint $\mathbf{J}_N = -\sum_{\alpha=1}^{N-1} \mathbf{J}_\alpha$. For a comparison of the two diffusion laws we consider the most simple constitutive model for the electrolyte. It is the so-called *incompressible simple mixture*, which Nernst and Planck presumably might have had in mind when postulating their fluxes (7). With the constant reference values for the chemical potentials μ_α^{R}, the pressure p^{R}, and the total particle densities n^{R}, the chemical potentials for an incompressible

simple mixture read

$$\mu_\alpha = \mu_\alpha^{\mathrm{R}} + \frac{1}{m_\alpha n^{\mathrm{R}}}(p - p^{\mathrm{R}}) + \frac{kT}{m_\alpha}\log\left(\frac{n_\alpha}{n^{\mathrm{R}}}\right). \tag{9}$$

Now we ignore cross diffusion and assume that the diagonal mobilities are proportional to the particle densities, i.e., $M_{\alpha\alpha} = (k^{-1} m_\alpha M_\alpha^{\mathrm{NP}}) n_\alpha$. Then the thermodynamically correct fluxes (8) are given by

$$\mathbf{J}_\alpha = -M_\alpha^{\mathrm{NP}}\left(\nabla n_\alpha + \frac{z_\alpha e_0}{kT} n_\alpha \nabla\varphi - \frac{m_\alpha n_\alpha}{m_N n_N}\nabla n_N + \frac{n_\alpha}{kT n^{\mathrm{R}}}\left(1 - \frac{m_\alpha}{m_N}\right)\nabla p\right). \tag{10}$$

Hence, only the first two terms of the correct fluxes agree with the Nernst–Planck fluxes (7).

Implications of the extended model

In the following, three examples are given to illustrate the large importance of the missing phenomena in the Nernst–Planck model.

Pressure dependence of mole fractions. Between two electrodes with given potentials φ_{L} and φ_{R} , we consider an electrolyte in equilibrium. Let the electrolyte consist of three constituents: positively charged cations C, negatively charged anions A, and the neutral solvent S. The corresponding mole fractions $y_\alpha = n_\alpha / n^{\mathrm{R}}$ are y_{A} , y_{C} , and y_{S} . The domain Ω can be decomposed into the boundary layers and the bulk part where all quantities turn out to be constant. It is necessary to include the solvent into the model since its mole fraction is not constant in the layers, see Figure 5. In the extended model, the pressure restricts the mole fraction y_A, y_C of the ions to the physical range $0 \le y_\alpha \le 1$, contrary to the classical Poisson–Nernst–Planck model without the pressure correction, where the mole fractions leave the physical range.

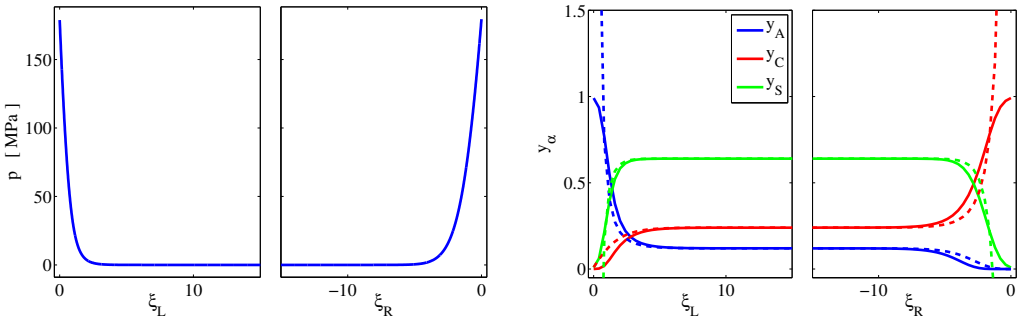

Fig. 5: *Left: high material pressure in the boundary layers. Right: comparison of mole fractions computed by the new proposed model (solid) and with the classical Poisson–Nernst–Planck model (dashed).*

Boundary layers. The new electrolyte model allows to resolve the boundary layer. Moreover, by applying the method of formal asymptotic analysis, it is now possible to derive a simple reduced model for the bulk region that is supplemented by modified boundary conditions arising from an exploitation of the full model within the boundary layer. The strategy is illustrated in Figure 6 for the variation of a typical variable u near to the actual interface between the electrolyte and a solid metallic electrode.

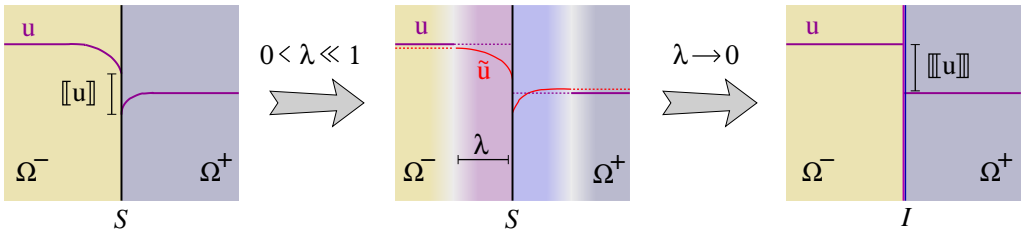

Fig. 6: The sharp limit $\lambda \to 0$ of the boundary layer changes the actual interface S into the interface I with new boundary conditions

The domains of the electrode, the electrolyte, and their (actual) interface are indicated by Ω^+, Ω^-, and S, respectively. Figure 6$_{\text{left}}$ shows the three domains. From left to right, we have the electrode (yellow), the interface (black solid line), and the electrolyte (purple). In the bulk domains left and right to the interface, we observe the indicated variation of u. Across the interface S, the field u has a discontinuity described by the double bracket $[\![u]\!]$. Its determination relies mainly on jump conditions that are established and exploited in [5]. The parameter λL_0 with $0 < \lambda \ll 1$ from above implies that the variation of u is restricted to a small neighborhood of the interface S. In other words, the parameter λ creates boundary layers left and right to S. This fact is indicated in Figure 6$_{\text{middle}}$. The description of the boundary layers in the limit $\lambda \to 0$ leads to a new interface I with a new jump that we denote by the triple bracket $[\![\![u]\!]\!]$. On the scale of the limiting case, the original interface S with its discontinuity $[\![u]\!]$ is not resolved anymore as it is indicated in Figure 6$_{\text{right}}$.

Among the results of the mathematical limit $\lambda \to 0$, we have in the bulk regions $\Omega^\pm$ local charge neutrality, which was postulated in the Nernst–Planck model in the whole domain. Moreover, the limit $\lambda \to 0$ uniquely determines new jump conditions (e.g., $[[[u]]]$) at the interface I, Figure 6$_{\text{right}}$, from the original jump conditions (e.g., $[[u]]$) at the interface S, Figure 6$_{\text{left}}$, and this result is the essential gain of our approach. In particular, the new jump conditions represent the basis for a rational derivation of the so-called *Butler–Volmer equations* describing interfacial electrochemical reactions.

Stern layer revisited. The failure of the Nernst–Planck model to adequately describe the phenomena within the boundary layers has lead many authors to introduce here artificial constructs like *molecular capacitors*. The most relevant version is due to Otto Stern who constructed in 1924 a double layer consisting of a serial connection of two layers. Stern first assumed an adsorption layer with a linear potential drop toward the electrolyte at the interface of the electrode and the electrolyte, Figure 7. Nowadays, the adsorption layer is called *Stern layer*. That layer is followed by a so-called *diffuse layer* with exponential decay. The ad hoc decomposition of the boundary layer into Stern layer and diffuse layer is necessary in the Poisson–Nernst–Planck setting: If we assume local equilibrium in both layers, which is a good approximation, the Nernst–Planck model implies that the charge density n^{F} becomes a function of the electric potential φ alone, and the equation for the potential within the layer is $\lambda^2 \Delta\varphi = -n^{\mathrm{F}}(\varphi)$, which has been in strong disagreement with experimental data for over 70 years.

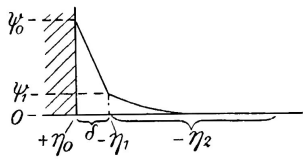

Fig. 7: The Stern layer from the famous 1924 paper of Otto Stern

In the same context, our improved electrolyte model implies that the charge density is a function of the electric potential and (!) of the pressure. Thus, here we have the coupled system

$$\lambda^2 \Delta\varphi = -n^{\mathrm{F}}(\varphi, p) \quad \text{and} \quad \nabla p = -n^{\mathrm{F}}(\varphi, p)\nabla\varphi, \tag{11}$$

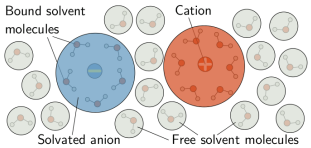

Fig. 8: *Solvated ions reduce the density of the solvent*

which allows to predict the experimental data for the first time. However, the use of a simple mixture is not sufficient. There is a further phenomenon, viz. the formation of solvated ions illustrated in Figure 8, that is not represented by the Nernst–Planck model, whereas the new model incorporates the phenomenon by recalculating the free energy function on the basis of Figure 8.

Figures 9 show the potential and the particle densities within the boundary layer between a metallic electrode and the bulk region of an electrolyte consisting of a 0.5 molar solution of KCl in water. The applied voltage between the electrode and the electrolyte is low in the left figure and high on the right-hand side. In the low voltage regime, we observe exclusively a diffuse layer, whereas we may identify a decomposition into two different layers in the high-voltage regime. Here, there is indeed a second layer between the electrode and the diffuse layer as it was proposed by Stern. However, the origin and the properties of our Stern layer differ from Stern's original idea. In the new setting, the Stern layer is characterized by a strong decrease of solvent molecules, which is accompanied by a saturation of solvated anions. Thus, the new model does not rely on an a priori assumed decomposition of the boundary layer. In fact, that decomposition is implied by the equations of balance and the corresponding constitutive equations.

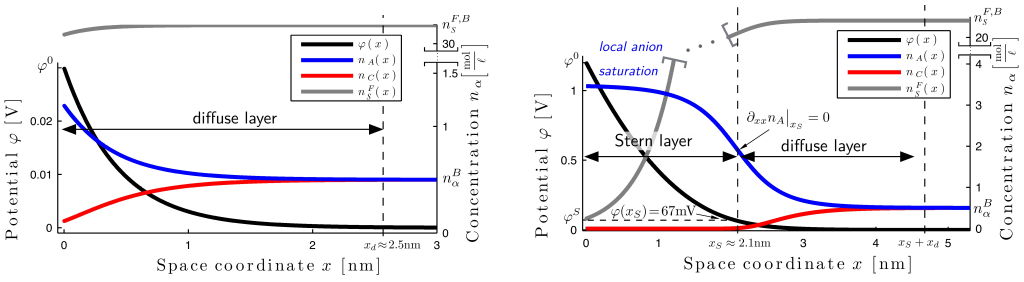

Fig. 9: *Potential and the particle densities within the boundary layer. Left: low-potential regime. Right: high-potential regime.*

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2.7 Modeling, Analysis and Simulation of Multi-frequency Induction Hardening

Dietmar Hömberg, Thomas Petzold, and Elisabetta Rocca

Introduction

In most structural components in mechanical engineering, the surface is particularly stressed. Therefore, the aim of surface hardening is to increase the hardness of the boundary layers of a workpiece by rapid heating and subsequent quenching. This heat treatment leads to a change in the microstructure, which produces the desired hardening effect. Depending on the respective heat source, one can distinguish between different surface hardening procedures. Induction heat treatments can easily be integrated into a process chain. Moreover, they are energy efficient since the heat is generated directly in the workpiece. That is why induction hardening is still the most important surface treatment technology.

Its mode of operation relies on the transformer principle. A given current density in the induction coil induces eddy currents inside the workpiece. Because of the Joule effect, these eddy currents lead to an increase in temperature in the boundary layers of the workpiece. Then the current is switched off, and the workpiece is quenched by spray-water cooling producing the desired hard, martensitic microstructure in the boundary layer. Due to the skin effect, the eddy currents tend to distribute in a small surface layer. The penetration depth of these eddy currents depends on the material and essentially on the frequency. Therefore, it is difficult to obtain a uniform contour hardened zone for complex workpiece geometries such as gears using a current with only one frequency.

If, for example, a high frequency (HF) is applied, then the penetration depth is small, and it is possible to harden only the tip of the gear. With a medium frequency (MF), it is possible to heat the root of the gear, but not the tip. With a single frequency, a hardening of the complete tooth can only be achieved by increasing the heating time. But then, the complete tooth is heated beyond the austenitization temperature, which results in a complete martensitic structure of the tooth after quenching, which is not desirable since this will foster fatigue effects.

Recently, a new approach was developed, which amounts to supplying medium and high frequency powers simultaneously to the induction coil. This concept is called *multi-frequency induction hardening*; see also Figure 1.

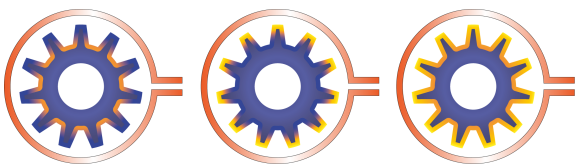


Fig. 1: *The effect of medium-, high- and multi-frequency induction heating. MF (left): only the root of the gear is heated, HF (middle): only the tip of the gear is heated, MF+HF (right): tip and root of the gear are heated.*

The inductor current consists of a medium frequency fundamental oscillation superimposed by a high-frequency oscillation. The amplitudes of both frequencies are independently controllable, which allows separate regulation of the respective shares of the output power of both frequencies according to the requirements of the workpiece. This fact provides the ability to control the depth of hardening at the root and at the tip of the tooth individually [6]. Owing to the complex interplay of nonlinear material data and system parameters, there is a high demand for simulation and control of this process. This was the starting point for the project "Modeling, simulation and optimization of multifrequency induction hardening", coordinated by WIAS within the Federal Ministry of Education and Research's Priority Program "Mathematics for Innovations in Industry and Services". In the sequel, the main achievements of the WIAS subproject will be presented.

The model

The main parts of the model are a vector potential formulation of Maxwell's equations to describe the evolution of eddy currents, strongly coupled to the energy balance through the Joule heat term, and a rate law for the high-temperature phase, austenite, in the workpiece. It is assumed that during the quenching process following inductive heating, austenite transforms completely into martensite and is therefore an indicator of the hardening profile. The austenitization behavior is directly linked to the temperature distribution by the transformation kinetics.

The following slightly idealized geometric setting is considered (cf. Figure 2), a hold-all domain D, containing the inductor Ω, the workpiece Σ, and the surrounding air. We call $G = \Omega \cup \Sigma$ the set of conductors and define the space-time domain as $Q = \Sigma \times (0,T)$; see Figure 2. Following [5], the mathematical model of multi-frequency induction hardening amounts to finding the magnetic vector potential A, temperature ϑ, and austenite phase fraction z, satisfying the following nonlinear coupled boundary value problem:

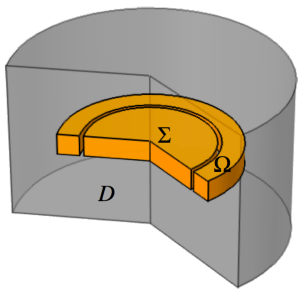


Fig. 2: *Domain D consisting of the inductor Ω, the workpiece Σ, and the surrounding air*

$$\sigma A_t + \operatorname{curl}\left(\frac{1}{\mu}\operatorname{curl} A\right) = J_0(x)u(t) \quad \text{a.e. in } D \times (0,T), \tag{1}$$

$$\vartheta_t - \Delta\vartheta = -L(\vartheta,z)z_t + \sigma(x,z)|A_t|^2 \quad \text{a.e. in } Q, \tag{2}$$

$$z_t = \frac{1}{\tau(\vartheta)}\left(z_{eq}(\vartheta) - z\right)^+ \quad \text{a.e. in } Q, \tag{3}$$

$$\frac{\partial\vartheta}{\partial\nu} + \vartheta = g \quad \text{a.e. on } \partial\Sigma \times (0,T), \tag{4}$$

$$A(0) = A_0, \quad \text{a.e. in } D, \quad \vartheta(0) = \vartheta_0, \quad z(0) = 0 \quad \text{a.e. in } \Sigma. \tag{5}$$

Here, μ is the permeability and σ the electric conductivity. Since the latter vanishes in non-conducting regions, (1) is a degenerate parabolic equation. J_0 is a precomputed spatial source current in the inductor, and $u(t)$ is the time-dependent control imposing the different frequencies. The other physical parameters were normalized to one.

Analysis

(1)–(5) is a strongly coupled system of evolution equations. The main analytical challenges are the quadratic Joule heating term in (2) and the nonlinearities in σ and μ. While the former depends on temperature and phase, the latter in addition also depends on the vector potential.

In two recent papers, the simpler frequency domain situation of Joule heating was studied. In [4], the Boccardo–Galluet approach was applied to prove existence of a weak solution, while in [3], new regularity results were used to prove existence and stability in the frequency domain setting. In [5], the existence of a weak solution to a fully coupled electro-thermo-mechanical model was proven. Recently, existence and stability of solutions to (1)–(5) could be shown in the case that μ, σ depend on the phase fraction z (see WIAS Preprint no. 1910, 2014). Since the phase fraction grows with increasing temperature, still the effect of changing temperature is maintained.

Simulation

The system (1)–(5) is also numerically challenging. One has to deal with two different time scales, one for the heat equation and one for the rapidly oscillating magnetic vector potential. Owing to the skin effect, the eddy currents have to be resolved in a boundary layer, so one is also faced with two spatial scales. A further difficulty is imposed by the nonlinearities, especially the (ϑ, A)-dependent permeability.

Fig. 3: *Gear geometry*

While the temperature ϑ was approximated with standard P1 elements, the natural space for the vector potential A is the Hilbert space $H(\mathrm{curl}, D)$. To discretize A, curl-conforming finite elements of Nédélec type were implemented in the finite element and finite volume toolbox `pdelib`. To account for the skin effect, the computational grid has to resolve the small surface layer of the workpiece in which eddy currents are distributed. Therefore, an adaptive grid was chosen for A governed by a residual-based a posteriori error estimator developed in [1].

The temperature changes on a time scale much larger than that of its right-hand side $\sigma|A_t|^2$, which is governed by the frequency of the source current. Hence, we can approximate the Joule heat term by its average over one period. Then we can solve the heat equation together with the ordinary differential equation describing the phase transition using time steps $\Delta t \gg \delta t$, where δt denotes the time step for the time discretization of (1). We replace the rapidly varying Joule heat by an averaged Joule heat term, which is obtained from the solution of the vector potential equation.

To deal with the (ϑ, A)-dependency of the permeability, we proceed as in [2]. We first determine the magnetic field with constant relative permeability $\hat{\mu}_r$, assuming that only a time-averaged value of the permeability affects the magnetic field. Since the magnetic field is periodic, this approach induces a periodic permeability $\mu(\vartheta(x,t), H(x,t)) = \mu_0\mu_\mathrm{r}(\vartheta(x,t), H(x,t))$. Averaging over one period yields an effective permeability that is space dependent but independent of the magnetic field, i.e., we choose

$$\frac{1}{\mu_{\mathrm{r,av}}(x)} = \frac{1}{T}\int_0^T \frac{1}{\mu_\mathrm{r}(\vartheta(x,t), H(x,t))}\,dt.$$

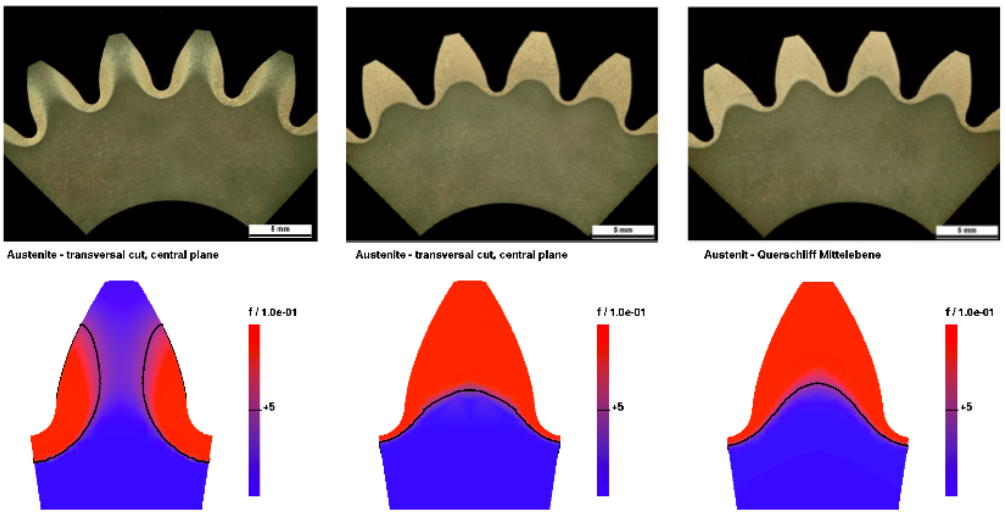


Fig. 4: *Simulated and experimental hardening profile using MF (left), HF (middle), and multi-frequency approach, MF+HF (right)*

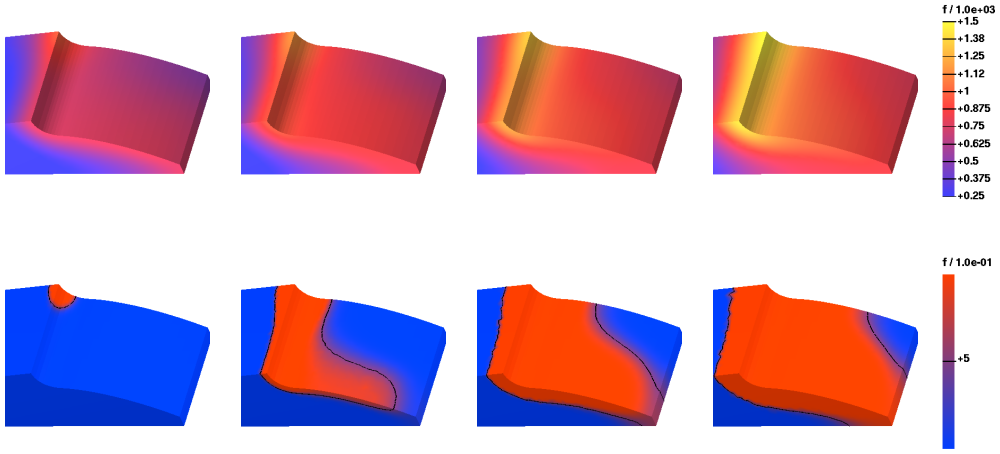
Experimental verification

The experimental verification was performed by our project partner *Foundation Institute of Materials Science (IWT)*, Bremen. Discs with different cross sections and a spur-gear with 21 teeth and a diameter of 47.7 mm were used; see Figure 3. All the samples were heated by single-frequency power, MF and HF separately, and by the multi-frequency approach in order to achieve a contour hardening. The temperature at the surface was measured by a pyrometer and compared to the simulation. In addition, metallographic analyses were performed and compared to the simulated austenite fraction, which by assumption transforms completely to martensite during the quenching process.

Figure 4 depicts a comparison for MF, HF, and the multi-frequency approach. It shows a good coincidence between simulation and experiment; however, no contour hardening could be achieved due to technical limitations of the hardening equipment at IWT.

Industrial validation

To validate the developed code in an industrial setting, further experiments at our project partner's *EFD Induction*, Freiburg, were conducted. For the numerical validation of the experiments, at first the maximal power for MF and HF in the simulation code was adjusted to reproduce the corresponding mono-frequency experiments at EFD. The company's experiments showed that with machine specific power parameters of 53 % MF and 22 % HF, corresponding to approximately 300 kW MF and 100 kW HF, a contour hardening could be achieved with a heating time set to 0.25 s. Without any further fitting except for the mentioned fitting of the maximal mono-frequency powers, the corresponding simulations were run. The heating phase simulation is shown in Figure 5 on page 59.



(a) $t = 0.1$ s (b) $t = 0.15$ s (c) $t = 0.2$ s (d) $t = 0.25$ s

Fig. 5: *Heating of a gear with the multi-frequency approach. Temperature profile (top row) and austenite profile (bottom row) for different time snapshots. For symmetry reasons, only a quarter of the tooth is considered.*

A comparison of experimental and simulated hardening profiles is depicted in Figure 6, showing the desired contour hardening effect and an excellent accordance between experiment and simulation. Stimulated by these promising results, follow-up projects are in preparation aiming at the solution of related optimal control and shape design problems.

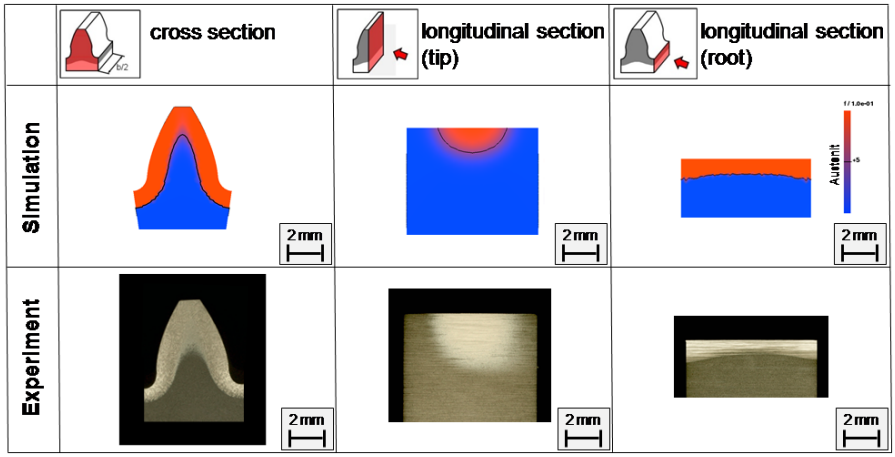


Fig. 6: *Simulated and experimental hardening profile using the multi-frequency approach, MF+HF*

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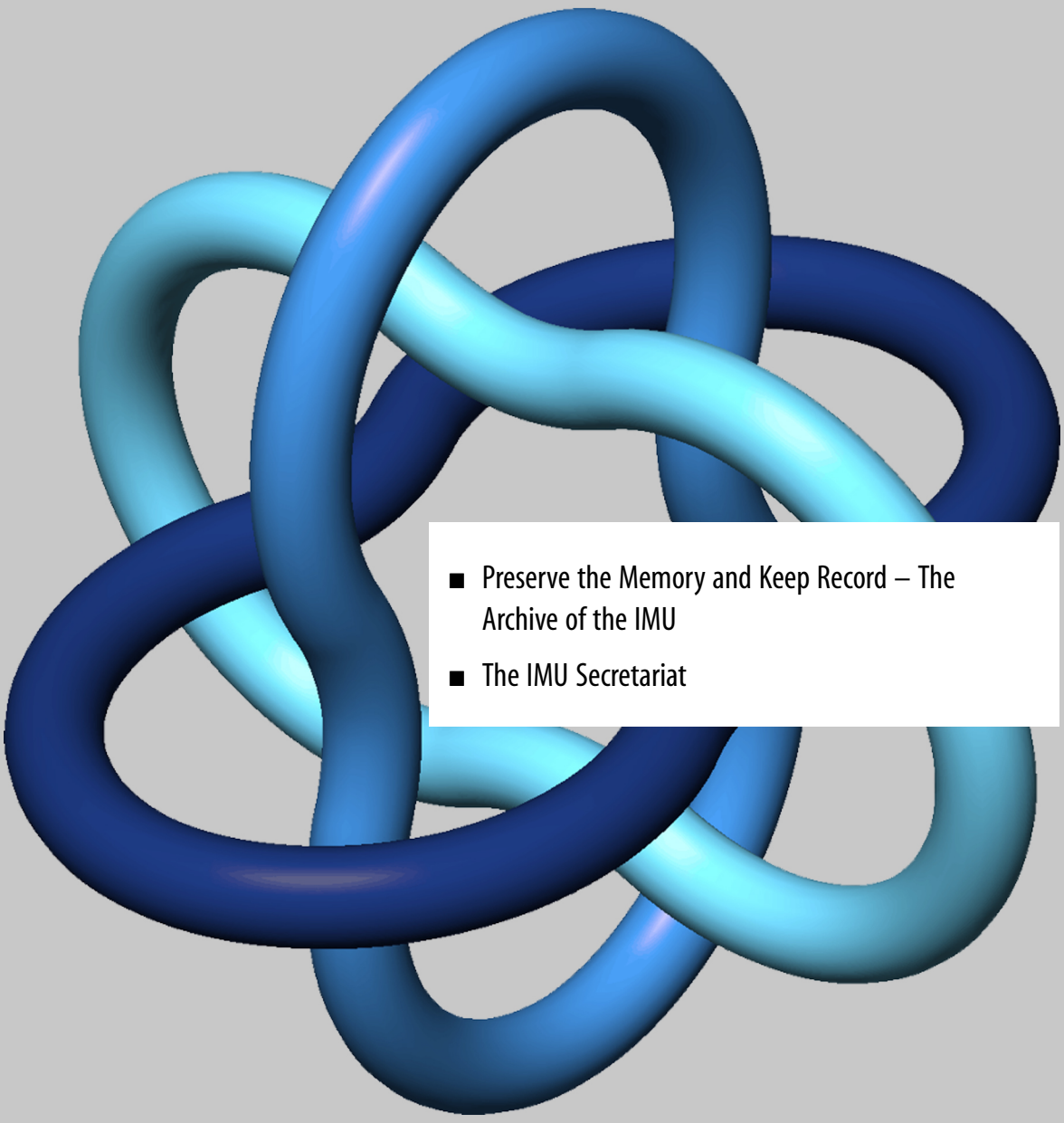
3 IMU@WIAS



- Preserve the Memory and Keep Record – The Archive of the IMU
- The IMU Secretariat

3.1 Preserve the Memory and Keep Record – The Archive of the IMU

Birgit Seeliger and Sylwia Markwardt

Setting up the IMU Archive

Since 2011, when the Secretariat of the International Mathematical Union has been permanently located at WIAS, also the IMU Archive (with the ICMI Archive being a subset of the IMU Archive) including the physical resources like a room and archival equipment, IT facilities, as well as a professional archivist are in Berlin. After the Secretariat opening ceremony in February 2011, preparations started to procure appropriate furniture for the archive room and archival software. In June 2011, the move of the IMU Archive from Helsinki to Berlin was completed.

Until that point in time, no Union archive in a strict sense had existed. The documents giving evidence of the activities and history of the IMU and its commissions were collected more or less accidentally and stored at those places where the then IMU presidents and secretaries were based institutionally. It is true that there was no formal obligation to deliver documents to an IMU archive (that officially not existed), but former IMU officers nevertheless tried to capture and store relevant material during their terms of service for IMU. The archive of ETH Zurich was a "shelter" for collected IMU material before it was moved in 1994 to the archive of the University of Helsinki, which continued to host IMU material until 2011. Looking back, this was the birth of a real IMU archive. Olli Lehto, IMU Secretary during 1983–1990, revised and organized all the material with the professional help of the archivist Tuulikki Mäkeläinen. A first archival overview was produced in 1996; see `http://www.mathunion.org/Publications/Bulletins/40/catalogue.html`, revised in 1998.

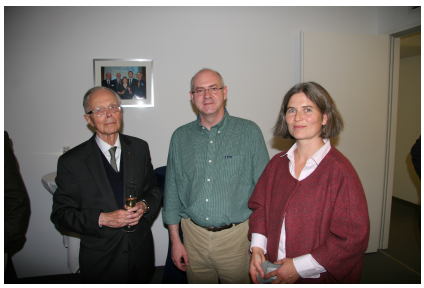


Fig. 1: *Left: IMU Archives in 1996, Central Archives of the Helsinki University. Chief Archivist E. Vallisaari, O. Lehto, and T. Mäkeläinen. Photo: Ilmar Jöutvald. Right: IMU Archivists power (O. Lehto, G. Curbera, B. Seeliger) in 2011.*

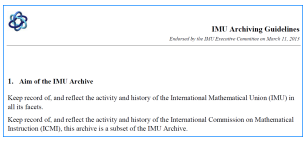
In 2008, Livia Giacardi (U Turin) visited the Helsinki University Archive to revise the part of ICMI's material, see `http://www.icmihistory.unito.it/documents/archives.pdf`.

Lehto's book "Mathematics without borders, a history of the International Mathematical Union" (Springer Verlag) is a valuable source of information about this "story".

In November 2011, when the setup of the IMU Archive in Berlin was basically finished, an official opening ceremony took place, which was attended among other guests by Guillermo Curbera, Curator of the IMU Archive, Olli Lehto, and archive staff of Helsinki. On this occasion, Olli Lehto gave a speech addressing the history of the IMU Archive as well as his personal experience from that time.

Archiving guidelines

More than 15 years have elapsed since the archive of the IMU has been revised for the last time. During that period, the way to produce and forward written material changed to a great extent from hard copy to digital medium, which had as a result that collecting and archiving became much more difficult, and the IMU Archive could run the risk that at lot of the material gets lost. The IMU Archive needed a strategy to tackle the problem. In a joint effort, the IMU EC, the ICMI EC, the IMU and ICMI Archive Curators, and the IMU Secretariat drafted "IMU Archiving Guidelines" that were endorsed by the IMU EC in March 2013 (Figure 2) and will be presented to the IMU General Assembly in 2014. These guidelines describe the general principles for archiving IMU material.


IMU Archiving Guidelines

Endorsed by the IMU Executive Committee on March 15, 2013

1. Aim of the IMU Archive

Keep record of, and reflect the activity and history of the International Mathematical Union (IMU) in all its facets.

Keep record of, and reflect the activity and history of the International Commission on Mathematical Instruction (ICMI), this archive is a subset of the IMU Archive.

Fig. 2: *IMU Archiving Guidelines ...*

As a preliminary measure an inventory list of documents still missing and/or to be archived in the future was compiled. The IMU Bulletins, the ICM Proceedings, and the World Directory of Mathematicians were identified to be the most important printed chronicles of IMU. The series of these editions available in the IMU Archive were incomplete, but almost all the gaps could be filled with the help of IMU representatives, institutions like the Weierstrass Institute, the Austrian Mathematical Society, and the Library of the Humboldt Universität Berlin.

Other material eligible for archiving are documents from IMU officers and commissions. All former IMU presidents, secretaries, representatives, and prize committee chairs who could be expected to provide material to the IMU Archive were approached to submit relevant stuff. A number of submissions have been received, but there are still gaps to fill. Additionally, the IMU Archive got material from other sources, e.g., Springer Publishing, WIAS, and ICM2006.

Fig. 3: *Gallery of former IMU Presidents and Secretaries*

Special collections

Documents such as correspondence, minutes, speeches, or communication in general form the central part of the IMU Archive. Besides, the collection includes objects like bags, cups, posters, or other promotional items that reflect a particular time, spirit, and atmosphere of IMU's "life".

A new arena will be entered with the currently ongoing photo archive project. This project aims to make available photographs of people, events, or other items of importance for IMU. Part of the project is a collection of pictures of all former IMU presidents and secretaries. Using contacts to persons or archives around the world made it possible to trace many pictures in real detective work. An impressive photo gallery is on show in the IMU Secretariat now (Figure 3).

Archiving strategies

The aim of any archive is, among others, to collect, store, and preserve "things" for a long time. This aim can be achieved only if there is a strategy that makes those things preserved, detectable, and accessible.

The "REFERENCE MODEL FOR AN OPEN ARCHIVAL INFORMATION SYSTEM (OAIS)", see `http://public.ccsds.org/publications/archive/650x0m2.pdf`, is a general recommendation for archives and sort of a quality management handbook that provides a structure and sets focal points for the overall archive management in order to ensure the workflow between the input and output of archival information. The IMU Archive decided to follow the suggestions of this model and adapted it to its needs (Figure 4).

The information path between the producer and the consumer is the way from the Submission Information Package (SIP) to the Dissemination Information Package (DIP). In between SIP and DIP is the archive, the flow chart makes one realize why archiving strategies are indispensable.

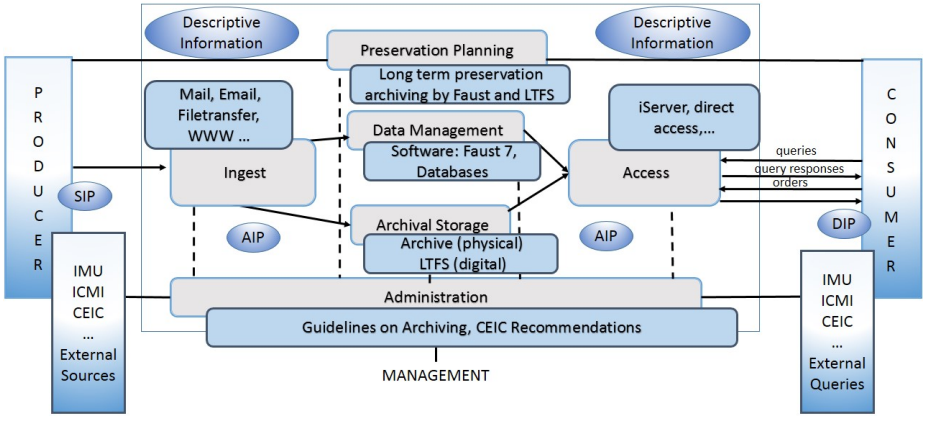


Fig. 4: *OAIS reference model for archiving, adapted to the IMU Archive's workflow*

The core functions of the OAIS model are Preservation Planning, Data Management, Archival Storage, and Administration. Below is a short description of how these core functions are applied to the IMU Archive environment.

Preservation Planning implies to plan which technology, software, and data formats as well as which migration plans and media choices are to be considered for long-term preservation. For the IMU Archive, it was decided to use the archival software FAUST. FAUST is independent of import formats and quantities of incoming information; the software is able to export its metadata in nonproprietary formats as XML (Extensible Markup Language) or METS (Metadata Encoding and Transmission Standard). The IMU Secretariat decided to use an LTFS (Linear Tape File System) as a long-term preservation archive medium.

The Data Management provides the services and functions around the descriptive information that identifies and describes the archive holdings as well as system information used to support archive operations including query responses or database updates. In the IMU Archive, FAUST is used in flexible applications that guarantee the description of different objects like paper documents, books, or photos in compliance with an archival description standard. The software allows the implementation of descriptive information of any analogical or digital objects and formats without touching or changing the objects. It stores the metadata and descriptions in databases and connects the data to the archived original permanently. This is the requirement to support and to enable the access to archival information.

The Archival Storage is like the “heart of the archive”. It provides the services and functions needed to store, maintain, and retrieve the archive holdings. The archive room in the IMU Secretariat, equipped with shelves and a fireproof safe, is the place of storage of physical items. Digital storage (implemented through LTFS) will be increasingly applied in the future.

The Administration manages the operations of the OAIS and its connections to the environment of the archive, its restrictions and configurations. At this point, the IMU Archiving Guidelines come into play. Advice from IMU’s Committee on Electronic Information and Communication (CEIC), the Curators of the IMU Archive, and the Executive Committee has also be taken into consideration.

The OAIS reference model is a useful instrument to structure and explain the IMU archiving system. The complexity of the workflow and the interdependency of administration, IT systems, and archive knowledge are adequately illustrated.

Archiving service

Since the IMU Archive has been installed in Berlin, a lot of inquiries on IMU “affairs” have been received. Dealing with the matter in question and replying to such inquiries is another way of preserving memory and keeping record.

3.2 The IMU Secretariat

Grants

DFG grant for International workshop "Elementary Mathematics from an Advanced Standpoint – Felix Klein and Mathematics for Teachers". The IMU Secretariat hosted the ICMI Klein Workshop from September 17 to 20, 2013. As part of the workshop a secondary teacher training (public lecture day) was held. The workshop contributed to the Klein Project, a major project of the International Mathematical Union and the International Commission on Mathematical Instruction. It aimed to link research mathematics with school mathematics in the spirit of Felix Klein's famous book "Elementary Mathematics from an Advanced Standpoint" that was published in 1908.

IMU won ICSU grant 2013. IMU's proposal for the project entitled "Mathematics of Climate Change, Related Natural Hazards and Risks" had been awarded €30,000 by the International Council for Science (ICSU) under its grants program 2013.

The workshop was joint venture of the three scientific unions IMU, IUGG (International Union of Geodesy and Geophysics), IUTAM (International Union of Theoretical and Applied Mechanics), as well as ROLAC (ICSU Regional Office for Latin America & The Caribbean), ICIAM (International Council for Industrial and Applied Mathematics), IRDR (Integrated Research on Disaster Risk), WCRP (World Climate Research Programme), the National Academy of Sciences in the US, and the Mexican Academy of Sciences. It was hosted by Centró de Investigación en Matemáticas (CIMAT) in Mexico. The workshop was held as a satellite activity of the first Mathematical Congress of the Americas (MCA 2013) from July 29 – August 2, 2013, Guanajuato, Mexico.

Fig. 1: *IMU booth at MCA2013*

The IMU also run a booth at the MCA 2013 (Figure 1) to provide information material about the IMU, its commissions and activities and to advertise the forthcoming International Congress of Mathematicians ICM 2014 in Seoul, Korea.

Abel Visiting Scholar Program. The Norwegian Abel Board and the International Mathematical Union installed the Abel Visiting Scholar Program inviting applications from mathematicians professionally based in developing countries to visit an international research collaborator. The program is designed for postdoctoral mathematicians in the early stages of their professional careers. The grant covers health insurance, visa cost, travel and living expenses including accommodation for one month for up to a total maximum amount of $5,000 per mathematician. Three grants are given per year.

IMU-Simons Travel Fellowship Program. The Simons Foundation has made a grant to IMU's Commission for Developing Countries to support mathematicians working in a developing or economically disadvantaged country (as determined by the IMU CDC). $75,000 are granted for a three-year period for collaborative research visits of mathematicians working in the developing world to a "center of excellence" in any part of the world for collaborative research.

Meetings

IMU – EFP Reception. A meeting gathering fellows of the IMU Berlin Einstein Foundation Program (EFP), EFP supervisors and others involved in the work of the EFP as well as the IMU Secretariat people took place at the IMU Secretariat on January 26, 2013. The EFP is supported by a grant given by the Einstein Stiftung Berlin to the Berlin Mathematical School on the occasion of the establishment of the IMU Secretariat at WIAS.

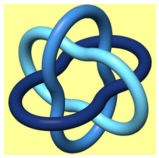
IMU Executive Committee meeting, CDC meeting, ICMI Executive Committee meeting. The IMU Executive Committee (EC) held its annual meeting at the IMU Secretariat in Berlin on March 11–12, 2013.

The meeting was preceded by a gathering of the members of the Commission for Developing Countries (CDC) and several guests.

The IMU EC and CDC jointly decided, e.g., to host with the support of the ICM 2014 organizers a MENAO event (MENAO stands for "Mathematics in Emerging Nations: Achievements and Opportunities") on August 12, 2014, in Seoul, Korea, aiming at finding additional support for mathematics in developing countries.

The newly elected Executive Committee of the International Commission on Mathematical Instruction (ICMI) held its annual meeting at the IMU Secretariat on May 22 – 24, 2013.

Events



MPE Day 2013. Mathematics of Planet Earth (MPE2013) was a joint enterprise of over 130 scientific societies, universities, research institutes, and organizations to dedicate 2013 as a special year for the Mathematics of Planet Earth. The European Launch of MPE2013 was on March 5, 2013, at the UNESCO headquarters in Paris. MPE2013 got the patronage of UNESCO and was endorsed, among others, by the International Mathematical Union. C. Rousseau, IMU Vice President, was the initiator and coordinator of MPE2013.

Heidelberg Laureate Forum. The first Heidelberg Laureate Forum (HLF) took place from September 23 – 27, 2013, in the city of Heidelberg, Germany. The HLF brings together winners of the Abel Prize, the Fields Medal, the Nevanlinna Prize, and the Turing Award with outstanding young scientists from all over the world for a one-week conference. The meeting is modeled after the annual Lindau Nobel Laureate Meetings established more than 60 years ago. The IMU who is a partner of the HLF nominated two members of the HLF Scientific Committee.

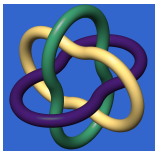
Guests of the IMU Secretariat. The table below gives an overview of guests who visited the IMU Secretariat this year.

Date	Guests	Event
Jan 25, 2013	Martin Rumpf, Germany	Individual visit

Jan 29, 2013	Peter Deuflhard, Germany; Hélène Esnault, Germany; Anne Jordan, Germany; Christian T. Martin, Germany; Volker Mehrmann, Germany; Dany Pascal Moualeu-Ngangue, Cameroon; Marion Müller, Germany; Ludovic Ndounkeu Tangpi, Cameroon; Konrad Polthier, Germany; Ozren Sekulović, Serbia; John M.Sullivan, Germany; Živorad Tomovski, Macedonia; Nadja Wisniewski, Germany; Linghui Zeng, China; Günter M. Ziegler, Germany	EFP-IMU Gathering
March 9 – 12, 2013	Ferdinando Arzarello, Italy; John Ball, UK; Carla Cederbaum, Germany; Herb Clemens, USA; Ingrid Daubechies, USA; José A. de la Pena, Mexico; Manuel de León, Spain; Helge Holden, Norway; Srinivasan Kesavan, India; Dongsu Kim, Korea; Yiming Long, China; László Lovász, Hungary; Joseph Mugisha, Uganda; Wandera Ogana, Kenya; Hyungju Park, Korea; Hoang Xuan Phu, Vietnam; Ragni Piene, Norway; Angel R. Pineda, USA; Cheryl Praeger, Australia; Christiane Rousseau, Canada; Vasudevan Srinivas, India; Polly W. Sy, Philippines; John F. Toland, UK; Yuri Tschinkel, USA; Sheung Tsun, UK; Marcelo Viana, Brazil; Wendelin Werner, France	IMU EC Meeting, CDC Meeting
May 22 – 24, 2013	Abraham Arcavi, Israel; Ferdinando Arzarello, Italy; Yuriko Baldin, Brazil; Bill Barton, New Zealand; Ingrid Daubechies, USA; Jean-Luc Dorier, Switzerland; Zahra Gooya, Iran; Gabriele Kaiser, Germany, Anjum Halai, Tanzania; Roger Howe, USA; Cheryl Praeger, Australia; Angel Ruiz, Costa Rica	ICMI EC Meeting
June 17 – 24, 2013	Bernard Hodgson, Canada	ICMI Archive
July 16, 2013	Carol Hutchins, USA	Individual visit
Sep 17 – 20, 2013	Michèle Artigue, France; Ferdinando Arzarello, Italy; Yuriko Baldin, Brazil; Bill Barton, New Zealand; Ehrhard Behrends, Germany; Samuel Bengmark, Sweden; Regina Bruder, Germany; Graeme Cohen, Australia; Paul Drijvers, Netherlands; Herbert Koch, Germany; Henning Körner, Germany; Ulli Kortenkamp, Germany; Jürg Kramer, Germany; Manfred Lehn, Germany; Andreas Loos, Germany; Daniel Lordick, Germany; William McCallum, USA; Jörg Meyer, Germany; Stefan Müller-Stach, Germany; Reinhard Oldenburg, Germany; Konrad Polthier, Germany; Jürgen Richter-Gebert, Germany; Bettina Rösken-Winter, Germany; Christiane Rousseau, Canada; Thilo Steinkrauß, Germany; Robert Teichert, Germany; Hans-Georg Weigand, Germany; Günter M. Ziegler, Germany	ICMI Klein Workshop

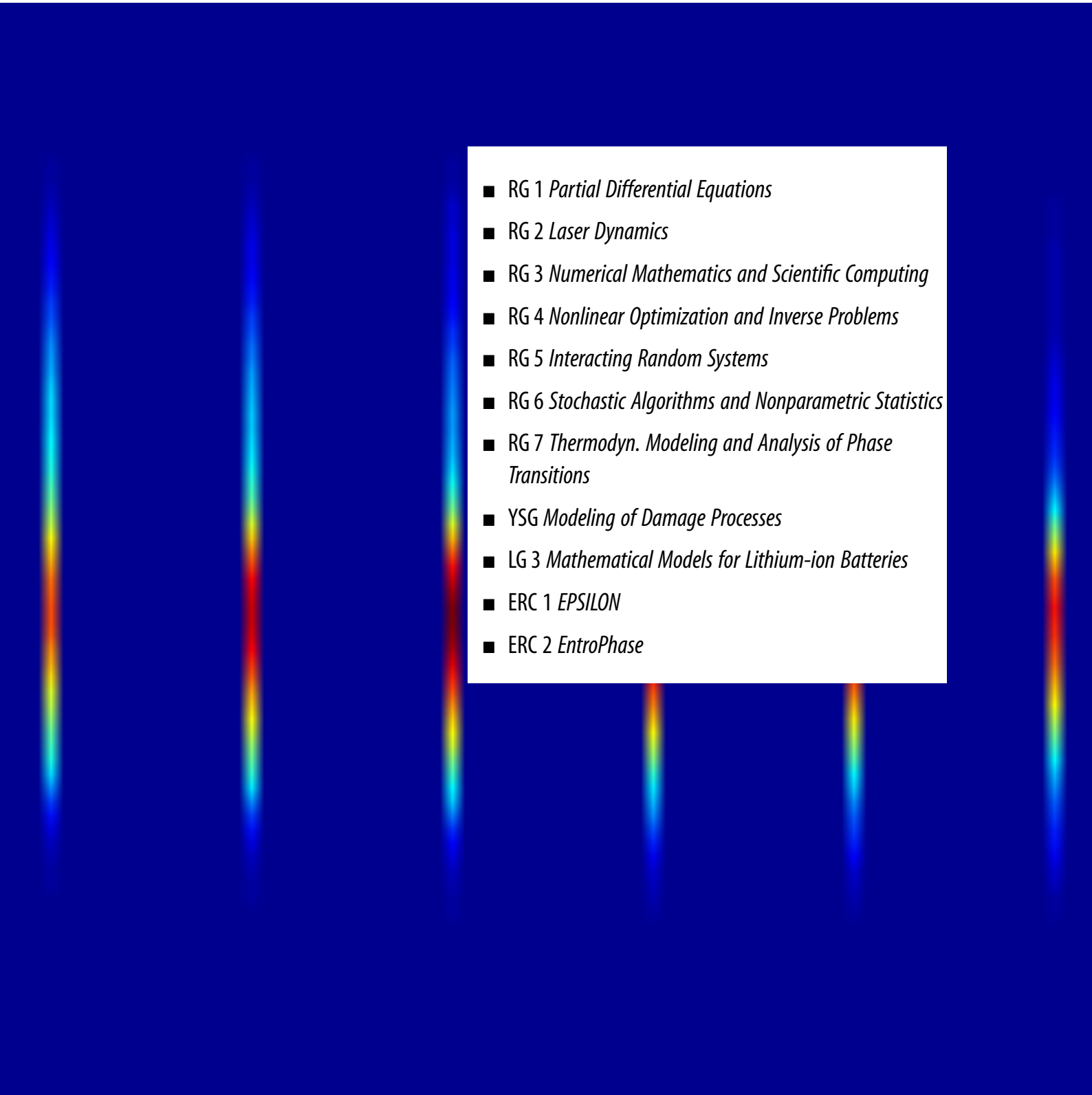
Oct 10, 2013	Martin Brokate, Germany; Mario Bukal, Croatia; José Antonio Carillo, Spain; Elisa Davoli, Italy; Manh Hong Duong, Vietnam; Michael Herrmann, Germany; Daniel Matthes, Germany; Maria Giovanna Mora, Italy; Stefan Neukamm, Germany; Elisabetta Rocca, Italy; André Schlichting, Germany; Ulisse Stefanelli, Austria; Florian Theil, UK; Rodica Toader, Italy; Nicolas van Goethem, Belgium	EEDSA 2013 – ERC workshop
Nov 1, 2013	Carol Wood, USA	Women in Mathematics
Dec 9, 2013	Hans Föllmer, Germany	Individual visit

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



- Mathematics of Planet Earth (MPE2013), European Launch at UNESCO, Paris, France (M. Grötschel)
- Friends of Mathematics Education (FOME), Berlin, Germany (M. Grötschel, L. Koch)
- 6th East Asia Regional Conference on Mathematics Education (EARCOME6), Phuket, Thailand (L. Koch)
- Scientific Program Committee meeting of the 8th International Congress of Industrial and Applied Mathematics (ICIAM 2015), Beijing, China (M. Grötschel)
- Abel Prize events, Oslo, Norway (M. Grötschel)
- CEIC meeting, Bath, UK (B. Seeliger, G. Telschow)
- Heidelberg Laureate Forum, Heidelberg, Germany (M. Grötschel)
- International Conference on Mathematics and Its Applications (IICMA) 2013, Yogyakarta, Indonesia (M. Grötschel)

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*
- ERC 1 *EPSILON*
- ERC 2 *EntroPhase*

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:

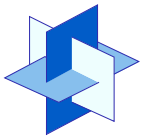
- Modeling of optoelectronic devices, also including quantum effects
- Reaction-diffusion systems, also including temperature coupling
- Multifunctional materials and elastoplasticity

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, including models derived from stochastic particle systems

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. Within the MATHEON project D22 "Modeling of electronic properties of interfaces in solar cells", interface conditions for thermionic emission were rigorously derived using a bulk layer approximation. Thermionic emission describes the transport of charge carriers with sufficiently high energy over a potential barrier at a hetero-interface. By suitable scalings of the mobilities in the bulk layer, one is able to pass to the limit in the energy dissipation formulation of the drift-diffusion system with the free energy as driving functional. The newly derived evolution equations consist of nonlinear parabolic equations in the bulk and on the interfaces with nonstandard coupling conditions. Further activities within the MATHEON project D22 were concentrated on the numerical analysis of reaction-diffusion systems in heterostructures. In cooperation with the Research Group *Numerical Mathematics and Scientific Computing* (RG 3), such nonlinear problems were studied in the setting of the implicit Euler Voronoi finite-volume method. Based on uniform global upper and lower bounds of the solutions for all Voronoi diagrams, the convergence of a subsequence of discrete solutions to a weak solution of the continuous problem was derived; compare the report of RG 3, too.

Electrothermal modeling of organic semiconductors. Organic light-emitting diodes (OLEDs) play a central role in modern lighting concepts, because of their energy efficiency. The self-heating of organic semiconductor devices based on Arrhenius-like conductivity laws were investigated in an intensive cooperation with the Institut für Angewandte Photophysik (IAPP) of Technische Universität Dresden and RG 3. In the spatially homogeneous situation, the self-consistent calculation explains thermal switching, bistability, and hysteresis resulting from S-shaped current-voltage characteristics with regions of negative differential resistance (NDR); see [1].

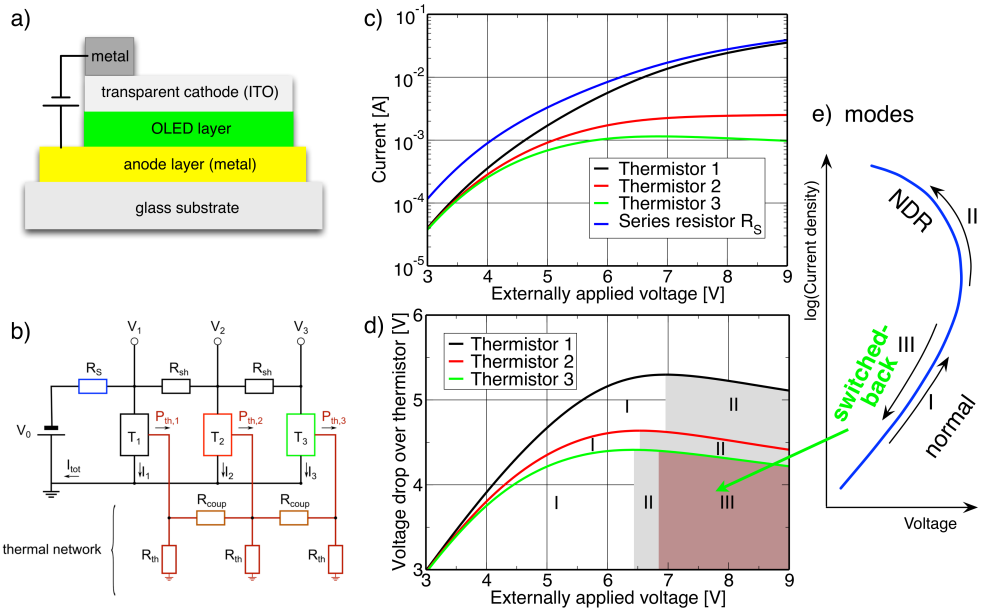


Fig. 1: Switched-back phenomenon induced by self-heating and negative differential resistance in OLEDs

The influence of this thermistor-like behavior on the current flow through a large-area thin-film device like an organic LED was studied by multi-physics circuit simulation. The simulation revealed a new effect caused by the spatial inhomogeneity induced by the voltage drop along the transparent cathode (ITO): Besides the expected normal (I) and NDR operation modes (II)—known from the spatially homogeneous theory—regions in the device can be "switched back", meaning that both, local current and local voltage, decrease for increasing externally applied voltage (operation mode III); see Figure 1 (c)–(e). This phenomenon can already be demonstrated by a chain of three electrothermally coupled thermistors; see Figure 1 (b)–(d). If a thermistor in the chain, e.g., T_2, enters the NDR mode, its current I_2 is increased, while the voltage drop V_2 decreases, leading to reduced voltage drop V_3 and current I_3 that corresponds to switching back T_3.

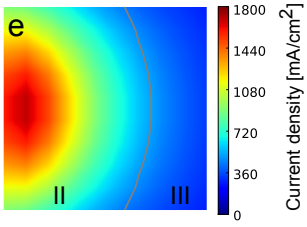


Fig. 2: Simulated current distribution and operation modes of an OLED

The appearance of spatially localized NDR and switched-back regions (see Figure 2) as well as their evolution in dependence on the total current was studied by comprehensive electrothermal circuit simulations for large-area thin-film devices. The good agreement between simulation and experiment for different OLEDs at IAPP suggests that these effects are responsible for the spatially inhomogeneous luminance in organic light-emitting diodes at high brightness.

Quantum modeling of cylindrical nanowire heterostructures. The quantum point contact is a typical mesoscopic system that shows conductance quantization in units of e^2/h, called *contact conductance*. It is due to the contact between a ballistic conductor, where elastic processes take place, and two reservoirs where dissipative processes take place. In [2], a detailed quantum mechanical description of electronic transport in a cylindrical nanowire with two quantum point contacts is considered. It is shown that this system could provide a very simple experimental evidence for quasi-bound states of evanescent channels, which is still an open issue in mesoscopic physics. They should appear as clear dips in the linear conductance at low temperatures.

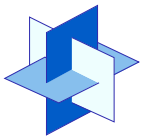
The tunnel injection structures are of great interest for future diode laser devices. They consist of a quantum well (QW), playing the role of a collector for the charge carriers, located close to the quantum dot (QD) layer, playing the role of the light emitter. Electronic structure calculations were performed for this complex low-dimensional system to optimize these structures. It is shown in the WIAS Preprint no. 1898 that, due to the interaction between the eigenvalues, hybrid states appear for small distances between QW and QD. This phenomenon may be an explanation for the additional photoluminescence peak measured for these structures.

Quantum modeling of light-emitting and absorbing devices. One of the main tasks in this year was to model a quantum dot that interacts with photons and is coupled to leads. This situation is typical for solar cells and light-emission diodes, which justifies their high topicality.

For the quantum dot interacting with photons, the well-investigated Jaynes–Cummings model was chosen, a model well known in quantum optics. The Jaynes–Cummings model (JM model) was completed by attaching two leads, which makes an electron current through the JM model possible. The arising Jaynes–Cummings-lead model (JCL model) [3] allows to study the interplay between photon and electron currents. Choosing the parameters of the model in a suitable manner, one gets either a solar cell or a light-emission diode. The main technical tool to compute the electron and photon currents is an abstract Landauer–Büttiker formula, which allows to rigorously compute also the photon current besides the electron current. The results were summarized and generalized in Lukas Wilhelm's Ph.D. "A rigorous Landauer–Büttiker formula and its application to models of a quantum dot LED", defended at the Humboldt-Universität zu Berlin in March 2013.

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).



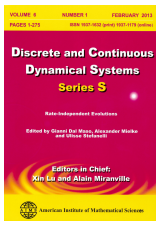
Shape memory alloys, elastoplasticity, and damage. The MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape memory alloys"

studied rate-independent models of dimension-reduced shape memory alloys. Furthermore, using the tools of Γ-convergence for hyperelastic materials with cracks, linearization methods in general space dimension were developed in order to obtain small-strain models as the limit of finite-strain models.

The subproject P5 “Regularizations and relaxations of time-continuous problems in plasticity” is a part of the DFG Research Unit FOR 797 “Analysis and Computation of Microstructure in Finite Plasticity”. A model for phase separation with application to elastoplasticity was analyzed. In order to deal with the non-convexity of the model, no regularization was used. Instead, a strategy was developed to control the oscillations directly and, thus, to show the existence of solutions. Within the project, a key concept is that of “rate-independent evolution”, which is the central theme of a Special Issue in the journal Discrete and Continuous Dynamical Systems Series S, **6**, 2013.

MICROPLAST

In the application area of damage, a model for the rate-independent evolution of brittle delamination was analyzed as the limit of adhesive contact models in the framework of local solutions. In contrast to energetic solutions, which are required to satisfy an energy equality and a global stability condition, i.e., minimality, to hold jointly in all variables and which have been intensively studied during the last years, local solutions are defined via an energy inequality and separate minimality, only. This wider concept of solutions seems to overcome the drawback of “too early” jumps. Moreover, it is possible to describe fracture in terms of stresses for the adhesive contact approximation of brittle delamination .



A coupled reaction-diffusion system on two scales. The derivation of effective equations and the study of pattern formation and instabilities is the central topic of the project A5 "Pattern formation in systems with multiple scales" within the Collaborative Research Center 910 “Control of Self-organizing Nonlinear Systems”. In [4], a new class of effective reaction-diffusion systems is rigorously derived via two-scale convergence. One species diffuses and reacts with respect to the macroscopic length scale, whereas a further species diffuses solely microscopically, but depends on both, the macro- and the micro-scale, due to a coupling via nonlinear reaction terms. This novel effective parabolic two-scale system will open the basis for the investigation of an unknown spectrum of patterns and competing instabilities with respect to the different scales.

SFB 910

Analysis of multiscale systems driven by functionals

erc

The ERC project “Analysis of multiscale systems driven by functionals” is devoted to the study of systems acting on multiple scales, which are defined in terms of energy or entropy functionals and of suitable geometric structures. One aim is to apply new multiscale methods to problems from material modeling that include nonlinearities and randomness. For example, in [5] the homogenization of the nonlinear bending theory for plates is investigated. A second application area of the project is optoelectronics. Using the modeling concept of GENERIC, a Maxwell–Bloch-type system was derived, coupling the evolution of electric and magnetic fields and of the density matrix for electron states. In contrast to widely used formulations, the resulting system is damped Hamiltonian, but preserves the positivity of the density matrix. In [6], a limit passage from an entropic

Ana Multi Scale

gradient structure for time-continuous Markov chains on a discrete domain to the Wasserstein Fokker–Planck equation is proved, making use only of the (nonlinear) metric structures.

The *ERC Workshop on Energy/Entropy-Driven Systems and Applications* took place at WIAS from October 9 – 11, 2013. It was organized by Karoline Disser, Alexander Mielke (both RG 1), and Ulisse Stefanelli (University of Vienna, Austria).

Fig. 3: *ERC Workshop EEDSA 2013: Berlin, October 9–11*

Further Highlights 2013

GAMM Junior. Marita Thomas has been selected as a GAMM Junior for the period 2013–2015. The GAMM Juniors are young researchers and members of the Gesellschaft für Angewandte Mathematik und Mechanik (International Association of Applied Mathematics and Mechanics, GAMM) who graduated with exceptional achievements in their final thesis and/or Ph.D. thesis in the field of applied mathematics or mechanics. The first 10 GAMM Juniors have been nominated at the end of 2011, and after a starting period of three years the group will consist of 30 persons.

Young Researchers' Minisymposium at the 84th Annual Conference of GAMM. At the GAMM conference 2013 in Novi Sad (Serbia), a Young Researchers' Minisymposium with the topic "Analytical and Engineering Aspects in the Material Modeling of Solids" was organized by Marita Thomas and Riccarda Rossi (University of Brescia, Italy). Five talks provided insight into recent developments in the analytical and computational investigation of dissipative phenomena in solids, which influence the elastic behavior of the material, such as magneto-electric effects, dislocations and plasticity, fracture and damage.

BMS Intensive Course on Evolution Equations and their Applications. This intensive course for young researchers took place at the Technische Universität Berlin from November 27–29. It was organized by Maciek Korzec (TU Berlin) and Matthias Liero (RG 1) within the Excellence Graduate School Berlin Mathematical School (BMS). The course was devoted to new methods for the

treatment of partial differential equations describing the evolution of physical systems and processes. The program included the presentation of thin-film models, homogenization of reaction-diffusion systems, Wasserstein gradient flows, dislocation theory, crack and delamination models, variational methods, and many more. Talks were given by Ph.D. students and PostDocs from all over the world. Additionally, keynote lectures by Andreas Münch (University of Oxford/UK) and Dorothee Knees (YSG) were given. The course was closed with the talk of Martin Burger (Westfälische Wilhelms-Universität Münster) in the BMS Friday Colloquium. There were about 40 participants coming from China, France, Germany, the Netherlands, Portugal, Russia, Spain, and the United Kingdom.

Fig. 4: *BMS Intensive Course on Evolution Equations and their Applications*

Summit on *Women in Leadership* hosted by Angela Merkel on May 7, 2013. What is holding women back from obtaining senior leadership positions? What needs to change in society, business, and politics so that more women reach top positions? These and other questions were discussed by Chancellor Angela Merkel and Christina Schröder (Federal Minister of Family Affairs, Senior Citizens, Women and Youth) with about 75 female leaders and executives from business, academia, the media, the world of arts and culture, the health sector, local politics, and administration. Among the guests were also about 25 students and young professionals mainly from MINT research fields (mathematics, informatics, natural sciences, and technology), amongst them Marita Thomas (RG 1).

Fig. 5: *Foto: Bundesregierung / Steffen Kugler (Photograph: Federal Government / Steffen Kugler)*

Women in leadership positions were “still a rarity”, Merkel said in her address. Though progress had been made, there is a need to move beyond the current “snail’s pace”. Merkel also emphasized that with a view to demographic change and challenges, full use needed to be made of the

potential offered by women. In the discussion, the participants spoke of their personal experience along their career paths to the leadership positions they now hold. On one issue in particular the participants agreed: Role models and networks are incredibly important and invaluable for increasing the visibility of women, for learning from each other, and for developing shared strengths.

This summit was declared not to be a one-time activity before the elections, but rather a signal initiative to further steps. Merkel's goal is to take what was discussed and use it to develop strategies for change, which will be presented in a follow-up meeting.

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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), the Marie Curie Initial Training Network PROPHET, the DFG Individual Grant "Ab-initio description of optical nonlinearities in femtosecond filaments", and the bilateral cooperation project MANUMIEL (supported by BMBF) between the Technical University of Moldova, the Ferdinand Braun Institute for High Frequency Technology, Berlin, and WIAS.

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 "Modeling, Analysis, and Simulation of Optical Modes in Photonic Devices", organized by the Research Groups RG 1 *Partial Differential Equations*, RG 2 *Laser Dynamics*, and RG 4 *Nonlinear Optimization and Inverse Problems*, where applied mathematicians and scientists from semiconductor laser physics initiated an in-depth discussion of the concept of resonances as a basis for the description of optical modes in lasers.

Mode-locking. In the Marie Curie Initial Training Network PROPHET, hybrid mode-locking in two-section edge-emitting semiconductor lasers was studied numerically and analytically, using a set of three delay-differential equations. Estimation of the locking range where the pulse repetition frequency is synchronized with the frequency of the external modulation was performed numerically and the effect of the modulation shape and amplitude on this range was investigated. The numerical simulations indicated that hybrid mode-locking can also be achieved in the cases when the frequency of the external modulation is approximately either twice or half the pulse repetition frequency of the free-running passively mode-locked laser [4].

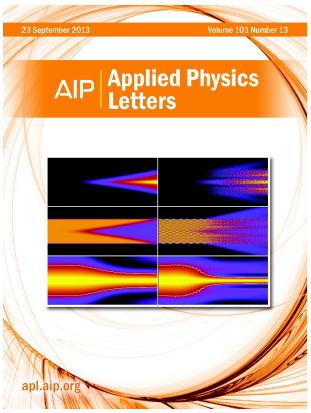

Fig. 1:
Cover of APL ***103****(13), 2013, showing a figure from [1]*

Broad-area lasers and amplifiers. Within this topic, optical beam propagation, amplification, and shaping in longitudinally and laterally modulated broad-area (BA) amplifiers were analyzed [1]. The study was based on simulations and analysis of a (2+1)-dimensional traveling wave model for the spatial-temporal dynamics of the optical field, the induced material polarization, and the carrier density; see Figure 1.

An efficient modeling approach was developed for the simulation of gain-guided BA laser diodes [5]. It is based on the idea of mesh decimation that allows the possibility of recasting traveling

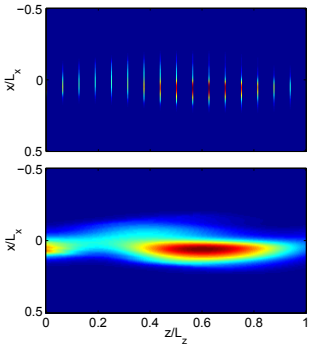

Fig. 2: *Mesh reconstruction of optical intensity from the past values of the mesh decimated by a factor of 16 [5]*

wave models into coupled delay-algebraic equations leading to an improvement of the integration time between one and two orders of magnitude, which may alleviate the necessity of using complex parallel code to simulate the dynamics of BA lasers; see Figure 2.

A reduced model for the dynamics of a multistripe laser array with an external cavity formed by either a single or two off-axis feedback mirrors was derived and analyzed, based on a set of delay-differential equations that takes into account the transverse carrier grating in the semiconductor medium [3].

Furthermore, the impact of the phase of the time-delayed optical feedback and carrier lifetime on the self-mobility of localized structures of light in BA semiconductor cavities was studied. It was shown both analytically and numerically that the feedback phase strongly affects the drift instability threshold as well as the velocity of cavity soliton motion above this threshold.

Ring lasers. A novel multimode instability in semiconductor ring lasers was theoretically predicted that provokes a periodic deterministic directional reversal, involving jumps between consecutive longitudinal modes, following the modal frequencies from blue to red. It was shown that, due to the extra degree of freedom that stems from the directional bistability, the threshold for this instability is much lower than it is in Fabry–Perot lasers, and it can hinder the performance of semiconductor ring lasers already at relatively low bias current.

Fourier-domain mode-locked lasers. A delay-differential equations (DDE) model to describe a Fourier-domain mode-locked (FDML) laser was proposed and investigated numerically and analytically. It was demonstrated that a slightly detuned FDML operation is formally equivalent to the case of an adiabatically slow sweep rate, but with the transitions between frequency-swept FDML modes instead of the standard longitudinal laser modes. The analysis of the DDE model explained why the change of the sign of the frequency sweep detuning from the inverse cavity round-trip time is equivalent to the reversal of the sweep direction. An explanation of experimentally observed regimes was given: A modulational instability was shown to be responsible for the transitions to the complex oscillating outputs, and a Turing-type instability for the abrupt frequency jumps [6].

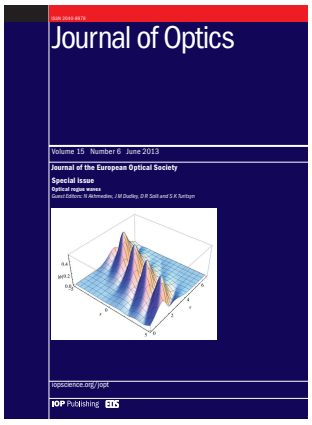

Fig. 3: *Cover of J. Opt.* ***15****, 2013, special issue on rogue waves, figure taken from [7]*

Pulses in nonlinear optical media

A novel method of producing octave-spanning optical supercontinua with exceptionally good correlation properties was proposed. Also, a new combined analytical/numerical approach was derived that yields ultrashort localized solitary solutions to Maxwell equations in a bidirectional framework. For more details, we refer to the Scientific Highlights article "Calculating Pulses in Optical Fibers: Short, Shorter, the Shortest" on page 22.

A wide class of exact solitary solutions to the Sasa–Satsuma equation with a nontrivial background was studied, which has a rich structure and admits several limiting cases that are important for applications. Among them are rogue waves and classical solitons; see Figure 3. Furthermore, the zero-background limit contains, as particular cases, previously known soliton solutions [7].

In collaboration with Raimondas Ciegis from TU Vilnius, Lithuania, different aspects of *numerical methods* for the nonlinear Schrödinger equation were investigated [2], as well as for the generalized nonlinear Schrödinger problem, and for the (2+1)-dimensional traveling wave model of broad-area semiconductor lasers and amplifiers.

An important event was the Workshop "Extreme Nonlinear Optics and Solitons" that was organized at WIAS with the support of the DFG Research Center MATHEON; see Figure 4. It brought together international experts from the theoretical and from the experimental side and led to new collaborations, e.g., in the upcoming field of optical turbulence. A project application by RG 2 on this topic within the new Berlin Research Center ECMath was already successfully approved.

Fig. 4: *Participants of the Workshop "Extreme Nonlinear Optics and Solitons"*

Dynamical systems

New contributions to the mathematical theory of large-size systems' synchronization were obtained. An important result was the comprehensive classification of coherence-incoherence patterns, so-called *chimera states*, relying on a bifurcation analysis in terms of the relevant infinite-dimensional thermodynamic limit equation. Moreover, novel types of such patterns featuring a less symmetric spatial structure were discovered in a system of non-locally coupled realistic limit-cycle oscillators [8].

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

The research group studies the development of numerical methods, their numerical analysis, and it works at implementing software tools for the numerical solution of partial differential equations and differential-algebraic systems. Many of the research topics have been inspired by problems coming from applications. These topics include three-dimensional tetrahedral mesh generation, see the Scientific Highlights article by Hang Si on page 44, and newly launched topics like uncertainty quantification, in collaboration with the Research Group *Nonlinear Optimization and Inverse Problems*, and model reduction for Navier–Stokes equations. Here, a short overview of selected fields of the group's research will be presented.

Finite volume methods for reaction-diffusion processes in semiconductor photoresists

Within the framework of the EU FP7 funded project MD3 "Material Development for Double Exposure and Double Patterning", the group developed and implemented numerical methods for the simulation of several new approaches to achieve higher resolution in optical lithography for semiconductor manufacturing. The focus was mainly on two processes: post exposure bake and double patterning. They can be described by systems of reaction-diffusion equations with nonlinear diffusion, spatially varying coefficients, and extremely varying time scales.

Afterwards, the numerical approach applied in the project was investigated and improved. A robust, accurate, and efficient fully implicit Voronoi finite volume discretization for reaction-diffusion systems was constructed in [5].

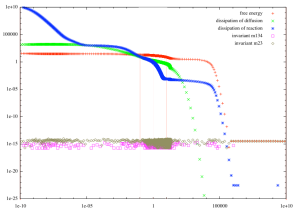
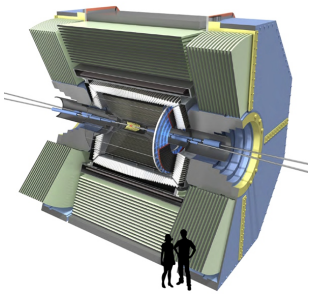


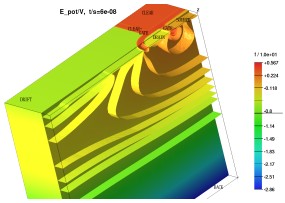
Fig. 1: *Evolution of the relative free energy (red) and the reactive (green) resp. diffusive (blue) contributions to the dissipation rate*

Due to several favorable properties of the discretization like mass conservation, positivity, monotone and exponential decay of the free energy, the proposed algorithm allows to perform long-term simulations over several magnitudes of time, until the thermodynamic equilibrium is reached; see Figure 1. The mathematical highlight is the (two-dimensional) proof of uniform upper and positive lower L^∞ bounds for reaction-diffusion systems with at most quadratic reactions in [4], which includes, e.g., the famous Michaelis–Menten–Henri kinetics. The challenge of the proof was that reaction-diffusion systems do not satisfy maximum principles. Nevertheless, depending on the order of the reactions and the space dimension, L^∞ bounds could be proved for some cases by a Moser iteration technique. This technique was transferred for the first time to a discrete finite volume setting. These uniform bounds allowed also to prove convergence for the fully discretized nonlinear problem.

Semiconductor device simulation

This WIAS application area was extended in collaboration with the Research Group *Partial Differential Equations*, the Technische Universität Dresden, and others to organic semiconductors,





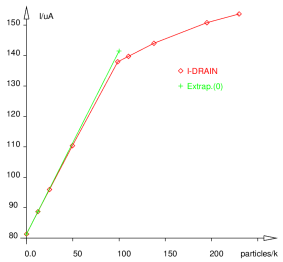


Fig. 2: *(a) Belle2 detector: The double layer DEPFET pixel detector occupies the central region,*
(b) the most expensive cola can of the world shown with a known counterpart,
(c) electrostatic potential in one half-pixel,
(d) a computed "lin-log"-like amplification curve, one design goal is to minimize perturbation effects.

OLEDs, and different transistor types. New concepts to handle general distribution functions, aiming mainly at III-V semiconductors (VCSEL, SFB 787) and organic materials, got attention. On the other hand, the three-year collaboration project with Halbleiterlabor München (HLL) of the Max Planck Society, in some aspects a continuation of the European XFEL detector collaboration, was aiming in its first year at contributions to the design of the innermost detector of the international high energy physics experiment Belle2 at KEK in Japan, see Figure 2.a. Its goal is to test the limits of the standard model of particle physics mainly by improving the measurement precision. That means especially smaller errors in particle position and momentum close to the origin of the first particle cascade, hence better detectors to get the results without tremendously increasing the particle energy.

One should imagine a cylindrical "camera" with 2 cm radius surrounding the vacuum tube and taking 50 000 pictures per second, each frame consisting of the multi-bit information from eight million pixels; Figure 2.b. A best-possible signal-to-noise ratio favors a DEPFET (DEPleted Field Effect Transistor)-based pixel design. That means each pixel has its own amplifier and a reset switch, hence the data is amplified before it reaches the large noisy metal layers. Furthermore, the influence of the detector on secondary particle cascades has to be minimized, hence the silicon is thinned to 75 μm. The detector must be radiation hard, fast, and it has a limited power budget that is imposed by the cooling conditions. Finally, it has to collect at least 90% of the electrons generated in the silicon by any event.

The three-dimensional simulations at WIAS helped to improve the charge collection, the speed, and verified a sufficient distance of the initial working conditions to all operational limits, including especially the expected shifts of the working conditions due to radiation damage. The typical time scales in the simulations are: generation of the electron-hole cloud: 1 ps; shortest electron travel time from bottom to top: 1 ns; charge collection time: smaller than 30 ns, distance of the slowly changing quasi-steady states to the steady state: seconds. The devices are now in production at HLL.

The working scheme of a DEPFET is based on a depleted volume with two MOSFETs (Metal Oxide Semiconductor Field Effect Transistors) on "top". The amplifier MOSFET has two gates, the applied voltage of the ordinary one defines the amplification. The buried "internal" gate of positively charged ions beneath the channel has to collect the electrons created in the lower 95% of the silicon, they change the electrostatic potential below the hole-conducting MOSFET channel and change the amplification, hence modulate the measured current roughly proportionally to the number of electrons stored in the "internal" gate. To collect the electrons from the next collision of positrons and electrons in the accelerator beams, the electrons in the "internal" gate have to be removed. That is done by applying a high voltage at the clear contact and the clear gate, which form, together with the "internal" gate, the switching MOSFET. This working cycle is studied in the numerical simulations; see Figure 2.c, d.

The next algorithmic challenge is to handle pixel-pixel interaction in cases where the amplifier characteristics have to approximate a "lin-log" behavior instead of being close to linear. The status of neighboring pixels will influence the very small potential barriers that control the "log" branch of the amplifier. The goal is to deduce the number of collected electrons in the pixel of interest by including the status of all its neighbors.

Computational hemodynamics and biological tissues modeling

Backflow stabilization. In computational fluid dynamics, open boundaries are typically treated imposing stress boundary conditions, neglecting convective effects at the outlets, and assuming that the flow velocity is mainly one-directional. In oscillatory regimes, as in the case of blood flows in the main arteries, this assumption is not always fulfilled, and instabilities might appear at the Neumann boundaries during backflow, i.e., when the flow enters the computational domain from the open boundaries (see, e.g., Figure 3). In [1], a stabilization was proposed that, besides fitting naturally in a finite element framework, is able to robustly control backflow instabilities. The method is based on a stabilization term aimed at regularizing the tangential derivative of the velocity at the open boundary, introducing an additional dissipation proportional to the backflow. Through several numerical examples, the performance and the accuracy of the method have been validated in classical benchmarks, against analytical solutions, and in a physiological aortic blood flow, against existing up-to-date methodologies.

Multiscale hemodynamics in cerebral veins. A further research topic, carried out in collaboration with the University of Trento, focuses on the numerical simulation of cerebral venous hemodynamics in the presence of *stenosis*, a pathological reduction of the blood vessel's cross-sectional area. In order to approach this problem, a multiscale model was developed in [3], coupling a three-dimensional finite element solver for blood flow in the major cervical veins with a one-dimensional finite volume scheme for the upstream cerebral network. Furthermore, the effect of different levels of occlusion of the internal jugular veins on the cerebral venous flow was investigated through a computational model of stenotic configuration starting from a patient-specific geometry.

Multiscale modeling of soft tissues. The main focus of this research, developed in the framework of a DFG program for the *Initiation of a Bilateral Cooperation* between WIAS and the *Pontificia Universidad Catolica de Valparaiso* (PUCV, Chile), is the study of biological tissues in *Magnetic Resonance Elastography* (MRE), a non-invasive technique used by clinicians to estimate mechanical properties of tissues through harmonic excitations. In collaboration with the research group MRE of the *Charité* (Berlin), a computational model for soft tissues composed of an incompressible elastic matrix and several small (compressible) gaseous inclusions was studied in [2]. Through an asymptotic expansion and a two-scale homogenization, the original problem was simplified, deriving an effective equation for a macroscale compressible material. In [2], it was shown that this multiscale approach can be used to efficiently solve inverse problems in time-harmonic regime, to recover tissue properties depending on the microscale (such as porosity) using only macroscale computations.

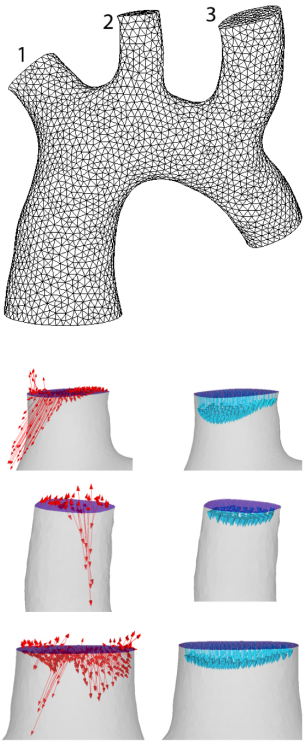


Fig. 3: *Effect of tangential stabilization. Top: computational mesh of an ascending aorta. Bottom: velocity profiles at three different outlets during backflow with (cyan) and without (red) stabilization.*

Macroscopic modeling of transport and reaction processes in magnesium-air batteries

Starting mid 2013, the group participates in the interdisciplinary research network "Perspectives for Rechargeable Magnesium-Air Batteries", which is funded by the German Ministry of Education and Research in the framework of the Research Initiative Energy Storage Systems of the German

Federal Government. Project partners are experimental and theoretical groups in the field of electrochemistry at the Universities of Bonn and Ulm, and the Center for Solar Energy and Hydrogen Research Baden-Württemberg. The investigation of magnesium-air batteries is part of the research efforts in the broader field of post-lithium-ion batteries. Principal advantages of such batteries would be the higher energy density, due to the replacement of the insertion cathode by a lighter air electrode, and the potentially higher availability of magnesium as raw material. The network intends to perform basic research on possible electrode and electrolyte materials for this kind of batteries.

The WIAS subproject is primarily aimed at the development of macroscopic models for components of magnesium air batteries. Topics of particular interest are pore models for the gas cathode, which shall improve the understanding of the coupling between species transport and oxidation reactions. These reactions involve precipitation of magnesium peroxide, influencing the available transport cross section. Another part of the WIAS project is devoted to the quantitative interpretation of measurements in electrochemical thin-layer flow cells with the aim to extract transport, solubility, and reaction parameters.

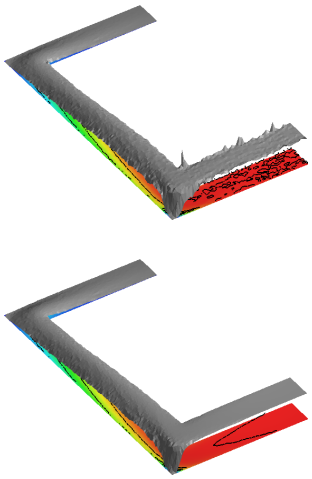


Fig. 4: *Concentration of dissolved species flowing into an U-shaped channel. Top: flow computation with Crouzeix–Raviart element. Bottom: flow computation with additional velocity field reconstruction.*

Currently, the underlying simulation tool for coupled fluid flow and species transport is improved. It will be based on a novel divergence-free discretization approach for the solution of the Navier–Stokes equations that uses the Crouzeix–Raviart finite element with appropriate velocity postprocessing [6]. The method is coupled to the Voronoi box-based finite volume method for species transport. This approach will allow for a more efficient solution of the Navier–Stokes equations in comparison to the previously used Scott–Vogelius finite element while guaranteeing the discrete maximum principle for the concentration of the transported species; see Figure 4.

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4.4 Research Group 4 "Nonlinear Optimization and Inverse Problems"

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

In 2013, the group continued its participation in the DFG Priority Program SPP 1204, and it was actively engaged in the DFG Research Center MATHEON with four projects (B20, C7, C11, and C30). The group was involved in two privately funded projects with industrial partners. In addition, it coordinated two collaborative projects with scientific and industrial partners; see also pages 119 ff. One is funded by the Central Innovation Program for small and medium-sized enterprises ZIM. The other was part of the BMBF Program "Mathematics for Innovations in Industry and Services" and was concluded last year with a successful final meeting, held on September 26 at ZF Friedrichshafen AG. Some achievements of the project are presented in the Scientific Highlights article on page 55.

A special highlight of last year's work was the organization of the IFIP TC7.2 Workshop "Electromagnetics — Modelling, Simulation, Control and Industrial Applications", May 13–17, 2013, together with the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*. Researchers from academia and industry discussed recent achievements in electromagnetics ranging from finite and boundary element discretization methods for the electromagnetic field equations in frequency and time domain to analysis, optimal control, and model reduction for multi-physics problems involving electromagnetics to direct and inverse scattering problems.

In the following, further scientific achievements of the research group in 2013 are detailed.

Inverse Problems

The group's work on elastic wave scattering by diffraction gratings and rough surfaces was continued [3]. The rough surface is supposed to be the graph of a bounded and uniformly Lipschitz continuous function on which the total elastic displacement satisfies either the Dirichlet or the impedance boundary condition. Based on a variational approach in weighted Sobolev spaces, uniqueness and existence results at arbitrary frequency were established for both elastic plane wave and point source (spherical) wave incidence in the two-dimensional case. In particular, the approach covers the elastic scattering from periodic structures (diffraction gratings), and quasi-periodicity of the scattered field is proved whenever the incident field is quasiperiodic. Moreover, the diffraction grating problem is also uniquely solvable in weighted Sobolev spaces for a broad class of non-quasiperiodic incident waves.

For the scattering of electromagnetic plane waves by rough surfaces, the surface is supposed to be the graph of a modulated almost-periodic function. A low contrast between cover material and substrate is assumed so that the Born approximation can be applied. For this situation, new formulas for the reflected and transmitted far fields were derived in the challenging case where the

singularity of the Fourier-transformed parametrization is enhanced by the singularity of the reciprocal symbol of the partial differential operator. The implementation of these formulas into a Monte Carlo algorithm allows to generate plots of the scattered far field for stochastic rough surfaces (cf. Figure 1). In other words, measuring the diffuse extreme uv field scattered by rough interfaces, parameters of these stochastic interfaces can be detected.

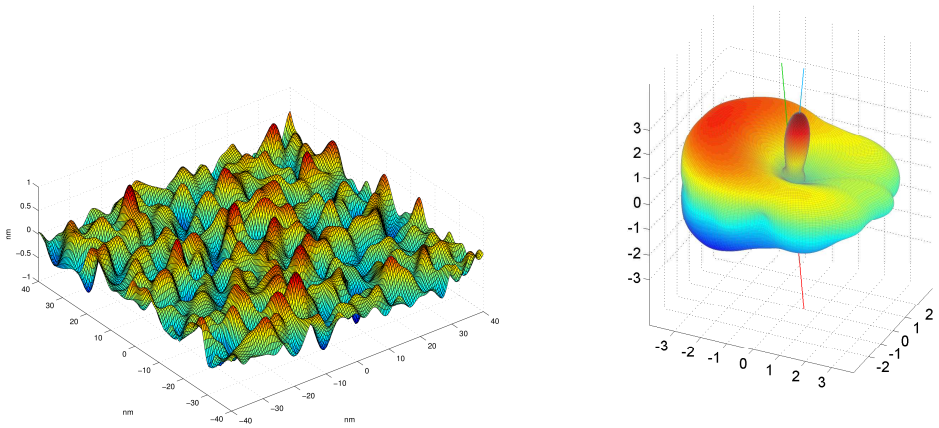

Fig. 1: *Left: example of an almost periodic rough surface. Right: averaged power density of the non-specular scattered wave.*

In connection with the joint ZIM project "Grating simulation in field tracing" with LightTrans GmbH Jena, the work on new features of the integral equation solver for conical diffraction was continued. The aim is the development of an enhanced and robust simulation method for diffraction gratings based on the integral method and its subsequent adaption to the field tracing approach and its software realization by the project partner. A very convenient spline representation of curved profiles with corners was developed. The goal is the parametric spline interpolation of periodic and closed (nonsmooth) curves in the plane that is determined only by the interpolation nodes, but should respect corners of curves and certain convexity properties. Several tests suggested to use an extension of the Steffen spline interpolation, designed for the approximation of monotonic functions. For large classes of curved grating profiles with corners, this new spline interpolation method achieves rather impressive approximation results and will be part of the preprocessing steps of the "Virtual Lab" software of LightTrans GmbH Jena.

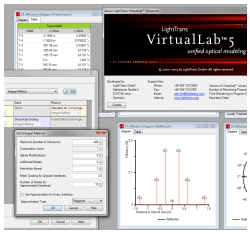

Fig. 2: *Screenshot of the VirtualLab software with the WIAS integral equation solver*

Motivated by the interests of LightTrans GmbH, integral methods for solving biperiodic grating problems were studied. An integral formulation of the corresponding transmission problem for Maxwell's equations was established, which exhibits similar properties as the integral formulation for conical diffraction, employed in the project. The analysis of this single equation approach shows the equivalence to the electromagnetic formulation and provides conditions ensuring that the corresponding singular integral equation acting on tangential fields of the grating surface is Fredholm and admits a possibly unique solution. The single equation formulation for one-surface problems is the basis of integral methods for biperiodic multi-surface gratings. Using known marching approaches for the periodic setting [6], two recursive approaches for the simulation of biperiodic multi-surface gratings were developed and analyzed.

Optimization and optimal control

The group continued its research in the areas of stochastic and nonsmooth optimization associated with 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 with Open Grid Europe GmbH. Benefitting from previous theoretical results, the work on probabilistic constraints shifted its focus to implementing algorithmic solution approaches. These approaches were applied to optimization problems with renewable energies under uncertainty. Major challenges in this respect were the embedding of probabilistic constraints into SQP solvers or the solution of stochastic mixed-integer nonlinear programs (SMINLPs). As an instance, Figure 3 illustrates the optimized operation profile of a water turbine in either off state or within positive working limits. Here, on/off switching is modeled by binary decision variables. The progress achieved in the numerical treatment of probabilistic constraints was presented in a plenary talk at the 13th International Conference on Stochastic Programming. Moreover, a Ph.D. thesis associated with Electricité de France and co-supervised by this research group was successfully defended and led to several joint publications.

Another topic of intensive research arose from second-order subdifferential calculus, which is of particular interest for the derivation of stationarity conditions in mathematical programs with equilibrium constraints (MPECs). Major progress was achieved along the following directions: a) computation of the graphical derivative and the Fréchet coderivative for the solution map to generalized equations; b) explicit formula for the second-order limiting subdifferential of maximum functions; c) conditioning of two-stage stochastic optimization problems using tools from second-order variational analysis. This last work [4] will appear in a special volume dedicated to the 50th anniversary of convex analysis.

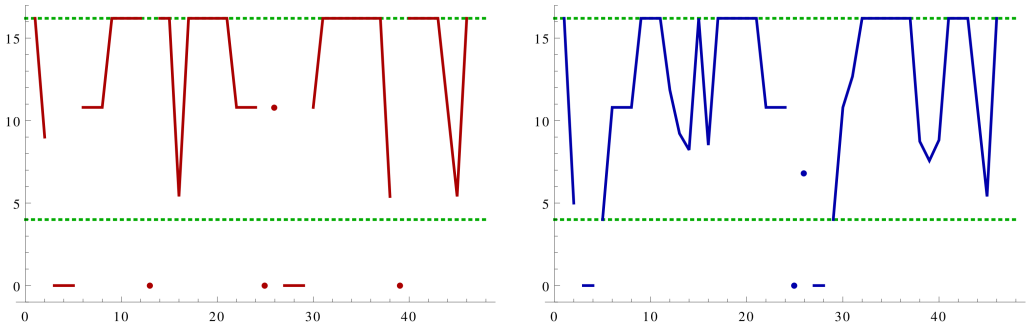

Fig. 3: *Optimal working profiles (affected by uncertainty) for a water turbine with positive operation limits (green) when switched on. Expected value solution (red) vs. robust solution using probabilistic constraints (blue).*

In the MATHEON project C30 "Automatic reconfiguration of robotic welding cells", a new approach was developed to find the fastest collision-free trajectory of a robot moving between two given positions [5]. The optimal trajectory is obtained by solving an optimal control problem. A direct method was used to solve this problem. The convergence of the solving method highly depends on the initialization of the control variables. Therefore, the main focus of the new approach was on the computation of a good initial trajectory. For that purpose, a two-step method was developed leading to a faster and more robust computation of the optimal trajectory. The new approach was then integrated into the algorithm that minimizes the makespan of robotic welding cells.

Phase field models give an alternative to shape calculus in treating structural optimization problems. In collaboration with the group of Harald Garcke (Universität Regensburg) and Vanessa Styles (University of Sussex), a phase field approach was developed to model structural optimization problems. It covers both mean compliance and compliant mechanism problems. A formal asymptotic analysis was performed to investigate the asymptotic limit (sharp interface limit) of the optimality system. Comparing this result with results obtained by the group of Grégoire Allaire (École Polytechnique, Palaiseau) for a simplified case, the authors could show that the phase field model was a good approximating model for structural topology optimization. Several numerical examples confirmed this investigation [1].

In the MATHEON project C11 "Modeling and optimization of phase transitions in steel", a new theorem on the differentiability of a minimax function was proposed. This fundamental new result simplifies the derivation of necessary optimality conditions of PDE-constrained optimization problems. It represents a generalization of the celebrated theorem of Correa–Seeger for the special class of Lagrangian functions.

In the framework of the DFG SPP 1204 project "Simulation, optimization and control of microstructure evolution and mechanical properties during hot rolling of multiphase steels", a SQP solver for the optimal control of a cooling line for the production of hot-rolled dual-phase steel was developed. Numerical results and an experimental validation are published in [2]. A preprint with further algorithmic details is in preparation.

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4.5 Research Group 5 "Interacting Random Systems"

The group continued its research activities on a number of topics like branching random walks in random environment (see the Scientific Highlights article on page 39), metastability of certain disordered systems, interacting many-body systems, random walks among random conductances, connectivity in large mobile ad-hoc systems, and the topics described below. In this way, a number of timely applications of large interacting random systems are under study in various areas like kinetic theory, biological evolution, statistical mechanics, and telecommunication networks.

In 2013, some successful long-term activities of the group came to their end, like the nationwide DFG Research Unit FOR 718 *Analysis and Stochastics in Complex Physical Systems*, headed by Wolfgang König, and three Ph.D. projects supervised by him (Tilman Wolff, Michele Salvi, and Mathias Becker). On the other hand, two new young researchers joined the group, Luca Avena in the DFG Priority Program (SPP) 1590 "Probabilistic Structures in Evolution", and Marion Hesse, who is in charge of fostering the bonds between the fields of analysis and probability at WIAS.

In 2013, the group was very active and successful in the submission of applications for third-party grants. The biggest success was the award of a new Leibniz group entitled "Probabilistic Methods for Mobile Ad-hoc Communication Systems". This group will take up its activities in summer 2014, jointly with our strategic partner, the IHP – Innovations for High Performance Microelectronics (Frankfurt/Oder). Furthermore, a DFG grant for one postdoc position for two years was awarded in the field "Random mass flow through random potential". Moreover, two members of the group are involved in a new proposal for a Collaborative Research Center (CRC), led by the Freie Universität Berlin, on "Scaling Cascades in Complex Systems". One of the two projects in this CRC proposes a close collaboration with the Research Group RG 3 *Numerical Mathematics and Scientific Computing*.

Jointly with other WIAS research groups, RG 5 also organized some interdisciplinary international workshops, the conference "QMath12 – Mathematical Methods in Quantum Mechanics" (also jointly with Humboldt-Universität zu Berlin), and the WIAS Workshop "Partial Differential Equations with Random Coefficients", jointly with the Research Groups RG 3 *Numerical Mathematics and Scientific Computing*, RG 4 *Nonlinear Optimization and Inverse Problems*, RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, and the Young Scientists' Group *Modeling of Damage Processes*.

A closer description of some of the group's achievements in 2013 follows.

Coagulation processes with transport

Many processes in chemical engineering have been successfully modeled by stochastic particle systems in recent years. For example, the formation of soot particles in combustion systems is a highly complex process, which needs rather sophisticated modeling of the resulting soot particle populations (see Figure 1). The stochastic approach allows for very detailed models of individual particles to be included with little additional impact on computation times. Another example is the process of formation and growth of silica nanoparticles. In collaboration with the Department

of Chemical Engineering and Biotechnology (University of Cambridge, UK), a mathematical model for such processes was developed. In this model, each particle is described by its constituent primary particles and the connectivity between these primaries. Each primary, in turn, has internal variables that describe its chemical composition. In [4], stochastic weighted algorithms were applied to this multidimensional particle model. The weighting mechanisms are designed in such a way that various physical processes changing individual particles (such as growth, or other surface reactions) can be 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.

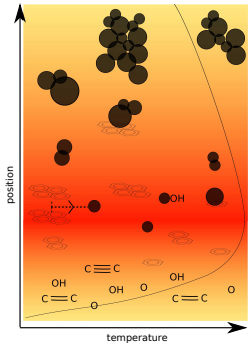

Fig. 1: *Flame diagram*

A common tool for the mathematical treatment of the subject are nonlinear partial integro-differential equations. The close connections between these equations and stochastic interacting particle systems provide the basis both for analytical studies and for numerical approximations. Convergence of the particle system to a deterministic limit was proved. A particular achievement was the treatment of bounded domains with realistic boundary conditions. A challenging problem is to understand the qualitative approximation properties of the algorithms. Stochastic particle methods depend on several discretization parameters, due to the finite number of particles, the decoupling of transport and interaction (time step), and the spatial delocalization of the interaction (cell size). The paper [5] studies the dependence on the cell size of the steady-state solution obtained in the infinite-particle-number limit. Sufficient conditions for second-order approximation are provided. Examples are given, where only first-order approximation is observed.

The mass of super-Brownian motion upon exiting balls

Branching particle systems are stochastic population models whose individuals live and reproduce independently of each other and identically in distribution. During their lifetime, the individuals move in space according to some Markov process. Superprocesses are measure-valued branching processes that arise as the short-lifetime and high-density limit of a certain discrete branching particle system.

In [3], a so-called super-Brownian motion X is considered, which is a superprocess with underlying Brownian spatial motion in $\mathbb{R}^d$. One is interested in the total mass of X as it first exits an increasing sequence of balls B_r of radius r. This is described by the processes $Z = (Z_r, r > 0)$ defined as $Z_r = ||X_{B_r}||$, where $||X_{B_r}||$ denotes the total mass of the so-called *exit measure* X_{B_r}. Intuitively, the exit measure X_{B_r} is a random measure that is supported on the boundary of B_r and obtained by "freezing" the mass of X when it first exits B_r. The radii r of the sequence of increasing balls become the time parameter of Z.

The total mass process Z turns out to be a time-inhomogeneous continuous-state branching process, meaning that it is a $[0, \infty]$-valued branching process whose law is determined by a branching mechanism, say $\Psi(\cdot, r)$, which changes as time evolves. The research group was able to characterize the branching mechanism $\Psi(\cdot, r)$ and show that it converges, as time goes to infinity, towards the branching mechanism of the total mass of a super-Brownian motion in $\mathbb{R}$ as it first crosses an increasing sequence of levels. This result allows the group to give a probabilistic interpretation for a well-known analytical condition regarding compactness of the support of X.

Random partitioning and well-distributed points in a graph

Consider a finite weighted oriented connected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. Denote by $\mathcal{F}$ the set of spanning oriented rooted forests on $\mathcal{G}$. In [1], the group studied a certain natural probability measure $\mathbb{P}$ on $\mathcal{F}$. Several results were derived, relating this measure to the random walk X associated with the weighted graph $\mathcal{G}$, with the spectrum of its generator and with hitting times of subsets of the graph. In some sense, the random forest Φ sampled from the measure $\mathbb{P}$ induces a "good" random partition of the graph.

Among other results, the group proved that the set of roots $\rho(\Phi)$, i.e., the set of points that are the roots of the trees constituting Φ (the distinguished red points in Figure 2), is a determinantal process. Roughly speaking, this means that these roots are random points that repel each other. In other words, the points in $\rho(\Phi)$ are "well" distributed in the graph. For example, it turns out that on average, no matter where the random walk X starts, it hits the set of roots $\rho(\Phi)$ in the same amount of time, independently of the geometry of the graph.

The same property still holds when conditioning the law $\mathbb{P}$ on a given number of roots. For practical purposes, the so-called *Wilson algorithm* and variants of it provide a way to sample the measure $\mathbb{P}$ with and without conditioning. The "nice" properties of this measure allow to use it for some sub-sampling procedures that may have applications in metastability and signal treatment (wavelets). Morever, in [1], the group introduced two different coalescence and fragmentation processes in which trees of a forest can merge or can be fragmented. The latter may have applications in theoretical biology. Together with co-authors, the group is currently investigating these directions.

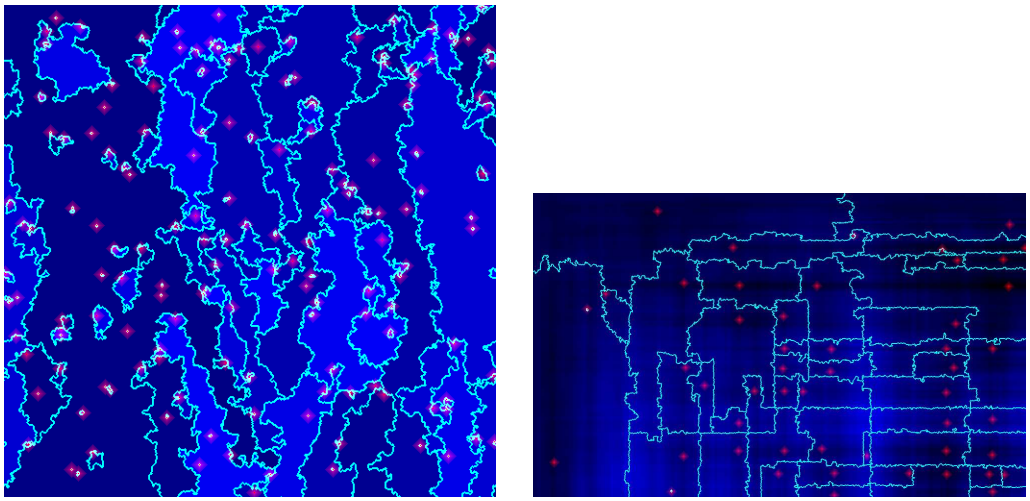

Fig. 2: *Two examples of a partition induced by a realization of this random forest when the underlying graph is a square lattice box with two different weights. Each component of these partitions is constituted by points of the graph belonging to the same tree. The distinguished red points represent the roots of the trees.*

Anderson localization at the spectral boundary of a random Schrödinger operator

The random Schrödinger operator $\Delta + \xi$, where Δ is the standard Laplace operator on $\ell^2(\mathbf{Z}^d)$, and $\xi = (\xi(z))_{z \in \mathbf{Z}^d}$ is a random i.i.d. potential, describes conductance properties of metal alloys

or optical properties of glasses with impurities. For decades, the phenomenon of Anderson localization has been of great interest, i.e., the fact that the total mass of its eigenfunctions, at least for eigenvalues close to the boundaries of its spectrum, are strongly concentrated at random locations. There are two main proof methods known, both of which do not give any description of geometric properties of the random field in the localization regions.

In [2], the group derived a third, independent proof method for Anderson localization that gives a clear picture of the random landscape ξ in the relevant regions, but, however, works only directly at the edge of the spectrum. This restriction is due to a crucial use of (probabilistic) extreme value theory, which yields a description of the limiting point process of localization centers and corresponding rescaled eigenvalues as an explicit Poisson point process. The shape of the potential ξ in the relevant regions had been known previously; it is described as the solution to a certain characteristic variational problem. The result will be employed in future work for proving that the solution to the (time-dependent) Cauchy problem for $\Delta + \xi$ is concentrated in just one of these regions, which was the original motivation.

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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 120 ff. Members of the research group participate in the DFG Research Unit 1735 "Structural Inference in Statistics: Adaptation and Efficiency".

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 2013 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 2013:

- Prolongation of the mega grant with the Moscow Institute of Physics and and Technology for two more years 2014–2015
- Jörg Polzehl was elected Fellow of the Institute of Mathematical Statistics (IMS)
- Book publication by Thorsten Dickhaus [3]
- Distinguished paper (with discussion) in the Journal of Statistical Planning and Inference

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 situations with large parameter sets under possible model misspecification was developed further and applied to solving some important problems in statistical inference, including the Fisher expansion for the (quasi) maximum likelihood estimator, the Wilks expansion for maximum likelihood, the Bernstein–von Mises theorem for the posterior distribution of the parameter, etc. A particularly important problem is the so-called *dimensional asymptotics*; to know how fast can the parameter dimension grow with the

sample size so that the important parametric results are still valid. The new approach appeared to be very helpful and efficient in this question and allowed to find the critical dimension for different problems and models.

The power of the new methodology is well illustrated by the application to the problem of estimating the conditional quantile curve. [1] provides a rigorous solution to the prominent problem of pointwise bandwidth selection in nonparametric quantile estimation, and it is published as a distinguished paper with discussion in the Journal of Statistical Planning and Inference.

A reformulation of the criterion for parameter selection enabled further insight into theoretical properties of the Propagation-Separation approach in exponential families.

Many complex models in various fields of applications are built on stochastic differential equations driven by Brownian motion. It turned out that the classical maximum likelihood techniques for the statistical analysis of these models exhibit stability problems when they are investigated in a pathwise manner. Explicit examples were constructed for which the classical estimators explode in sup-norm although the observation path is well behaved. This very undesirable property can be overcome by using rough paths theory, which was employed to obtain a new class of estimators that are stable in sup-norm and still have the strong optimality properties that the classical theory yields. These results are a first step in applications of rough paths to statistical problems, and it seems to be a very promising new field of interaction.

Another line of research is on a forward-reverse algorithm for the simulation of conditional expectations of a general Markov chain and its applications to the widely used expectation-maximization (EM) algorithm. Due to its popularity, an extension of the EM algorithm to a Markov chain setting will be of great value for many models where explicit inference techniques are not applicable.

The investigation of efficient estimation methods for stochastic differential equations driven by Lévy processes remains an active topic. In [2], the efficiency of maximum likelihood estimators for the drift in a general Lévy setting was demonstrated when a jump filtering approach is used to recover the continuous part of the process before the maximum likelihood estimator is employed. These theoretical results are now applied in system biology in a joint project with groups at the University of St Andrews and the Leibniz Institute for Zoo and Wildlife Research in Berlin (IZW).

A new collaboration with the Wellcome Trust Center for Neuroimaging at the University College London was established, leading to several joint publications. Among the results were new algorithms for structural adaptive signal enhancement in multi-shell diffusion-weighted magnetic resonance experiments and for diffusion kurtosis imaging. Preliminary work for a new neurostatistical approach to the dynamics of learning was started with colleagues from the Leibniz Institute for Neurobiology in Magdeburg. Former results on adaptive segmentation in functional magnet resonance imaging were licensed to Brain Innovation, Maastricht, as part of their BrainVoyager QX software.

Further new results demonstrated the potential of binary classification methods employing multiple testing-based loss criteria for the analysis of multivariate stationary time series. These were applied in brain-computer interfacing, in cooperation with the Berlin Brain-Computer Interface group at Technische Universität Berlin. A randomization scheme for p-values corresponding to multiple tests of composite null hypotheses that enables an accurate estimation of the proportion of true nulls was developed. A formal mathematical foundation of effective numbers of tests was provided

based on probability bounds of higher order. These results were applied to genetic association studies, a next-generation genotype sequencing approach, in brain-computer interfacing, and in epigenetics.

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. Also there is a strong expertise in financial (interest rate) modeling, effective calibration, and the modeling of financial derivatives, such as interest rate and energy derivatives.

Highlights 2013:

- Successful defense of Ph.D. thesis by Jianing Zhang ("summa cum laude")
- Cooperation contract with HSH Nordbank

The innovative multilevel approach in the context of dual valuation for American options was elaborated in the publication [5]. In this approach, the multilevel idea was used for significantly reducing the complexity due to sub-simulations necessary for constructing the dual martingale. Before, the multilevel idea was virtually exclusively applied to the size of the time steps used in the simulation of stochastic differential equations. Further, the linear Monte Carlo algorithm for optimal dual martingales developed for American options in the preceding year (Schoenmakers, Huang, Zhang (2013)) was generalized to standard multiple exercise options, such as chooser interest rate products (e.g., chooser caps) by Balder, Mahayni, Schoenmakers (2013).

Nowadays in finance, asymptotic theory and the need for asymptotic formulas for option prices is emerging more and more. In this respect, the work [6] is considered a breakthrough. It is based on density expansions for projections of hypoelliptic diffusion processes and depends on a fine understanding of the geometry induced by the diffusion. On the theoretical side, the work obtains a much finer understanding of the expansion of the terms and a new geometrical sufficient condition for the expansion to hold. This work led to new asymptotic formulas for option pricing in popular stochastic volatility models such as the Stein–Stein model as well as for basket or spread options in general hypoelliptic diffusion models. Moreover, new insights into the classical problem of the sum of log-normal random variables were consequently obtained by Bayer, Friz, and Laurence (2013).

Another important task of financial engineers is the calibration of (asset) models to market data, which requires fast algorithms for option pricing. Gatheral and Karlsmark have shown that a properly extended version of the Ninomiya–Victoir method (due to Bayer, Friz, and Loeffen) can greatly improve the calibration speed of the double-mean-reverting model when calibrated against typical market products like European options on the S & P 500 index and the volatility index VIX, reducing the computational time of such a calibration by a factor five as compared to classical approximation methods (Euler–Maruyama).

The research on the simulation of conditional diffusions started in 2012 was continued in the present period and culminated in the key publication [4]. This approach turned out to be very useful in the evaluation of derivatives that involve the traded variance of underlying assets, for example, and is based on the forward-reverse simulation developed by Milstein, Schoenmakers, and Spokoiny back in 2004. As such, it may be considered a completely new approach to the problem of conditional simulation. Subsequently, the method was adapted to the setting of discrete time Markov chains, and in a first study, jointly with the project Statistical Data Analysis, applied in the context of parameter estimation for partially observed Markov chains. Indeed, it is a common problem in statistics that only partial observations of a process under consideration are available, for instance, due to coarse observation times. The celebrated EM algorithm is often used in such situations, which basically consists in simulating the missing observations conditioned on the actual observations. Hence, in a Markov model, it requires the simulation of conditional Markov processes or Markov bridges (e.g., Markov chains or diffusions), which is precisely the scope of the new forward-reverse algorithm by [4].

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

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

- Production and application of modern materials
- Energy technology
- Multiscale problems and 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

The origin of Onsager–Casimir reciprocity relations identified. The local nonnegative entropy production ζ of continuum thermodynamics is represented by a sum of binary products $\zeta = \sum_m D_m F_m \geq 0$. The sum runs over all included dissipative mechanisms, and the previous literature calls the factors contributing to the products *driving forces* and *fluxes*. If cross effects between the dissipative mechanisms are ignored, linear constitutive relations may be formulated as $F_m = \lambda_m D_m$ with $\lambda_m > 0$ for each m. If cross effects are taken into account, the linear constitutive relations are written as $F_m = \sum_n L_{mn} D_n$ with L_{mn} positive definite. The Onsager–Casimir reciprocity relations give a characterization of the matrix L_{mn} as either $L_{nm} = L_{mn}$ or $L_{nm} = -L_{mn}$, depending on the corresponding fluxes and driving forces. In the literature, there is the opinion that Onsager has delivered a microscopically based proof of the Onsager–Casimir reciprocity relations. However, it is overlooked that Onsager's reasoning exclusively concerns ordinary differential equations on the macroscopic scale. If partial differential equations are macroscopically involved, the corresponding reasoning is still outstanding, except for simple constitutive models where an underlying kinetic theory is available. A prominent example is the Boltzmann equation for monatomic ideal gases.

In this context, Wolfgang Dreyer, jointly with Dieter Bothe from the Center of Smart Interface at TU Darmstadt, achieved a breakthrough. In the monographic article [1], they identified the origin of Onsager–Casimir reciprocity relations completely within the setting of continuum thermodynamics.

To this end, they removed the notions of *driving forces* and *fluxes*, because these are not uniquely defined, and showed that the entropy production is represented by $\zeta = \sum_m \mathcal{N}_m \mathcal{P}_m$, where $\mathcal{N}_m$ and $\mathcal{P}_m$ indicate quantities of negative and positive parity, respectively. The parity of a quantity can simply be read off from its physical dimension. A quantity has negative parity if its time unit *second* appears with an uneven power and positive if it appears with an even power. Next, they sharpened the dissipation axiom by requiring $\mathcal{N}_m \mathcal{P}_m \geq 0$ for all m and observed: *Mixing within one parity group that leaves the entropy production invariant implies Onsager symmetry.*

The following example with only two dissipative mechanisms serves for illustration. More details and the general case, where also nonlinear constitutive relations are considered, are found in [1].

$$\zeta = \mathcal{N}_1 \mathcal{P}_1 + \mathcal{N}_2 \mathcal{P}_2 = (\mathcal{N}_1 - D\mathcal{N}_2)\mathcal{P}_1 + \mathcal{N}_2(\mathcal{P}_2 + D\mathcal{P}_1) \tag{1}$$

According to the sharpened dissipation axiom, the linear constitutive relations are

$$\mathcal{N}_1 - D\mathcal{N}_2 = \lambda_1 \mathcal{P}_1, \quad \mathcal{N}_2 = \lambda_2(\mathcal{P}_2 + D\mathcal{P}_1) \quad \text{with} \quad \lambda_1,\ \lambda_2 > 0. \tag{2}$$

Thus, there is Onsager symmetry

$$(\mathcal{P}_1, \mathcal{P}_2)^T = \begin{pmatrix} \lambda_1^{-1} & -D\lambda_1^{-1} \\ -D\lambda_1^{-1} & \lambda_2^{-1} + D^2\lambda_1^{-1} \end{pmatrix} (\mathcal{N}_1, \mathcal{N}_2)^T. \tag{3}$$

Then antisymmetry trivially follows by regrouping

$$(\mathcal{N}_1, \mathcal{P}_2)^T = \begin{pmatrix} \lambda_1 & D \\ -D & \lambda_2^{-1} \end{pmatrix} (\mathcal{P}_1, \mathcal{N}_2)^T. \tag{4}$$

Diffusive phase segregation. In 2013, the analysis of a new model for diffusive phase segregation due to Paolo Podio-Guidugli (Rome), given by the phase field system

$$(\varepsilon + 2g(\rho))\,\mu_t + \mu\, g'(\rho)\,\rho_t - \operatorname{div}(\kappa(\mu, \rho)\,\nabla\mu) = 0\,, \tag{5}$$

$$\delta\rho_t - \sigma\,\Delta\rho + \partial f_1(\rho) + f_2'(\rho) \ni \mu\, g'(\rho), \tag{6}$$

was continued. 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 (6) 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).

In the paper *"An asymptotic analysis for a nonstandard viscous Cahn–Hilliard system"*, authored by Pierluigi Colli, Gianni Gilardi, Paolo Podio-Guidugli, and Jürgen Sprekels, that appeared in Disc. Cont. Dyn. Syst. Series S, **6** (2013), pp. 387–400, an asymptotic analysis for the solutions of system (5), (6) was performed as $t \to +\infty$ and as $\varepsilon \searrow 0$. New regularity and continuous dependence results were proved in [4] and in the submitted WIAS Preprints no. 1779 *"Regularity of the solution*

to a nonstandard system of phase field equations" and no. 1784 *"Analysis of a time discretization for a nonstandard Cahn–Hilliard system"*. A full error analysis, with optimal error orders, was carried out for a time discretization of system (5), (6).

In addition to the study of phase field systems of the form (5), (6), the analysis of optimal control problems for Allen–Cahn systems with dynamic boundary condition involving the *Laplace–Beltrami operator* Δ_Γ and bulk and surface potentials of logarithmic type, which was begun in 2012, was in [5] extended to the non-differentiable case of double obstacle potentials involving indicator functions. More precisely, the following state system was studied:

$$y_t - \Delta y + \xi + f_2'(y) = u \quad \text{a. e. in } Q, \tag{7}$$

$$y_{|\Gamma} = y_\Gamma, \quad \partial_t y_\Gamma - \Delta_\Gamma y_\Gamma + \partial_{\mathbf{n}} y + \xi_\Gamma + g_2'(y_\Gamma) = u_\Gamma \quad \text{a. e. on } \Sigma, \tag{8}$$

$$\xi \in \partial I_{[-1,1]}(y) \quad \text{a. e. in } Q, \quad \xi_\Gamma \in \partial I_{[-1,1]}(y_\Gamma) \quad \text{a. e. on } \Sigma, \tag{9}$$

$$y(\cdot,0) = y_0 \quad \text{a. e. in } \Omega, \quad y_\Gamma(\cdot,0) = y_{0\Gamma} \quad \text{a. e. on } \Gamma, \tag{10}$$

with smooth functions f_2, g_2 and given initial datum y_0 with $y_{0\Gamma} = y_{0|\Gamma}$, and where u and u_Γ represent distributed and, respectively, boundary controls. Here, $Q = \Omega \times (0,T)$, $\Sigma = \Gamma \times (0,T)$, where $T > 0$ is given and Γ denotes the boundary of an open and bounded three-dimensional domain Ω.

Owing to the non-differentiability of the indicator functions, it is a very challenging problem to establish ("first-order necessary") conditions that possible optimal controls have to satisfy. In [5], a new so-called *deep quench approach* was devised to derive such necessary optimality conditions. The main idea of this new approach is to approximate the graph of the subdifferential $\partial I_{[-1,1]}$ by the graphs of functions of the logarithmic form $h_\alpha(y) = \alpha\,[(1-y)\,\ln(1-y) + (1+y)\,\ln(1+y)]$ for $\alpha > 0$; a delicate analysis then shows that the known necessary optimality conditions for the approximating differentiable case yield in the limit $\alpha \searrow 0$ corresponding conditions for the non-differentiable case.

Secret of a grease drop decrypted. Under this headline, several daily newspapers reported on an interesting observation made by Barbara Wagner's group jointly with Ralf Seemann from Universität des Saarlandes.

The scientific content of the subject is described in detail in the article *"Droplets on liquids and their long way into equilibrium"* [2]. It concerns the modeling, analysis, and simulation of the late stages of dewetting processes of a thin multi-layer system. It consists of liquid polymethyl methacrylate (PMMA) on a substrate and short-chained polystyrene (PS) above. After some time, PS droplets are formed on the liquid PMMA layer. The mathematical model unexpectedly predicts that the droplets synchronize their evolution independently of the initial geometry and long before the equilibrium state has been reached. The possible equilibria of a liquid droplet with constant

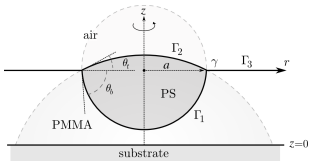


Fig. 1: *Sketch of an axisymmetric liquid lens in equilibrium with $\Gamma_1, \Gamma_2, \Gamma_3$ being the PS/PMMA, PS/air, PMMA/air interface, respectively, and the triple junction*

surface tensions σ_α are established by minimizing the surface energy,

$$E = \sum_{\alpha=1,2,3} \sigma_\alpha \int_{\Gamma_\alpha} d\Gamma, \tag{11}$$

via a deformation of the underlying liquid substrate by the droplet.

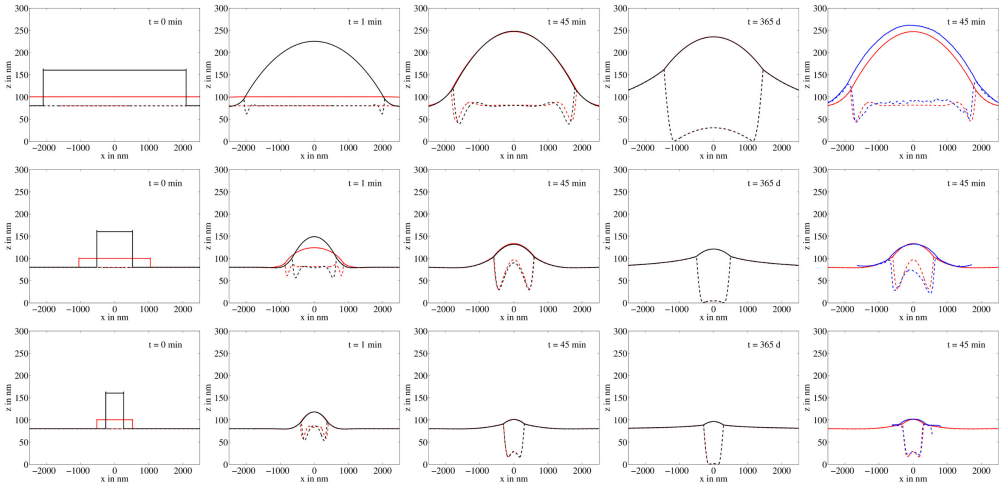


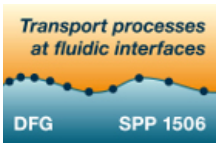
Fig. 2: *Numerical simulations and experimental data. The first plot of each row shows two polystyrene geometries, red and black, having the same volume. The next three plots depict corresponding predicted evolutions of the dewetting process. The solid and dashed lines show the height functions h_1 and h_2, respectively. The fifth plot compares at time 45 minutes the simulations with experimental data.*

In non-equilibrium, the corresponding evolution is described by two coupled degenerate parabolic equations for the height functions (h_1, h_2) of the two liquids,

$$\partial_t h_i = \sum_{j=1}^{2} \nabla \cdot (Q_{ij}(h_1, h_2) \nabla \frac{\delta E}{\delta h_j}), \qquad i = 1, 2. \tag{12}$$

Figure 2 shows for the selected initial values extremely good coincidence between predicted and measured data.

Funded under Priority Programs of the German Research Foundation



Gradient flow perspective of thin-film bilayer flows 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"*. Robert Huth from the Leibniz Group *Mathematical Models for Li-Ion Batteries*, Sebastian Jachalski and Dirk Peschka, jointly with Georgy Kitavtsev from the Max Planck Institute for Mathematics in the Sciences in Leipzig, studied the evolution of a liquid bilayer within the thin-film approximation. Particularly the triple points between both liquids and the surrounding air, which are mostly ignored in the literature, are taken into account. To this end, the thin film equations are rewritten as an evolution driven by a gradient structure, as it has already been done for the corresponding Stokes equations. The details are described in the WIAS Preprint no. 1814 *"Gradient flow perspective of thin-film bilayer flows"*.

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 2013, they developed with Jan Giesselmann a new diffuse-interface model for a liquid electrolyte with N constituents where the solvent may undergo a transition from the liquid to the vapor phase. The model consists of N mass balance equations for the constituents, the momentum equation for the barycentric velocity of the mixture, and an Allen–Cahn equation describing the phase transition. These equations are coupled to the Poisson equation for the quasi-static electric potential. In this case, there are two small parameter that one must send to zero to establish the sharp-interface limit. A parameter δ appears in the Allen–Cahn equation and controls the width of the interface. Moreover, there is a parameter ϵ in front of the Laplace operator in the Poisson equation. ϵ is related to the Debye length and usually leads to boundary layers. However, here there is a delicate interaction between the two parameters. Their ratio determines whether the liquid-vapor interface is a carrier of charged species. The mathematical treatment of the new model is the same as in [6], where the neutral case is considered.

The International Workshop "Two-Phase Fluid Flows – Modeling, Analysis and Computational Methods", organized by Christiane Kraus (YSG) and Wolfgang Dreyer (RG 7), took place at WIAS, February 6–8, 2013. The lectures focused on the diffuse and sharp interface modeling (kinetic relations/configurational forces, generalized Riemann problems), analytical investigations of liquid-vapor flow models, asymptotic regimes (low Mach number, flows in special geometries, boundary interaction), efficient numerical techniques (space/time adaptivity, approximate Riemann solvers, ghost fluid and level-set approach, discontinuous Galerkin), and applications (cavitation, bubble collapse, cooling and boiling, liquid jets).

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"

Project C9, headed by Olaf Klein and Jürgen Sprekels, jointly with Fredi Tröltzsch, Technische Universität Berlin, may serve as an example of a typical MATHEON research project. In recent years, the main focus concerned optimal control problems for crystal growth applications. In 2013, theoretical questions in the same context were mainly addressed. Pierre-Etienne Druet studied the

regularity of the elliptic transmission problem

$$-\mathrm{div}(k_S \nabla\theta) = f \quad \text{in} \quad \Omega \setminus S, \quad [[\theta]]_S = 0, \quad -[[k_S \nabla\theta \cdot \nu]]_S = q \quad \text{on } S, \tag{13}$$

with $S \subset \Omega$ – given interface, k_S – material-dependent interface, f, q – given functions. Here, the interface S has the structure $S = \cup_{i=1}^{m} S_i$, where the surfaces $S_1, S_2, ..., S_m$ have twofold derivatives and may meet at a closed contact line. For $m = 2$, the results are published in [3], while the general case is carefully described and solved in the WIAS Preprint no. 1875 *"Regularity of second derivatives in elliptic transmission problems near an interior regular multiple line of contact"*.

Another investigation addresses the mathematical problems of generalized potential theory. To this end, divergence and curl operators are introduced as functionals in Sobolev spaces. It is proved in the WIAS Preprint no. 1870 *"Higher L^p regularity for vector fields that satisfy divergence and rotation constraints in dual Sobolev spaces, and application to some low-frequency Maxwell equations"* that these functionals yield a higher integrability of vector fields on Lipschitz domains. The new methods introduced are best suited to solve many problems in generalized potential theory. The electrotechnical approximation of the Maxwell equations serves here to illustrate the higher regularity and compactness of the solution operator for rather weak conditions on the data.

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 high complexity. Mainly initial-boundary value problems for nonlinear coupled systems of partial differential equations are involved.

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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. Collaborations exist with the Research Groups RG 1 *Partial Differential Equations* and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* on the modeling and analysis of multifunctional materials.

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.

Analytical investigations on a nonlocal Cahn–Hilliard system with damage were accompanied by numerical simulations within the DFG Research Center MATHEON project C32. Integrated within the nonlocal separation process of interacting particles, the damage process is modeled by the diffusion of voids, representing a special type of noninteracting particles of the multi-component system. The analytical results for the continuous evolution system were carried over to construct a stable and highly accurate numerical scheme for approximate solutions to an appropriately time-discretized system.

Local multi-component systems for describing phase separation and damage processes in solids were analytically studied, for instance, in [2]. The introduced model consists of a parabolic diffusion equation of fourth order for the concentration coupled with an elliptic system with material-dependent coefficients for the strain tensor and a doubly nonlinear differential inclusion for the damage function. The main aim was to show existence of weak solutions for the introduced model, where, in contrast to existing damage models in the literature, different elastic properties of damaged and undamaged material are regarded. This highly nonlinear model covers the intermediate case between incomplete and complete damage that takes care of different deformation properties of damaged and undamaged material. Christian Heinemann very successfully defended his Ph.D. thesis in 2013 on coupled phase separation and damage models.

In addition, hyperbolic-parabolic evolution inclusions defined on Lipschitz domains with mixed boundary conditions were investigated, describing, for instance, damage processes and elasticity

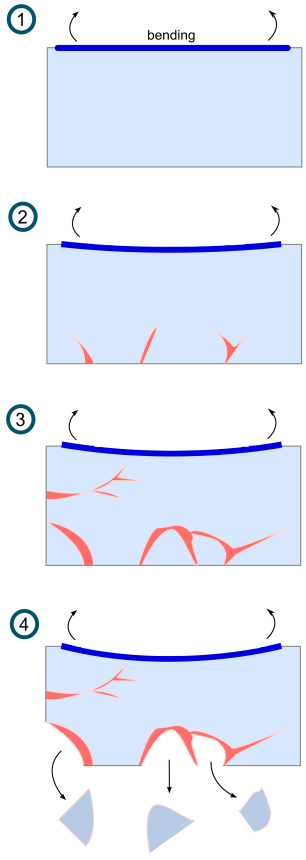

Fig. 1: *Damage formation due to bending, resulting in weakened and completely separated parts*

with inertial effects. Existence results for such systems were shown; cf. [3]. To this end, a suitable weak formulation had to be introduced in order to deal with such evolution inclusions. Then, existence of weak solutions was shown by utilizing time-discretization, H^2 regularization, and variational techniques.

A different question was in the focus of [4], where a vanishing viscosity analysis was carried out for quasilinear damage systems on nonsmooth domains. Relying on refined spatial and temporal regularity estimates for both the displacement field as well as for the damage variable, in a first step, the existence of solutions to a doubly nonlinear evolution inclusion of parabolic type was shown. Thanks to the regularity estimates, for positive viscosity parameters the energy is absolutely continuous along solutions, which allows for switching between different equivalent characterizations of solutions via chain rule arguments. The vanishing viscosity analysis then was carried out in a reparametrized setting.

Typically, in damage models the dependence of the elastic parameters on the damage state is given by phenomenological constitutive relations. One part of the group focuses on the derivation of effective macroscopic damage models, where the influence of the microscopic damage state on the effective macroscopic behavior is justified rigorously using multiscale convergence techniques for evolutionary systems. For further details, the reader is referred to the Scientific Highlights article on page 27.

As a further topic, phase field models for flows of multi-component compressible fluids were investigated. A new thermodynamically consistent diffuse interface model of Allen–Cahn/Navier–Stokes type for multi-component flows with phase transitions and chemical reactions was deduced. For the introduced diffuse interface model, physically admissible sharp interface limits were studied. In particular, two scaling regimes were considered, i.e., a non-dissipative and a dissipative regime, where a generalized Allen–Cahn/Euler system for mixtures with chemical reactions in the bulk phases equipped with admissible interfacial conditions was recovered in the sharp interface limit. The interfacial conditions satisfy, for instance, a Young–Laplace- and a Stefan-type law.

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 "Two-Phase Fluid Flows – Modeling, Analysis and Computational Methods" organized by Christiane Kraus (YSG) and Wolfgang Dreyer (RG 7), took place at WIAS, Febru-

ary 6–8, 2013. The lectures focused on the diffuse and sharp interface modeling (kinetic relations/configurational forces, generalized Riemann problems), analytical investigations of liquid-vapor flow models, asymptotic regimes (low Mach number, flows in special geometries, boundary interaction), efficient numerical techniques (space/time adaptivity, approximate Riemann solvers, ghost fluid and level-set approach, discontinuous Galerkin), and applications (cavitation, bubble collapse, cooling and boiling, liquid jets).

Fig. 2: *Participants of the workshop "Two-Phase Fluid Flows – Modeling, Analysis and Computational Methods", Berlin*

In 2013, Dorothee Knees, jointly with Krzysztof Chelminski (University of Warsaw), organized the Section "Applied Analysis" at the 84th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM) at Novi Sad, Serbia.

Christiane Kraus was also involved in the organization of the workshop "Partial Differential Equations with Random Coefficients" at WIAS, November 13–15, 2013.

References

[1] W. Dreyer, J. Giesselmann, C. Kraus, *A compressible mixture model with phase transition*, WIAS Preprint no. 1832, 2013, to appear in: Phys. D.

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[3] C. Heinemann, C. Kraus, *Existence of weak solutions for a hyperbolic-parabolic phase field system with mixed boundary conditions on non-smooth domains*, WIAS Preprint no. 1890, 2013, submitted.

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

The Leibniz group is externally funded 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

New electrolyte models. For 1.5 years, the Leibniz group has developed various new electrolyte models that significantly change the existing models of the literature in the context of boundary layers between an electrolyte and a solid electrode. A detailed description of the new findings is described in the Scintific Highlights article *"Crucial Revisions of Electro-Chemical Modelling"* on page 49.

The revisions of the classical models are mandatory because the classical models do not appropriately deal with a small parameter λ in the Poisson equation determining the quasistatic electric field. For example, in the electrolyte, λL_0 defines a length scale

$$\lambda L_0 = \sqrt{\frac{kT\epsilon_0}{e_0^2 n_0}}$$

that induces a thin boundary layer between the electrode and the bulk region of the electrolyte. Herein, we have k – Boltzmann constant, T – absolute temperature, e_0 – elementary charge, n_0 – typical particle density of the solute, and L_0 – typical length scale of the electrolyte. By means of formal asymptotic analysis, the Leibniz group derived new boundary conditions for the electrolyte-electrode interface so that many of the classical models will continue to apply, however, with new interface conditions that take care of the boundary layers; see [4], [6].

The basis electrolyte model, developed within LG 3 and published in *Physical Chemistry Chemical Physics* [4], was significantly extended to incorporate solvation effects [6]. Solvation, i.e., the agglomeration of solvent molecules around an ionic molecule, occurs in almost all polar fluids and is considered to be one main effect in the physical chemistry of electrolytic solutions. Even though this effect is well know in physical chemistry and theoretical chemistry, its rigorous incorporation

in continuum thermodynamic mixture theories was still outstanding. However, such mixture theories are the very basis for many model concepts in electrochemistry.

The lead-acid battery, a paradigm of the new model. A complex engineering application is the simulation of a lead-acid battery. Based on the new model and new boundary conditions, charging and discharging cycles were simulated. The lead electrode is modeled by a mixture of Pb^{2+} and free electrons e^-. The other electrode consists of lead oxide PbO_2. In between, there is sulfuric acid $E : H_2SO_4$ that in a solution in water $S : H_2O$ forms the anions $A : SO_4^{2-}$ and cations $C : H_3O^+$ of the electrolyte. Moreover, there are the surface reactions,

$$Pb^{2+} + SO_4^{2-} <=> PbSO_4, \tag{1a}$$

$$PbO_2 + 2e^- + SO_4^{2-} + 4H_3O^+ <=> PbSO_4 + 6H_2O. \tag{1b}$$

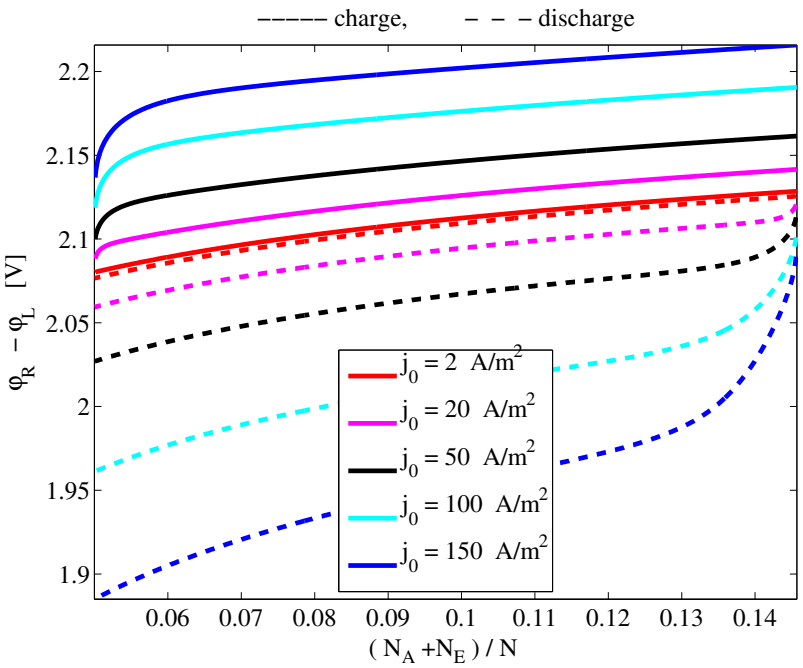

Fig. 1: *Charging–discharging cycles of a lead-acid battery computed with the new boundary conditions including new Butler–Volmer equations. The height of the hysteresis loop depends on the strength of the applied electric current.*

Dissertation

Manuel Landstorfer, member of the Leibniz group since November 2012, very successfully defended his Ph.D. thesis *"Mathematical modeling of batteries based on balance equations and coupled thermo-electrodynamics"* [1] in October 2013 at Ulm University. His Ph.D. thesis, under the supervision of Prof. Dr. Stefan Funken and Prof. Dr. Timo Jacob, is strongly related to his research work in the Leibniz group and covered a thermodynamically consistent derivation of the field equations to describe the instationary behavior of a porous lithium-ion battery cell.

Such porous cells, sketched in Figure 2 on the following page, are highly complex and exhibit inhomogeneous structures for which simplified or reduced models are desired in order to study the

cell behavior for various boundary conditions.

Manuel Landstorfer further showed that the widely used Newman model [2] uses an inadequate material model for lithium intercalation and identified this problem as the origin for the inconsistent prediction of the open circuit potential (OCP). Parts of his thesis were published in the comprehensive review article *"Mathematical modeling of intercalation batteries at the cell level and beyond"* in Chemical Society Reviews [3].

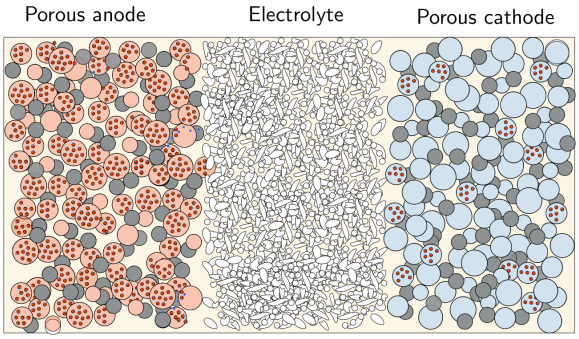

Fig. 2: *Sketch of lithium-ion battery cell, consisting of a porous anode and cathode that are bathed in a liquid electrolyte and separated by a polymeric sponge, which is also soaked with electrolyte.*

Miscellaneous

In 2012, Rüdiger Müller participated in the Volunteer Lecturer Program of the International Mathematical Union, which is developed and sponsored by the Commission for Developing Countries. He was invited as a guest professor by the Urgench State University, Urgench, Uzbekistan. In December 2013, he held a three-week compact course on Numerical Analysis for Partial Differential Equations for students and academic staff.

Wolfgang Dreyer was selected as a member of the Executive Committee of *The International Society for the Interaction of Mechanics and Mathematics*.

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4.10 ERC Group 1 "EPSILON – Elliptic PDEs and Symmetry of Interfaces and Layers for Odd Nonlinearities"

In the framework of the competition for European Research Council (ERC) grants, Enrico Valdinoci received a Starting Grant in January 2012 for a period of five years. At that time still a professor at Milan University, he decided to move his grant to the Weierstrass Institute. On June 1, 2013, he started his work at WIAS and began to build up his new group. In autumn, Stefania Patrizi took up her place as a new postdoc, and more coworkers will follow.

The investigations of the group are dedicated to the analysis of interfaces of layers that arise, e.g., in phase transitions and surface tension phenomena. The focus is on the geometry, structure, and regularity of the interfaces. Mathematically, elliptic variational problems are addressed, in particular, problems involving fractional Laplace operators.

In 2013, Enrico Valdinoci held several research courses and many invited seminars and talks. In the context of the ERC project, he organized and sponsored several events, such as the *International School on Recent Advances in Partial Differential Equations and Applications* in Milan in June, the *Conference on Qualitative and Geometric Aspects of Elliptic PDE's* in Bellaterra in September, and the *Workshop on Nonlinear Equations* in Madrid in October.

Fig. 1: *Bellaterra in September*

Jointly with Stefania Patrizi and many other international collaborators, several research projects were carried out, leading to a large number of papers on topics like asymptotics, Γ-convergence, and density estimates for some nonlocal phase transition equations; nonlinear analysis methods for nonlocal equations; regularity theory for nonlocal minimal surfaces; partial differential equations in anisotropic media; symmetry results and overdetermined problems; dislocation theory in periodic crystals.

Furthermore, Enrico Valdinoci acted as an advisor for the PhD students Alessio Fiscella, Nicola Abatangelo, and Matteo Cozzi, and for the masters students Davide Piazzoli and Luca Lombardini, and he coordinated the research of the postdoc Annalisa Massaccesi at Milan University.

References

[1] A. Chambolle, M. Novaga, E. Valdinoci, eds., *Geometric Partial Differential Equations*, vol. 15 of CRM Series, Scuola Normale Superiore, Pisa, 2013, 400 pages.

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4.11 ERC Group 2 "EntroPhase – Entropy Formulation of Evolutionary Phase Transitions"

In the framework of the competition for European Research Council (ERC) grants, Elisabetta Rocca received a Starting Grant in April 2011 for a period of five years on the above topic. In 2013, she took the decision to move her grant from Milan University to WIAS. Elisabetta Rocca is heading the new group as the principal investigator. The postdoc Sergio Frigeri is working with her. The group's main aim is to get relevant mathematical results and further insight into new models for phase transitions and the corresponding evolution partial differential equation (PDE) systems. Its new approach turned out to be particularly helpful for the investigation of issues like existence, uniqueness, control, and long-time behavior of the solutions to these evolutionary PDEs.

Fig. 1: *Binary mixtures of incompressible fluids*

The new theory of the group is important because phase transition phenomena arise in a variety of applied problems like, e.g., melting and freezing in solid-liquid mixtures, phase changes in solids, liquid crystal flows, soil freezing, damage in elastic materials, plasticity, food conservation, and collisions. In 2013, the group mainly focused on the following subjects:

- Nonlocal version of a phase separation model in binary mixtures of incompressible fluids (cf., e.g., [4]; Figure 1)
- Models for phase transitions in viscoelastic material and damaging phenomena including temperature dependence and complete damage (cf., e.g., [6])
- Evolution of liquid crystal flows (cf., e.g., [1, 2, 3, 5]) (Figure 2)
- Multifrequency induction hardening in steel (Figure 3)

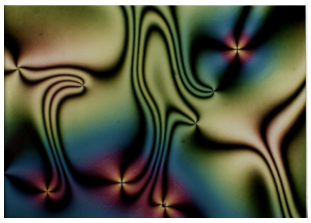

Fig. 2: *Nematic liquid crystals*

The main idea

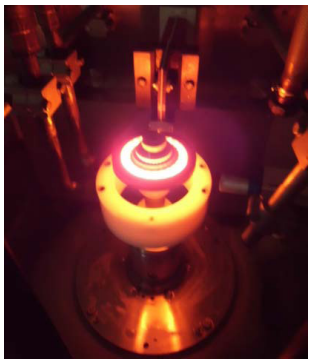

Fig. 3: *Induction hardening*

The main idea is to consider new notions of solution, the so-called *entropic* solutions, reinterpreting the concept of a weak solution satisfying a suitable energy conservation and entropy inequality, which were recently introduced by Eduard Feireisl (Prague) for a problem of heat conduction in fluids. These ideas turned out to be particularly useful in the analysis of highly nonlinear and possibly degenerating PDEs arising from different types of phase transition models. They were already successfully applied in [6], where such a suitable weak solvability notion was needed to analyze a weak formulation of a heat and momentum equation, and, for the phase/damage parameter, of a generalization of the principle of virtual powers.

Moreover, in [2, 3], a three-dimensional model describing the time evolution of nematic liquid crystals in the framework of Ericksen and the Landau–de Gennes theory was analyzed. The natural physical constraints were enforced by a singular free energy bulk potential proposed by John M. Ball and Apala Majumdar (Oxford). The thermal effects are present through the component of the free energy that accounts for intermolecular interactions. The models are consistent with the general principle of thermodynamics and mathematically tractable. The a priori estimates for the

associated system of evolutionary PDEs are identified and global-in-time *entropic* solutions for arbitrary physically relevant initial data are constructed.

Further activities

The group organized international schools and workshops, and group members participated in international conferences and workshops, but knowledge was also exchanged with international experts visiting WIAS, like Prof. Maria Schonbek (University of California, October 4–11, 2013) and Dr. Virginia Agostiniani (University of Oxford, December 10–12, 2013).

Main international meetings and schools organized in 2013.

- *CIRM-ERC Workshop DIMO2013 – Diffuse Interface Models*, Levico Terme, Italy, September 10–13, 2013 (organized with Pierluigi Colli and Giulio Schimperna (Pavia))
- *International School on Recent Advances in Partial Differential Equations and Applications*, University of Milan, Department of Mathematics, Italy, June 17–22, 2013 (coordinated with Enrico Valdinoci (WIAS))
- *Spring School on Rate-independent Evolutions and Hysteresis modelling*, Milan, Italy, May 27–31, 2013 (coordinated with Stefano Bosia (Milan), Michela Eleuteri (Milan), and Enrico Valdinoci (WIAS))

Fig. 4: *International School in Milan in June*

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A Facts and Figures

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

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

A.1 Calls, Awards and Distinctions, Ph.D. Theses, and Undergraduate-degree Supervision

A.1.1 Calls

1. D. Knees, W2 professorship, July 19, Universität Kassel, FB10 – Mathematik und Naturwissenschaften.
2. ———, W3 professorship, December 16, Universität Duisburg–Essen, Fakultät für Mathematik.

A.1.2 Awards and Distinctions

1. D. Knees, *Vice chair of the GAMM Activity Group "Analysis of Partial Differential Equations", Gesellschaft für Angewandte Mathematik und Mechanik*, December 10, 2013.
2. A. Mielke, *Head of the Secretariat of the International Mathematical Union (IMU)*.
3. ———, *Member of the IMU Berlin Einstein Foundation Program Committee*.
4. ———, *Treasurer of IMU*.
5. J. Polzehl, *Fellow of the Institute of Mathematical Statistics, Beachwood, USA*, August 5, 2013.
6. V. Spokoiny, *Mega-Grant of the Russian Government to establish a Research Group "Predictive Modeling" at the University of Physics and Technology in Moscow*.
7. M. Thomas, *GAMM Junior, Gesellschaft für Angewandte Mathematik und Mechanik*, 2013–2015.

A.1.3 Ph.D. Theses

1. M. Becker, *Asymptotische Resultate über Lokalzeiten von Irrfahrten im Z^d* , Universität Leipzig, Fakultät für Mathematik und Informatik, supervisor: Prof. Dr. W. König, November 13.
2. M. Salvi, *The random conductance model: Local times large deviations, law of large numbers and effective conductance*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 22.
3. W. van Ackooij, *Chance constrained programming with applications in energy management*, Ecole Centrale Paris, supervisors: Dr. R. Henrion, Prof. Dr. M. Minoux, December 12.
4. L. Wilhelm, *A rigorous Landauer–Büttiker formula and its application to models of quantum-dot LED*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, March 6.
5. Ch. Heinemann, *Phase separation coupled with damage processes*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisors: Dr. Ch. Kraus, Prof. Dr. J. Sprekels, November 19.
6. M. Hesse, *Branching diffusions on the boundary and the interior of balls*, University of Bath, Department of Mathematical Sciences, supervisors: Prof. Dr. A. Kyprianou, Dr. S. Harris, November 25.
7. M. Landstorfer, *Mathematical modeling of batteries based on balance equations and coupled thermo-electrodynamics*, Universität Ulm, Fakultät für Mathematik und Wirtschaftswissenschaften, supervisors: Prof. Dr. St. Funken, Prof. Dr. T. Jacob, October 11.

8. E. Schmeyer, *Numerische Verfahren zur Simulation von Mehrphasenströmungen mittels Populationsbilanzen*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, August 16.
9. C. Suciu, *Numerical methods based on direct discretizations for uni- and bi-variate population balance systems*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, September 28.
10. T. Wolff, *Random walk local times, Dirichlet energy and effective conductivity in the random conductance model*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 6.
11. J. Zhang, *Non-standard backward stochastic differential equations and multiple optimal stopping problems with applications to securities pricing*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Priv.-Doz. Dr. J.G.M. Schoenmakers, March 21.

A.1.4 Undergraduate-degree Supervision

1. L. Arnold, *Mischungseigenschaft des Random Waypoint Mobilitätsmodells* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 2.
2. F. Beck, *Mehrkriterielle Optimierung eines thermoelektrischen Generators im Fahrzeug* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, December 11.
3. L. Bonorden, *Stochastic homogenisation for the principal eigenvalue in the Anderson model with small disorder* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 16.
4. R. Breese, *Diffusivität gerichteter Polymere in zufälliger Umgebung bei schwacher Wechselwirkung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 11.
5. Ch. Brennecke, *Eine divergenzfreie Rekonstruktion für eine nicht-konforme Diskretisierung der inkompressiblen Stokes-Gleichungen* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Linke, June 5.
6. J. Diekmann, *Markovketten-Algorithmen für zufällige Graphenfärbungen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 13.
7. K.R. Dietsch, *Alterung in verschiedenen Modellen der statistischen Mechanik* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 19.
8. H. Dressel, *Boole'sches Modell mit beschränkter Reichweite* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 13.
9. J. Finke, *Large deviations for a discrete-time random walk in random environment* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 4.
10. P. Granzin, *Punktprozesskonvergenz von Ordnungsstatistiken bei divergierendem Parameter* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 18.

11. A. Hady, *Analysis und optimale Steuerung für ein Modell der Laserthermotherapie* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, December 15.
12. M. Hoffmann, *The Navier–Stokes–Darcy problem* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Caiazzo, December 19.
13. H.-T. Huynh, *Tieftemperaturverhalten eines eindimensionalen Vielteilchensystems mit Lennard-Jones-Potential* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 4.
14. M. Klare, *Mischungseigenschaften des Random Waypoint Models* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 16.
15. F. Litzinger, *Diskretisierung der stationären inkompressiblen Navier-Stokes-Gleichungen in 3D auf unstrukturierten Tetraedergittern* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Linke, December 19.
16. Ch. Marter, *Analyse des Martingallimes beim Galton-Watson-Prozess* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 10.
17. G.A. Müller, *Optimalsteuerung eines PKW-Hybridantriebs* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, June 1.
18. S. Reukauf, *Asymptotische Verteilung einer Ordnungsstatistik mit divergierendem Parameter* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 14.
19. S. Rockel, *Über Formen des konvektiven Terms in Finite-Elemente-Diskretisierungen der inkompressiblen Navier-Stokes-Gleichungen* (diploma thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, February 18.
20. D. Schindler, *Große Abweichungen für die Selbstüberschneidungslokalzeit einer positiv rekurrenten Markovkette* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, November 15.
21. A. Schölzel, *Perfekte Simulation von positiv konditionierten, korrelierten Poisson-Zufallsvariablen* (diploma thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 28.
22. L. Schumacher, *Isogeometric analysis for scalar convection-diffusion equations* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. V. John, May 30.
23. H. Wetzig, *Große Abweichungen für die Aufenthaltsmaße des Random Waypoint Models* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 27.
24. M. Wolff, *Vorkonditionierte Krylov-Unterraum-Verfahren zur Lösung linearer Gleichungssysteme* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. V. John, January 21.
25. K. Zaidi, *Kristallisierung bei positiver Temperatur in einem vereinfachten eindimensionalen klassischen Partikel-Modell* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 6.

A.2 Grants[1]

European Union, Brussels

- **Seventh Framework Programme**

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

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

  ERC Starting Grant "EPSILON – Elliptic partial differential equations and symmetry of interfaces and layers for odd nonlinearities" (E. Valdinoci in ERC 1)

  ERC Starting Grant "EntroPhase – Entropy formulation of evolutionary phase transitions" (E. Rocca in ERC 2)

  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)

- **Forschungsinitiative "Energiespeicher" der Bundesregierung** (Research Initiative Energy Storage Systems of the German Federal Government)

  Interdisziplinäres Forschungsnetzwerk "Perspektiven für wiederaufladbare Magnesium-Luft-Batterien" (Interdisciplinary research network "Perspectives for Rechargeable Magnesium-Air Batteries"), subproject „Makroskopische Modellierung von Transport- und Reaktionsprozessen in Magnesium-Luft-Batterien" (Macroscopic modeling of transport and reaction processes in magnesium-air batteries; in RG 3)

- **Strategie der Bundesregierung zur Internationalisierung von Wissenschaft und Forschung** (Strategy of the German Federal Government for the internationalization of science and research)

  "Verbundprojekt MANUMIEL: Mathematische Modellierung und numerische Simulation von Dioden-Lasern mit mikro-integrierten externen Resonatoren" (Joint project MANUMIEL: Mathematical modelling and numerical simulation of micro-integrated external cavity diode lasers; in RG 2, cooperation with Moldavia)

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

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)

  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 YSG)

  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)**, Technische Universität Bergakademie Freiberg

  “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)**, Freie Universität Berlin

  “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)**, Technische Universität Darmstadt and Rheinisch-Westfälische Technische Universität Aachen

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

  “Structure formation in thin liquid-liquid films” (in RG 7)

- **Priority Program SPP 1590: “Probabilistic Structures in Evolution”**, Universität Bielefeld

  “Branching random walks in random environmentwith a special focus on the intermittent behavior of the particle flow” (in RG 5)

- **Priority Program SPP 1679: “Dyn-Sim-FP – Dynamische Simulation vernetzter Feststoffprozesse” (Dynamic simulation of interconnected solids processes)**, Technische Universität Hamburg-Harburg

  “Numerische Lösungsverfahren für gekoppelte Populationsbilanzsysteme zur dynamischen Simulation multivariater Feststoffprozesse am Beispiel der formselektiven Kristallisation” (Numerical methods for coupled population balance systems for the dynamic simulation of multivariate particulate processes using the example of shape-selective crystallization; in RG 3)

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

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

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

- **Research Unit FOR 797 “Analysis and Computation of Microstructure in Finite Plasticity”**, Ruhr-Universität Bochum

  P5: “Regularisierung und Relaxierung zeitkontinuierlicher Probleme in der Plastizität” (Regularizations and relaxations of time-continuous problems in plasticity; in RG 1)

- **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)

  "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 YSG)

- **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** with Chile (Pontificia Universidad Católica de Valparaíso (PUCV)): "Modeling of poroelastic biological tissues in Magnetic Resonance Elastography (MRE): Numerical simulations and parameters estimation", supported by DFG and Comisión Nacional de Investigación Científica y Tecnológica (CONICYT, Chile), in RG 3)

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)

  "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)

Einstein Stiftung Berlin (Einstein Foundation Berlin)

- A scholarship holder of the IMU Berlin Einstein Foundation Program (in RG 1)

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)
- 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)
- 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, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
2. ———, Editorial Board, Monatshefte der Mathematik, Springer-Verlag, Berlin.
3. ———, Editorial Board, Stochastic Processes and Applications, Elsevier, Oxford, UK.
4. Th. Dickhaus, Editorial Board, Annals of the Institute of Statistical Mathematics, Springer-Verlag, Heidelberg.
5. ———, Editorial Board, Statistics, Taylor & Francis, Berlin.
6. R. Henrion, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
7. ———, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, The Netherlands.
8. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
9. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, The Netherlands.
10. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
11. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
12. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
13. D. Knees, Editorial Board, Discrete and Continuous Dynamical Systems — Series S (DCDS-S), American Institute of Mathematical Sciences, Springfield, Missouri, USA.
14. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
15. P. Mathé, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
16. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
17. A. Mielke, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin, Heidelberg.
18. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
19. ———, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
20. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
21. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
22. ———, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
23. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.

[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. ———, Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
25. H. Neidhardt, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
26. ———, Editorial Board, Journal of Operators, Hindawi Publishing Corporation, New York, USA.
27. ———, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russia.
28. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
29. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
30. J.G.M. Schoenmakers, Editorial Board, Applied Mathematical Finance, Taylor & Francis, Oxford, UK.
31. ———, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
32. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
33. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
34. J. Sprekels, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
35. ———, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
36. ———, Editorial Board, Applied Mathematics and Optimization, Springer-Verlag, New York, USA.
37. ———, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
38. 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

8th DFG-CNRS Workshop "Two-Phase Fluid Flows – Modeling, Analysis and Computational Methods"
Berlin, February 6–8
Organized by: WIAS (RG 7 and YSG)
Supported by: DFG, Centre National de Recherche Scientifique (CNRS), France

The workshop aimed at bringing together researchers from different disciplines to discuss recent insights and viewpoints on modeling, analysis, and numerical simulations of liquid-vapor flows.

The lectures focused on the diffuse and sharp interface modeling (kinetic relations/configurational forces, generalized Riemann problems), analytical investigations of liquid-vapor flow models, asymptotic regimes (low Mach number, flows in special geometries, boundary interaction), efficient numerical techniques (space/time adaptivity, approximate Riemann solvers, ghost fluid and level-set approach, discontinuous Galerkin), and applications (cavitation, bubble collapse, cooling, and boiling).

About 50 scientists, mainly from France and Germany, participated in the workshop. In seven invited lectures and 17 talks, a broad range of topics from modeling, analysis, and simulation were covered.

Modeling, Analysis, and Simulation of Optical Modes in Photonic Devices — MASOMO 2013
Berlin, April 10–12
Organized by: WIAS (RG 1, RG 2, and RG 4)
Supported by: DFG Research Center Matheon, DFG Collaborative Research Center 787 "Semiconductor Nanophotonics", WIAS

The aim of this three-day workshop was to focus on the problems arising in the modeling and simulation of optical modes in semiconductor lasers with open cavities. By bringing together applied mathematicians and scientists from semiconductor laser physics, an in-depth discussion of this topic was initiated. It resulted in a thorough survey of the pros and cons of the concept of resonances as a basis for the description of optical modes in lasers.

The topics of the presentations covered Maxwell equations for active materials, Maxwell–Bloch equations, Helmholtz equations, modeling based on optical modes, methods for the computation of optical modes and applications including cavities in photonic crystals, broad area lasers, VCSEL devices, and optical fiber lasers. In particular, the mathematical and computational problems related to the modeling of open cavities were highlighted in several talks as well as possible solutions. The workshop was attended by more than 50 participants from six countries.

IFIP TC7.2 Workshop "Electromagnetics – Modelling, Simulation, Control and Industrial Applications"
Berlin, May 13–17
Organized by: WIAS (RG 4 and RG 7)
Supported by: DFG Research Center Matheon, WIAS

The workshop brought together 69 researchers from academia and industry from 13 countries. The goal was to discuss recent achievements in electromagnetics. Mathematical topics included finite and boundary element discretization methods for the electromagnetic field equations in frequency and time domain, analysis, optimal control, and model reduction for multi-physics problems involving electromagnetics, as well as direct and inverse scattering problems. Among the industrial applications discussed in the workshop were electromagnetic flow control in crystal growth, multifrequency induction hardening, and problems in diffractive optics.

QMath 12 — Mathematical Results in Quantum Mechanics
Berlin, September 10–13
Organized by: WIAS (RG 1 and RG 5), Humboldt-Universität zu Berlin
Supported by: WIAS, DFG, DFG Research Center Matheon, IAMP (International Association of Mathematical Physics)
Sponsored by: AIP (Journal of Mathematical Physics), Birkhäuser Verlag, de Gruyter Verlag, Forum of Mathematics, Springer Verlag, Technology Consulting

The conference was the 12th in the QMath series devoted to the state of the art and new results in the "quantum part" of mathematical physics. This series has developed into one of the biggest and most visible periodic conferences within mathematical physics worldwide. The main topics this year were spectral theory of Schrödinger operators, spectra of random operators, quantum field theory, and relativistic quantum mechanics, interacting many-body systems, and numerical methods in mathematical physics.

The conference was attended by about 125 participants from about 18 countries from three continents. Eighty-five talks were given, including twelve invited plenary talks, 14 invited topical talks, and 59 contributed talks. The organizing and program committee consisted of Volker Bach (TU Braunschweig), Michael Demuth (TU Clausthal), Pavel Exner (TU Prague and Nuclear Physics Institute Rez), Marcel Griesemer (Universität Stuttgart), Wolfgang König (WIAS Berlin and TU Berlin), Alexander Mielke (WIAS Berlin and HU Berlin), Hagen Neidhardt (WIAS Berlin), Reinhold Schneider (TU Berlin), and Simone Warzel (TU München).

ERC Workshop on Energy/Entropy-Driven Systems and Applications
Berlin, October 9–11
Organized by: WIAS (RG 1), University of Vienna (Austria)
Supported by: ERC Advanced Grant "Analysis of Multiscale Systems Driven by Functionals

This workshop focused on methods and results for evolution problems driven by functionals, giving emphasis to gradient flows for free energy or entropy as well as to generalized gradient and rate-independent systems, also in a multiscale setting. Various applications of theses topics were discussed, including materials modeling, stochastic models, multi-particle systems, transition from discrete to continuum, fluid mechanics, and reaction-diffusion systems. The program featured 15 invited lectures and seven contributed talks, and the workshop was attended by 60 participants.

Extreme Nonlinear Optics & Solitons (ENOS 2013)
Berlin, October 28–30
Organized by: WIAS (RG 2)
Supported by: DFG Research Center Matheon, WIAS

This three-day workshop was aimed at bringing together applied mathematicians, theoretical and experimental physicists working in the field of nonlinear optical waves, soliton theory, and optical extreme phenomena, in order to initiate useful discussions, as well as to stimulate and strengthen fruitful collaboration between the scientists working in these fields. The topics of the presentations included optical rogue waves and modeling extreme pulses, formation of femtosecond filaments of light, solitons in optical fibers and mode-locked lasers, dissipative optical solitons in optics and other fields, cavity solitons in broad-area laser systems, optical turbulence, polariton solitons, formation of ultrashort few-cycle optical pulses. More than 30 speakers from 10 countries presented their scientific achievements at the workshop.

Partial Differential Equations with Random Coefficients
Berlin, November 13–15
Organized by: WIAS (RG 3, RG 4, RG 5, and YSG)
Supported by: DFG Research Center Matheon

This workshop was one of the strategic measures of WIAS for fostering the bonds between its different research areas, in this case between numerics, analysis, and probability. It was organized as a three-days fall school for

newcomers to the field, given by eminent experts with a particular weight on a pedagogical presentation of the material, combined with a series of research talks on the topic by practioners. The topic of the workshop was the modeling, analysis, and numerics of partial differential equations with random coefficients, in particular in view of the influence of randomness on questions like existence, uniqueness, and critical behavior of the solutions. The number of attendees reached all together some 60 interested people from all the three areas involved, including a substantial number of guests from outside WIAS or even outside Berlin.

Workshop "Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis"
Berlin, December 11–13
Organized by: WIAS (RG 6), Technische Universität Berlin, Oxford University
Supported by: WIAS, European Research Council

The workshop focused on Rough Path Analysis and its rapidly growing applications in Applied Stochastic Analysis, ranging from the resolution of ill-posed stochastic partial differential equations to new ways of handling high-dimensional data. More precisely, rough paths and related topics nowadays lead to significant progress in the following broad variety of fields:

- Nonlinear stochastic partial differential equations driven by space-time white noise
- Statistical descriptions of non-Markovian, non-martingale processes
- Stochastic Loewner evolution
- Statistics and machine learning
- Algorithms for stochastic and rough differential equations

The two-day workshop attracted around 50 participants and featured 28 invited speakers, mostly early career researchers from Berlin and Oxford, on topics related to the afore-mentioned fields. A second Berlin-Oxford meeting has been announced, taking place in Oxford on July 1–3, 2014.

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

Closing Workshop – "Analysis and Stochastics in Complex Physical Systems"
Universität Leipzig, March 20–22
Organized by: DFG Research Unit FOR 718 (hosted at WIAS)
Supported by: Max-Planck-Institut für Mathemmatik in den Naturwissenschaften, Leipzig, Universität Leipzig

This workshop was the closing event of the DFG Research Unit (FOR) 718 *Analysis and Stochastics in Complex Physical Systems*, which run from 2006 through Summer 2013 and was headed by Wolfgang König (head of RG 5 *Interacting Random Systems*). The topics of the talks covered a great deal of the main research subjects of the FOR 718 members evolving around several interfaces between analysis and probability, like random pinning models, Gaussian free fields, optimal mass transport, quantum systems, the Fokker–Planck equation, and much more. A number of distinguished speakers followed our invitations, like Alexander Mielke, Marek Biskup, Mark Peletier, and Barbara Niethammer. The number of talks given was 13, and about 40 participants were attending. The organizers were Max von Renesse and Stephan Luckhaus (Universität Leipzig) and Wolfgang König (WIAS).

PreMoLab: Advances in predictive modeling and optimization
Berlin, May 16–17
Organized by: WIAS (RG 6), Institute for Information Transmission Problems (Russian Academy of Sciences), Moscow Institute of Physics and Technology (MIPT)
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 world-leading scientists for building new research groups in Russia. Interactions of these new groups with established international groups are of special importance for the success of this project. This workshop was an important step in bringing together two groups lead by Vladimir Spokoiny: the WIAS Research Group '*Stochastic Algorithms and Nonparametric Statistics* and Premolab (MITP Moscow). It was attended by 16 members of the Berlin research group and 25 members of the Moscow group. The scientific program included 17 talks on the current research fields from each side and a lot of scientific discussion.

Information Meeting of the German Mathematical Society (DMV) for High-school Graduates

Berlin, September 17
Organized by: German Mathematical Society (DMV)

On September 17, about 40 high-school graduates of 2013 and 2012 who had received the *Abiturpreis* (graduation prize) of the German Mathematical Society (DMV) visited the Weierstrass Institute to participate in an information meeting of DMV. The DMV and also members of the WIAS staff and the institute's trainees presented their work.

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

1. P. Friz, co-organizer, *Stochastic Methods in Finance and Physics*, University of Crete, Department of Applied Mathematics, Heraklion, Greece, July 15–19.
2. ———, organizer, *29th European Meeting of Statisticians (EMS)*, Eötvös Loránd University, Budapest, Hungary, July 20–25.
3. G. Hu, co-organizer of the minisymposium "Recent Progress on Inverse Problems in Elasticity", *Applied Inverse Problem Conference*, Korea Advanced Institute for Sciences and Technology, Daejeon, Korea, July 1–5.
4. Th. Dickhaus, organizer, *Princeton-Humboldt Conference 2013*, Princeton University, Department of Operations Research and Financial Engineering, USA, November 1–2.
5. C. Guhlke, co-organizer, *Solid State Electrochemistry Workshop 2013 (SSE2013)*, Universität Heidelberg, July 22–24.
6. R. Hildebrand, organizer of the session "Convex Programming: Theoretical Results", *International Conference on Continuous Optimization (ICCOPT2013)*, Universidade Nove de Lisboa, Portugal, July 29 – August 1.
7. D. Hömberg, organizer of the minisymposium "Recent Trends in PDE-Constrained Control and Shape Design", *Equadiff13*, Charles University, Prague, Czech Republic, August 26–30.
8. V. John, organizer of the minisymposium "Finite Element Methods for Convection-dominated Problems", *14th Conference on Mathematics of Finite Elements and Applications (MAFELAP 2013)*, Brunel University, London, UK, June 11–14.
9. D. Knees, co-organizer of the section S14 "Applied Analysis", *84th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2013)*, University of Novi Sad, Serbia, March 18–22.
10. W. König, organizer, *Analysis and Stochastics in Complex Physical Systems, Closing Workshop of the DFG Research Unit FOR 718*, Universität Leipzig, Mathematisches Institut, March 20–22.
11. M. Liero, co-organizer, *BMS Intensive Course on Evolution Equations and their Applications*, Berlin Mathematical School, Technische Universität Berlin, November 27–29.
12. A. Mielke, member of the Programme Committee, *Equadiff13*, Charles University, Prague, Czech Republic, August 26–30.
13. O. Omel'chenko, organizer of the minisymposium "Emergent Dynamics in Coupled Oscillators", *XXXIII Dynamics Days Europe*, Madrid, Spain, June 3–7.
14. V. Spokoiny, program chair, *Information Technology and Systems – 2013*, Russian Academy of Sciences, Institute for Information Transmission Problems, Kaliningrad, September 1–6.
15. ———, member of the Scientific Committee, *Conference on Structural Inference in Statistics*, Universität Potsdam, Institut für Mathematik, September 17–19.
16. ———, organizer, *PreMoDay 2013*, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, November 7.

[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. M. THOMAS, co-organizer of the Young Researchers' Minisymposium "Analytical and Engineering Aspects in the Material Modeling of Solids", *84th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2013)*, University of Novi Sad, Serbia, March 19.

18. E. VALDINOCI, co-organizer, *International School on Recent Advances in Partial Differential Equations and Applications (AdvPDEs2013)*, University of Milan, Department of Mathematics, Italy, June 17–21.

19. ———, co-organizer, *Conference on Qualitative and Geometric Aspects of Elliptic PDE's*, Centre de Recerca Matemàtica, Bellaterra, Spain, September 2–6.

20. ———, member of the Organizing Commitee, *Workshop on Nonlinear Equations*, Università Carlos III de Madrid, Departamento de Matemáticas, Spain, October 17–18.

21. W. WAGNER, member of the Program Committee, *9th IMACS Seminar on Monte Carlo Methods*, Annecy, France, July 15–19.

A.6 Publications

A.6.1 Monographs

[1] W.K. Härdle, V. Spokoiny, V. Panov, W. Wang, *Basics of Modern Mathematical Statistics*, Springer Texts in Statistics, Springer, Berlin, 2013, 185 pages.

Monographs (to appear)

[1] Th. Dickhaus, *Simultaneous Statistical Inference*, Springer, Berlin et al.

A.6.2 Editorship of Proceedings and Collected Editions

[1] D. Hömberg, F. Tröltzsch, eds., *System Modeling and Optimization, 25th IFIP TC 7 Conference, CSMO 2011, Berlin, Germany, September 12–16, 2011*, vol. 391 of IFIP Advances in Information and Communication Technology, Springer, Heidelberg [et al.], 2013, 568 pages.

[2] G. Dal Maso, A. Mielke, U. Stefanelli, eds., *Rate-independent Evolutions*, vol. 6 (No. 1) of Discrete and Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences, Springfield, 2013, 275 pages.

[3] E. Bonetti, C. Cavaterra, E. Rocca, R. Rossi, eds., *Special Issue Dedicated to Michel Frémond on the Occasion of his 70th Birthday*, vol. 6 (No. 2) of Discrete and Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences, Springfield, 2013, 333 pages.

[4] A. Chambolle, M. Novaga, E. Valdinoci, eds., *Geometric Partial Differential Equations*, vol. 15 of CRM Series, Scuola Normale Superiore, Pisa, 2013, 400 pages.

A.6.3 Outstanding Contributions to Monographs

[1] J. Elschner, G. Hu, *Chapter: 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., vol. 14 of Radon Series on Computational and Applied Mathematics, de Gruyter, Berlin/Boston, 2013, pp. 101–134.

[2] J. Fuhrmann, *Chapter: Mathematical and Numerical Modeling of Flow, Transport and Reactions in Porous Structures of Electrochemical Devices, in: Simulation of Flow in Porous Media: Applications in Energy and Environment*, P. Bastian, J. Kraus, R. Scheichl, M. Wheeler, eds., vol. 12 of Radon Series on Computational and Applied Mathematics, de Gruyter, Berlin/Boston, 2013, pp. 139–164.

[3] A. Mielke, *Chapter 21: Dissipative Quantum Mechanics Using GENERIC, in: Recent Trends in Dynamical Systems – Proceedings of a Conference in Honor of Jürgen Scheurle*, A. Johann, H.-P. Kruse, F. Rupp, St. Schmitz, eds., vol. 35 of Springer Proceedings in Mathematics & Statistics, Springer, Basel et al., 2013, pp. 555–585.

[4] J.G.M. Schoenmakers, *Chapter 12: Coupling Local Currency Libor Models to FX Libor Models, in: Recent Developments in Computational Finance*, Th. Gerstner, P. Kloeden, eds., vol. 14 of Interdisciplinary Mathematical Sciences, World Scientific Publishers, Singapore, 2013, pp. 429–444.

A.6.4 Articles in Refereed Journals[4]

[1] D. Crisan, J. Diehl, P. Friz, H. Oberhauser, *Robust filtering: Correlated noise and multidimensional observation*, Ann. Appl. Probab., 23 (2013), pp. 2139–2160.

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[132] K. Tabelow, S. Mohammadi, N. Weiskopf, J. Polzehl, *POAS4SPM — A toolbox for SPM to denoise diffusion MRI data*, Preprint no. 1856, WIAS, Berlin, 2013.

[133] M. Thomas, *Uniform Poincaré–Sobolev and relative isoperimetric inequalities for classes of domains*, Preprint no. 1797, WIAS, Berlin, 2013.

[134] T. Roubíček, M. Thomas, Ch. Panagiotopoulos, *Stress-driven local-solution approach to quasistatic brittle delamination*, Preprint no. 1889, WIAS, Berlin, 2013.

[135] G. Albanese, A. Fiscella, E. Valdinoci, *Gevrey regularity for integro-differential operators*, Preprint no. 1844, WIAS, Berlin, 2013.

[136] B. Barrios, I. Peral, F. Soria, E. Valdinoci, *A Widder's type theorem for the heat equation with nonlocal diffusion*, Preprint no. 1798, WIAS, Berlin, 2013.

[137] L. Caffarelli, O. Savin, E. Valdinoci, *Minimization of a fractional perimeter-Dirichlet integral functional*, Preprint no. 1818, WIAS, Berlin, 2013.

[138] M. Cozzi, A. Farina, E. Valdinoci, *Gradient bounds and rigidity results for singular, degenerate, anisotropic partial differential equations*, Preprint no. 1803, WIAS, Berlin, 2013.

[139] S. Dipierro, A. Figalli, E. Valdinoci, *Strongly nonlocal dislocation dynamics in crystals*, Preprint no. 1894, WIAS, Berlin, 2013.

[140] S. Dipierro, G. Palatucci, E. Valdinoci, *Dislocation dynamics in crystals: A macroscopic theory in a fractional Laplace setting*, Preprint no. 1847, WIAS, Berlin, 2013.

[141] M.M. Fall, E. Valdinoci, *Uniqueness and nondegeneracy of positive solutions of* $(-\Delta)^s u + u = u^p$ *in* R^N *when* s *is close to 1*, Preprint no. 1804, WIAS, Berlin, 2013.

[142] A. Figalli, E. Valdinoci, *Regularity and Bernstein-type results for nonlocal minimal surfaces*, Preprint no. 1831, WIAS, Berlin, 2013.

[143] A. Fiscella, E. Valdinoci, *A critical Kirchhoff type problem involving a non-local operator*, Preprint no. 1801, WIAS, Berlin, 2013.

[144] O. Bäumchen, L. Marquant, R. Blossey, A. Münch, B. Wagner, K. Jacobs, *Influence of slip on the Rayleigh–Plateau rim instability in dewetting viscous films*, Preprint no. 1886, WIAS, Berlin, 2013.

[145] M.G. Hennessy, V.M. Burlakov, A. Münch, B. Wagner, A. Goriely, *Controlled topological transitions in thin film phase separation*, Preprint no. 1885, WIAS, Berlin, 2013.

[146] ———, *Propagating topological transformations in thin immiscible bilayer films*, Preprint no. 1887, WIAS, Berlin, 2013.

[147] M.D. Korzec, M. Roczen, M. Schade, B. Wagner, B. Rech, *Equilibrium shapes of poly-crystalline silicon nanodots*, Preprint no. 1884, WIAS, Berlin, 2013.

[148] T. Ahnert, A. Münch, B. Wagner, *Two-phase flow model for concentrated suspensions*, Preprint no. 1901, WIAS, Berlin, 2013.

[149] M. Dziwnik, M.D. Korzec, A. Münch, B. Wagner, *Stability analysis of non-constant base states in thin film equations*, Preprint no. 1883, WIAS, Berlin, 2013.

[150] W. Wagner, *A random cloud model for the Schrödinger equation*, Preprint no. 1851, WIAS, Berlin, 2013.

[151] ———, *Some properties of the kinetic equation for electron transport in semiconductors*, Preprint no. 1857, WIAS, Berlin, 2013.

[152] A. Wilms, P. Mathé, F. Schulze, Th. Koprucki, A. Knorr, U. Bandelow, *Influence of the carrier reservoir dimensionality on electron-electron scattering in quantum dot materials*, Preprint no. 1781, WIAS, Berlin, 2013.

[153] S. Yanchuk, L. Lücken, M. Wolfrum, A. Mielke, *Spectrum and amplitude equations for scalar delay-differential equations with large delay*, Preprint no. 1826, WIAS, Berlin, 2013.

A.7.2 WIAS Technical Reports Series

[1] H. Si, *TetGen: A quality tetrahedral mesh generator and a 3D Delaunay triangulator (Version 1.5 — User's Manual)*, WIAS Technical Report no. 13, WIAS, Berlin, 2013.

A.7.3 Preprints/Reports in other Institutions

[1] P. Friz, St. Gerold, M. Yor, *How to make Dupire's local volatility work with jumps*, arXiv:1302.5548, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[2] G. Hu, J. Li, H. Liu, H. Sun, *Inverse elastic scattering for multiscale rigid bodies with a single far-field measurement*, arXiv:1310.3516, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[3] G. Hu, H. Liu, *Uniqueness in determining refractive indices by formally determined far-field data*, arXiv:1308.5955, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[4] R. Allez, *Tracy Widom at high temperature*, arXiv:1312.1283, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[5] R. Allez, J.-P. Bouchaud, *Eigenvectors dynamic and local density of states under free addition*, arXiv:1301.4939, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[6] R. Allez, J. Touboul, G. Wainrib, *Index distribution of the Ginibre ensemble*, arXiv:1310.5039, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[7] T. Bodnar, Th. Dickhaus, *False discovery rate control under Archimedean copula*, arXiv:1305.3897, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[8] M. Eigel, C. Gittelson, Ch. Schwab, E. Zander, *Adaptive stochastic Galerkin FEM*, Report no. 2013-01, Eidgenössische Technische Hochschule, Seminar for Applied Mathematics, Zürich, Switzerland, 2013.

[9] S.P. Frigeri, M. Grasselli, E. Rocca, *A diffuse interface model for two-phase incompressible flows with nonlocal interactions and nonconstant mobility*, arXiv:1303.6446, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[10] C.G. Petra, O. Schenk, M. Lubin, K. Gärtner, *An augmented incomplete factorization approach for computing the Schur complement in stochastic optimization*, ANL/MCS-P4030-0113, Argonne National Laboratory, Lemont, IL, USA, 2013.

[11] St. Neukamm, A. Gloria, F. Otto, *An optimal quantitative two-scale expansion in stochastic homogenization of discrete elliptic equations*, Preprint no. 41, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 2013.

[12] A. Miranville, E. Rocca, G. Schimperna, A. Segatti, *The Penrose–Fife phase-field model with coupled dynamic boundary conditions*, arXiv:1301.5563, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

[13] D. Puzyrev, S. Yanchuk, A.G. Vladimirov, S.V. Gurevich, *Stability of plane wave solutions in complex Ginzburg–Landau equation with delayed feedback*, arXiv:1311.2414, Cornell University Library, arXiv.org, Ithaca, USA, 2013.

A.8 Talks and Posters

A.8.1 Main and Plenary Talks

1. J. Elschner, *Direct and inverse problems for diffraction gratings*, Symposium "Light Scattering: Simulation and Inversion", May 27–28, Bremen, May 28.
2. R. Henrion, *Optimisation sous contraintes en probabilité*, Journées annuelles 2013 du Groupe de Recherche MOA, June 17–19, Paris, France, June 17.
3. ———, *Stochastic optimization with probabilistic constraints*, International Conference on Stochastic Programming (SP XIII), July 8–12, Bergamo, Italy, July 9.
4. D. Knees, *Weak solutions for rate-independent systems illustrated at an example for crack propagation*, BMS Intensive Course on Evolution Equations and their Applications, November 27–29, Technische Universität Berlin, Berlin Mathematical School, November 28.
5. H. Si, *TetGen: A quality tetrahedral mesh generator*, Fourth Tetrahedron Workshop on Grid Generation for Numerical Computations (Tetrahedron IV), July 1–3, MOX – Dipartimento di Matematica, Politecnico di Milano, Verbania, Italy, July 1.

A.8.2 Scientific Talks (Invited)

1. P. Friz, *Marginal density expansions for diffusions and stochastic volatility and related stuff*, Large Deviations and Asymptotic Methods in Finance, April 9–11, Imperial College London, UK, April 10.
2. ———, *Some aspects of stochastic area*, UK Probability Easter Meeting; Geometry and Analysis of Random Processes, April 8–12, University of Cambridge, Department of Pure Mathematics, UK, April 11.
3. ———, *Les chemins rugueux*, 4 talks, École d'Été sur l'Équation KPZ et les Chemins Rugueux, June 3–13, Lebesgue Center of Mathematics, Rennes, France, June 10–13.
4. ———, *Rough path analysis*, Summer School "Numerical Methods for Stochastic Differential Equations", September 2–4, Vienna University of Technology, Institute for Analysis and Scientific Computing E 101, Austria, September 4.
5. ———, *Physical Brownian motion in magnetic field as rough path*, German-Japanese Meeting on Stochastic Analysis, September 9–13, Universität Leipzig, Mathematisches Institut, September 13.
6. ———, *(Rough) pathwise stochastic analysis: Old and new*, Stochastic Analysis and its Applications, 60th Birthday of Terry Lyons, September 23–27, University of Oxford, Oxford-Man Institute, UK, September 24.
7. ———, *On the probability density function of baskets*, Seminar, Vienna University of Technology, Financial and Actuarial Mathematics, Austria, October 30.
8. G. Hu, *Direct and inverse acoustic scattering by extended and point-like obstacles*, The Second International Conference on Interdisciplinary Applied and Computational Mathematics, June 19–22, Zhejiang University, Hangzhou, China, June 19.
9. ———, *On uniqueness in inverse elastic scattering from rectangular periodic structures*, Applied Inverse Problem Conference, July 1–5, Korea Advanced Institute for Sciences and Technology, Daejeon, Korea, July 1.
10. ———, *Direct and inverse acoustic scattering by extended and point-like obstacles*, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, July 15.

11. ———, *Direct an inverse acoustic scattering by extended and point-like scatterers*, Franco-German Summer School "Inverse Problems and Partial Differential Equations", October 7–11, Universität Bremen, October 9.
12. ———, *Elastic wave scattering from periodic structures*, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, November 25.
13. ———, *Inverse elastic wave scattering from rigid diffraction gratings*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, December 19.
14. S. Amiranashvili, *Mathematics and physics behind short pulses in optical fibers*, Habilitandenkolloquium, Humboldt-Universität zu Berlin, Institut für Physik, February 5.
15. R.M. Arkhipov, *Spectral and temporal characteristics of radiation from a periodic resonant medium excited at the superluminal velocity*, ICONO/LAT 2013 Conference, June 17–22, Russian Academy of Sciences, Moscow, June 20.
16. L. Avena, *Recent progresses in random walks in dynamical random environments*, Aix-Marseille Université, Laboratoire d'Analyse, Topologie, Marseille, France, September 13.
17. ———, *Recent progresses in random walks in dynamical random environments*, Workshop "Random Media", September 16–17, Technische Universität Berlin, September 17.
18. ———, *A local CLT for some convolution equations with applications to self-avoiding walks*, Università degli Studi di Roma "La Sapienza", Dipartimento di Matematica, Italy, December 17.
19. U. Bandelow, *Propagation of ultrashort pulses in nonlinear dispersive optical media: Solitons, rogue waves and horizons*, Technische Universität Wien, Institut für Theoretische Physik, Austria, June 4.
20. ———, *Semiconductor lasers for high speed applications: Modeling and simulation*, Technische Universität Wien, Institut für Photonik, Austria, June 7.
21. ———, *Ultrashort optical solitons in nonlinear media with arbitrary dispersion*, 13th International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD 2013, August 16–24, Vancouver, Canada, August 22.
22. ———, *Comprehensive mathematical modeling and simulation of semiconductor lasers*, 2013 International Nano-Optoelectronics Workshop (iNOW'2013), August 19–30, Cargèse, France, August 26.
23. ———, *Modeling and simulation of semiconductor lasers for high speed applications*, The Russell Berrie Nanotechnology Institute, Haifa, Israel, November 20.
24. ———, *Ultrashort solitons and rogue waves in nonlinear dispersive optical media*, Optics Seminar, Weizmann Institute, Rehovot, Israel, November 27.
25. ———, *Solitons on a background, rogue waves, and classical soliton solutions of the Sasa–Satsuma equation*, VI Rio de la Plata Workshop on Laser Dynamics and Nonlinear Photonics, December 6–13, Montevideo, Uruguay, December 17.
26. ———, *Horizons, ultrashort solitons, and rogue waves in nonlinear dispersive optical media*, National University of Mar de Plata, Department of Physics, Argentina, December 19.
27. Ch. Bayer, *Simulation of conditional diffusions via forward-reverse stochastic representations*, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, February 20.
28. ———, *Asymptotics can beat Monte Carlo*, 20th Annual Global Derivatives & Risk Management, April 16–18, The International Centre for Business Information (ICBI), Amsterdam, The Netherlands, April 18.
29. ———, *Asymptotics beats Monte Carlo: The case of correlated local volatility baskets*, Stochastik-Seminar, Universität Heidelberg, Institut für angewandte Mathematik, June 18.

30. ———, *Asymptotics beats Monte Carlo: The case of correlated local volatility baskets*, Stochastic Methods in Finance and Physics, July 15–19, University of Crete, Department of Applied Mathematics, Heraklion, Greece, July 19.

31. ———, *Simulation of conditional diffusions via forward–reverse stochastic representations*, Seminar in Mathematical Statistics, Linköping University, Division of Mathematical Statistics, Sweden, September 11.

32. ———, *Simulation of conditional diffusions via forward-reverse stochastic representations*, Forschungsseminar Stochastische Analysis & Stochastik der Finanzmärkte, Humboldt-Universität zu Berlin, Institut für Mathematik, October 31.

33. ———, *Asymptotics beats Monte Carlo: The case of correlated local volatility baskets*, Seminar Finanzmathematik, Universität Wien, Austria, November 28.

34. M. Becker, *Large deviation for self-intersection local times*, Young European Probabilists 2013 and School on Random Polymers, January 8–12, Technische Universiteit Eindhoven, European Institute for Statistics, Probability, Stochastic Operations Research and their Applications, Eindhoven, The Netherlands, January 8.

35. A. Caiazzo, *Asymptotic analysis of LBM: Algorithms for fluid-structure interaction*, International Conference on Scientific Computation and Differential Equation (SciCADE), September 16–20, University of Valladolid, Spain, September 17.

36. ———, *Reduced order modeling for finite element simulations of the cardiovascular system*, Universidad de Castilla-La Mancha, Departamento de Matematica, Cuenca, Spain, September 23.

37. K. Disser, *Passage to the limit of the entropic gradient structure of reversible Markov processes to the Wasserstein Fokker–Planck equation*, Oberseminar Analysis, Martin-Luther-Universität Halle-Wittenberg, Institut für Mathematik, Halle, November 20.

38. W. Dreyer, *Sharp limits of phase field models and thermodynamic consistency*, Prof. Dr. Hans Georg und Lieselotte Hahn Workshop: Phase Field Modeling, February 20–22, Freudenstadt, February 21.

39. ———, *Kinetic relations for moving phase boundaries – A purely sharp interface study*, Workshop "Hyperbolic Techniques for Phase Dynamics", June 10–14, Mathematisches Forschungsinstitut Oberwolfach, June 10.

40. ———, *On waves generated by phase transitions*, XVII International Conference on Waves and Stability in Continuous Media (WASCOM2013), June 17–21, Levico Terme, Italy, June 17.

41. ———, *On waves generated by phase transitions*, 11th Hirschegg Workshop on Conservation Laws, Mathematical Theory and Numerical Analysis for Conservation Laws, September 8–14, Hirschegg/Kleinwalsertal, Austria, September 5.

42. ———, *Six lectures on coupling of electrodynamics and thermodynamics*, 6 talks, Technische Universität Darmstadt, Center for Smart Interfaces, October 9–11.

43. ———, *Phase transition and hysteresis due to non-local and non-linear material behavior of lithium-ion batteries*, CeNoS-Kolloquium, Universität Münster, Center for Nonlinear Science, November 26.

44. M. Eigel, *On tensor approximations with adaptive stochastic Galerkin FEM*, Eidgenössische Technische Hochschule Zürich, Seminar für Angewandte Mathematik, Switzerland, September 25.

45. G. Faraud, *Connection times in large ad-hoc networks*, Ecole de Printemps "Marches Aléatoires, Milieux Aléatoires, Renforcements" (MEMEMO2), June 10–14, Aussois, France, June 13.

46. M.H. Farshbaf Shaker, *Relating phase field and sharp interface approaches to structural topology optimization*, Universität der Bundeswehr, Institut für Mathematik und Rechneranwendung, Neubiberg, March 13.

47. ———, *Relating phase field and sharp interface approaches to structural topology optimization*, The Fourth International Conference on Continuous Optimization (ICCOPT), July 27 – August 1, Universidade Nova de Lisboa, Lisbon, Portugal, July 31.

48. ———, *Relating phase field and sharp interface approaches to structural topology optimization*, 26th IFIP TC7 Conference 2013 on System Modelling and Optimization, September 8–13, Klagenfurt, Austria, September 10.

49. ———, *A deep quench approach to optimal control of an Allen–Cahn equation with dynamic boundary conditions and double obstacles*, 26th IFIP TC7 Conference 2013 on System Modelling and Optimization, September 8–13, Klagenfurt, Austria, September 13.

50. A. Fiebach, *Voronoi finite volume methods for reaction-diffusion systems*, Schlumberger, Technology & Product Centers, Aachen, March 13.

51. ———, *A Voronoi finite volume method for reaction-diffusion equations*, Physikalisch-Technische Bundesanstalt, Department 7 – Safety of Structures, Berlin, August 13.

52. J. Fuhrmann, *Voronoi box based finite volume methods: Advantages and challenges*, Simulation and Optimization Seminar, Széchenyi István University, Győr, Hungary, January 21.

53. ———, *Mathematical and numerical modeling of coupled processes in electrochemical devices*, Nečas Seminar on Continuum Mechanics, Charles University, Prague, Czech Republic, March 4.

54. ———, *Stable numerical methods for macroscopic models of electrochemical devices*, University of West Bohemia, Plzeň, Czech Republic, March 5.

55. ———, *Numerical strategies for electrolyte simulations*, Water Phenomena in PEM: Sorption, Swelling and Breakthrough Processes (PEM 2013), October 3–4, Trondheim, Norway, October 3.

56. K. Gärtner, *Approximation of best separators by eigenfunctions of p-Laplacian*, Celebrating 40 Years Nested Dissection, July 22–23, University of Waterloo, Computer Research Centre, Ontario, Canada, July 23.

57. J. Giesselmann, *Energy consistent DG schemes for compressible two-phase flows*, Workshop “Hyperbolic Techniques for Phase Dynamics”, June 10–14, Mathematisches Forschungsinstitut Oberwolfach, June 11.

58. A. Glitzky, *Continuous and finite volume discretized reaction-diffusion systems in heterostructures*, Asymptotic Behaviour of Systems of PDE Arising in Physics and Biology: Theoretical and Numerical Points of View, November 6–8, Lille 1 University – Science and Technology, France, November 6.

59. K. Götze, *Starke Lösungen für die Bewegung von Starrkörpern in Flüssigkeiten*, Oberseminar Analysis, Technische Universität Dresden, Institut für Analysis, January 24.

60. ———, *Free fall of a rigid body in a viscoelastic fluid*, Workshop “Geophysical Fluid Dynamics”, February 18–22, Mathematisches Forschungsinstitut Oberwolfach, February 20.

61. C. Guhlke, *Thermodynamics of electrolytes*, 2nd International Conference on Materials for Energy – EnMat II, May 13–15, Karlsruhe, May 14.

62. O. Gün, *Moment asymptotics for branching random walks in random environment*, Workshop on Disordered Systems, June 24–28, Centre International de Rencontres Mathématiques, Marseille, France, June 24.

63. H. Hanke, *Derivation of an effective damage model with evolving micro-structure*, Oberseminar zur Analysis, Universität Duisburg-Essen, Fachbereich Mathematik, Essen, January 29.

64. Ch. Heinemann, *On a PDE system describing damage processes and phase separation*, Oberseminar Analysis, Universität Augsburg, July 11.

65. ———, *Degenerating Cahn–Hilliard systems coupled with mechanical effects and complete damage processes*, Equadiff13, MS27 – Recent Results in Continuum and Fracture Mechanics, August 26–30, Prague, Czech Republic, August 27.

66. S. Heinz, *On a way to control oscillations for a special evolution equation*, Conference "Nonlinearities", June 10–14, University of Warsaw, Institute of Mathematics, Male Ciche, Poland, June 11.

67. R. Henrion, *Optimization problems with probabilistic constraints*, Universität Göttingen, Institut für Numerische und Angewandte Mathematik, January 8.

68. ———, *Optimization problems with probabilistic constraints*, Workshop "Numerical Methods for PDE Constrained Optimization with Uncertain Data", January 27 – February 2, Mathematisches Forschungsinstitut Oberwolfach, January 30.

69. ———, *Optimization problems with probabilistic constraints*, 2 talks, University of Ostrava, Department of Mathematics, Czech Republic, March 19–21.

70. ———, *Problèmes d'optimisation avec des contraintes en probabilité*, Electricité de France, Clamart, France, June 20.

71. ———, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen*, Technische Universität Darmstadt, Fachbereich Mathematik, September 16.

72. ———, *Dual stationarity conditions for MPECs*, 7 talks, CIMPA-UNESCO-MESR-MINECO-INDIA Research School "Generalized Nash Equilibrium Problems, Bilevel Programming and MPES", November 25 – December 6, University of Delhi, India, December 2–6.

73. D. Hömberg, *On a phase field approach to shape optimization*, Université de Paris-Sud, Laboratoire de Mathématiques, Equipe Analyse Numérique et EDP, France, January 16.

74. ———, *Sufficient optimality conditions for a semi-linear parabolic system*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, February 27.

75. ———, *An optimal shape design approach towards distortion compensation*, Fudan University, School of Mathematics, Shanghai, China, March 6.

76. ———, *Mathematics for the digital factory*, Mathematics for Industry and Society, July 4–5, French Embassy, Berlin, July 5.

77. ———, *An optimal shape design approach towards distortion compensation*, Equadiff13, MS21 – Recent Trends in PDE-constrained Control and Shape Design, August 26–30, Prague, Czech Republic, August 29.

78. ———, *Modelling, analysis and simulation of multifrequency induction hardening*, Forum Math-for-Industry 2013 "The Impact of Applications on Mathematics", November 4–8, Kyushu University, Fukuoka, Japan, November 7.

79. ———, *Identification of phase transition kinetics and the generalized Avrami–Kolmogorov model*, Nippon Steel & Sumitomo Metal Corporation, Tokyo, Japan, November 11.

80. ———, *Modern mathematical tools for process optimization*, Course on Trends in Rolling Technology, November 26–27, POHTO – The Institute of Management and Technological Training, Oulu, Finland, November 26.

81. S. Jachalski, *Structure formation in thin liquid bilayers*, BMS Intensive Course on Evolution Equations and their Applications, November 27–29, Technische Universität Berlin, November 27.

82. V. John, *On recent analytical and numerical investigations of the SUPG method*, Advances in Computational Mechanics (ACM 2013) – A Conference Celebrating the 70th Birthday of Thomas J.R. Hughes, February 24–27, San Diego, California, February 27.

83. ———, *Velocity-pressure reduced order models for the incompressible Navier–Stokes equations*, 14th Conference on Mathematics of Finite Elements and Applications (MAFELAP 2013), June 11–14, Brunel University, London, UK, June 14.

84. ———, *Assessments of discretizations of convection-dominated scalar problems*, SIAM Conference on Mathematical & Computational Issues in Geosciences, Minisymposium 1 "New Developments in the Modeling, Analysis and Stimulation of Oceanic Flows – Part I", June 17–20, Universitá Degli Studi di Pavoda, Italy, June 17.

85. ———, *Numerical solution methods for coupled population balance systems for the dynamic simulation of multivariate particle processes at the example of form-selective crystallization*, Kick-off Meeting of SPP 1679, TuTech GmbH Hamburg, August 29.

86. ———, *Direct discretizations of bi-variate population balance systems on tensor-product meshes*, The 5th International Conference on Population Balance Modeling (PBM 2013), September 11–13, Indian Institute of Science, Bangalore, September 11.

87. ———, *Finite element methods for the simulation of incompressible turbulent flows*, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, India, September 14.

88. ———, *Numerical methods for convection-diffusion equations – State of the art*, Tata Institute of Fundamental Research, Centre for Applicable Mathematics, Bangalore, India, September 17.

89. ———, *Finite element methods for the simulation of incompressible flows*, 10 talks, lecture for master students, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, October 15 – November 14.

90. ———, *Some analytical results for an algebraic flux correction scheme for a steady convection-diffusion equation in 1D*, Variational Multiscale and Stabilized Finite Elements (VMS 2013), November 6–8, International Center for Numerical Methods in Engineering, Barcelona, Spain, November 8.

91. L. Kamenski, *Stability of explicit time integration of linear parabolic equations with anisotropic finite element meshes*, University of Kansas, Department of Mathematics, USA, November 6.

92. ———, *Anisotropic finite element meshes and stability of explicit Runge–Kutta methods for linear parabolic equations*, University of Missouri-Kansas City, Department of Mathematics, USA, November 8.

93. O. Klein, *Representation of hysteresis operators for vector-valued monotaffine inputs by functions on strings*, Politecnico di Torino, DISMA Dipartimento di Scienze Matematiche "Giuseppe Luigi Lagrange", Italy, April 23.

94. ———, *A representation result for hysteresis operators with vector valued inputs and its application to models for magnetic materials*, 9th International Symposium on Hysteresis Modelling and Micromagnetics (HMM 2013), May 13–15, Taormina, Italy, May 13.

95. D. Knees, *A vanishing viscosity approach to a rate-independent damage model*, Seminar "Wissenschaftliches Rechnen", Technische Universität Dortmund, Fachbereich Mathematik, January 31.

96. ———, *Recent results in nonlinear elasticity and fracture mechanics*, Universität der Bundeswehr, Institut für Mathematik und Bauinformatik, München, August 13.

97. ———, *Global spatial regularity for elasticity models with cracks and contact*, Journées Singulières Augmentées 2013, August 26–30, Université de Rennes 1, France, August 27.

98. ———, *Modeling and analysis of crack evolution based on the Griffith criterion*, Nonlinear Analysis Seminar, Keio University of Science, Yokohama, Japan, October 9.

99. ———, *On energy release rates for nonlinearly elastic materials*, Workshop on Mathematical Aspects of Continuum Mechanics, October 12–14, The Japan Society for Industrial and Applied Mathematics, Kanazawa, Japan, October 12.

100. ———, *Crack evolution models based on the Griffith criterion*, Workshop on Mathematical Aspects of Continuum Mechanics, October 12–14, The Japan Society for Industrial and Applied Mathematics, Kanazawa, Japan, October 13.

101. ———, *Global spatial regularity results for crack with contact and application to a fracture evolution model*, Oberseminar Nichtlineare Analysis, Universität Köln, Mathematisches Institut, October 28.

102. W. König, *Upper tails of self-intersection local times: Survey of proof techniques*, Kyoto University, Research Institute for Mathematical Sciences, Japan, April 12.

103. ———, *A variational formula for the free energy of a many-boson system*, Random Combinatorial Structures and Statistical Mechanics, May 6–10, University of Warwick, Mathematics Institute, Warwick in Venice, Palazzo Pesaro-Papafava, Italy, May 10.

104. ———, *Eigenvalue order statistics and mass concentration for the parabolic Anderson model*, International Conference "Mathematical Physics of Disordered Systems – A Conference in Honor of Leonid Pastur", May 13–17, FernUniversität Hagen, May 16.

105. ———, *Large deviations for the local times of a random walk among random conductances*, Random Walks: Crossroads and Perspectives, Satellite Meeting of the Erdős Centennial Conference, June 24–28, Alfréd Rényi Institute of Mathematics, Budapest, Hungary, June 28.

106. ———, *Upper tails of self-intersection local times: Survey of proof techniques*, 12. Erlanger-Münchner Tag der Stochastik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, July 12.

107. ———, *Geordnete Irrfahrten*, Technische Universität Darmstadt, Fachbereich Mathematik, October 23.

108. ———, *Large deviations for the local times of random walk among random conductances*, 12th Workshop on Stochastic Analysis on Large Scale Interacting Systems, November 21–23, University of Tokyo, Japan, November 23.

109. ———, *Cluster size distribution in classical many-body systems with Lennard–Jones potential*, Warwick EPSRC (Engineering and Physical Sciences Research Council) Symposium on Statistical Mechanics: Computational Coarse-graining of Many-body Systems, December 9–13, University of Warwick, UK, December 11.

110. Th. Koprucki, *Discretization scheme for drift-diffusion equations with a generalized Einstein relation*, Matheon Workshop "6th Annual Meeting Photonic Devices", February 21–22, Konrad-Zuse-Zentrum für Informationstechnik Berlin, February 22.

111. ———, *Generalization of the Scharfetter–Gummel scheme*, 13th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2013), August 19–22, Vancouver, Canada, August 21.

112. Ch. Kraus, *Modeling and analysis of a nonlinear PDE system for phase separation and damage*, Università di Pavia, Dipartimento di Matematica, Italy, January 22.

113. ———, *Sharp interface limit of a diffuse interface model of Navier–Stokes–Allen–Cahn type for mixtures*, Workshop "Hyperbolic Techniques for Phase Dynamics", June 10–14, Mathematisches Forschungsinstitut Oberwolfach, June 11.

114. ———, *Damage and phase separation processes: Modeling and analysis of nonlinear PDE systems*, DIMO2013 – Diffuse Interface Models, September 10–13, Levico Terme, Italy, September 11.

115. M. Ladkau, *Multilevel policy iteration for pricing American options*, 26th European Conference on Operational Research, June 30 – July 4, Università La Sapienza, Rome, Italy, July 2.

116. Ch. Landry, *Collision detection between robots moving along specified paths*, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, May 15.

117. ———, *Optimizing work cells in automotive industry*, Mathematics for Industry and Society, July 4–5, French Embassy, Berlin, July 5.

118. M. Liero, *On gradient structures and geodesic convexity for reaction-diffusion systems*, Research Seminar, Westfälische Wilhelms-Universität Münster, Institut für Numerische und Angewandte Mathematik, April 17.

119. ———, *Gradient structures and geodesic convexity for reaction-diffusion system*, SIAM Conference on Mathematical Aspects of Materials Science (MS13), Minisymposium "Material Modelling and Gradient Flows" (MS100), June 9–12, Philadelphia, USA, June 12.

120. ———, *On gradient structures for drift-reaction-diffusion systems and Markov chains*, Analysis Seminar, University of Bath, Mathematical Sciences, UK, November 21.

121. A. Linke, *On the role of the Helmholtz-decomposition in mixed methods for incompressible flows and a new variational crime*, Clemson University, Department of Mathematical Sciences, South Carolina, USA, July 5.

122. ———, *On the role of the Helmholtz-decomposition in mixed methods for incompressible flows and a new variational crime*, Technische Universität Hamburg-Harburg, Institut für Mathematik, October 17.

123. A. Linke, *On the role of the Helmholtz-decomposition in mixed methods for incompressible flows and a new variational crime*, University of Reading, Department of Meteorology, UK, December 2.

124. ———, *On the role of the Helmholtz-decomposition in mixed methods for incompressible flows and a new variational crime*, Technische Universität Dresden, Fachbereich Mathematik, December 10.

125. ———, *On the role of the Helmholtz-decomposition in mixed methods for incompressible flows and a new variational crime*, Universität Hamburg, Fachbereich Mathematik, December 12.

126. H. Mai, *Efficient drift estimation for jump diffusion processes and jump filtering*, Séminaire de Statistique du CREST, École Nationale de la Statistique et de l'Administration Économique, Centre de Recherche en Économie et Statistique, Paris, France, February 18.

127. ———, *Applications of rough path analysis to robust likelihood inference*, Statistikseminar, Humboldt-Universität zu Berlin, Institut für Mathematik, October 18.

128. P. Mathé, *Signal detection in inverse problems*, Mathematical Modelling and Analysis (MMA2013) and Approximation Methods and Orthogonal Expansions (AMOE2013), May 27–31, University of Tartu, Institute of Mathematics, Estonia, May 29.

129. ———, *Projection schemes for signal detection in statistical inverse problems*, Inverse Problems and Regularization Theory, September 26–29, Fudan University, School of Mathematical Sciences, Shanghai, China, September 27.

130. ———, *Statistical Inverse Problems*, Applied Math Seminar, University of Warwick, Mathematics Institute, Coventry, UK, October 18.

131. A. Mielke, *Using gradient structures for modeling semiconductors*, Eindhoven University of Technology, Institute for Complex Molecular Systems, The Netherlands, February 21.

132. ———, *On entropy-driven dissipative quantum mechanical systems*, Analysis and Stochastics in Complex Physical Systems, March 20–22, Universität Leipzig, Mathematisches Institut, March 21.

133. ———, *Evolutionary Gamma convergence and amplitude equations*, Matheon Multiscale Seminar, Technische Universität Berlin, Institut für Mathematik, April 8.

134. ———, *Gradient structures and uniform global decay for reaction-diffusion systems*, Mathematisches Kolloquium, Universität Bielefeld, Fakultät für Mathematik, April 25.

135. ———, *Analysis, modeling, and simulation of semiconductor devices*, Kolloquium Simulation Technology, Universität Stuttgart, SRC Simulation Technology, May 14.

136. ———, *Coupling quantum mechanical systems with dissipative environments via GENERIC*, Applied Analysis Seminar, University of Bath, Department of Mathematical Sciences, UK, May 23.

137. ———, *Emergence of rate independence in gradient flows with wiggly energies*, SIAM Conference on Mathematical Aspects of Materials Science (MS13), Minisymposium "The Origins of Hysteresis in Materials" (MS56), June 9–12, Philadelphia, USA, June 12.

138. ———, *Deriving the Ginzburg–Landau equation as amplitude equation via evolutionary Gamma convergence*, ERC Workshop on Variational Views on Mechanics and Materials, June 24–26, University of Pavia, Department of Mathematics, Italy, June 26.

139. ———, *Rate-independent plasticity as vanishing-viscosity limit for wiggly energy landscape*, Workshop on Evolution Problems for Material Defects: Dislocations, Plasticity, and Fracture, September 30 – October 4, International School of Advanced Studies (SISSA), Trieste, Italy, September 30.

140. ———, *On the geometry of reaction-diffusion systems: Optimal transport versus reaction*, Recent Trends in Differential Equations: Analysis and Discretisation Methods, November 7–9, Technische Universität Berlin, Institut für Mathematik, November 9.

141. ———, *Introduction to evolutionary Gamma convergence for gradient systems*, 4 talks, School "Multiscale and Multi-field Representations of Condensed Matter Behavior", November 25–29, Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy, November 25–29.

142. ———, *Gradient structures and dissipation distances for reaction-diffusion systems*, Workshop "Material Theory", December 16–20, Mathematisches Forschungsinstitut Oberwolfach, December 17.

143. H.-J. Mucha, *Resampling techniques in cluster analysis: Is subsampling better than bootstrapping?*, European Conference on Data Analysis, July 10–12, University of Luxembourg, Luxembourg, July 11.

144. ———, *Assessment of stability in partitional clustering using resampling techniques*, Third Bilateral German-Polish Symposium on Data Analysis and Its Applications (GPSDAA 2013), September 26–28, Technische Universität Dresden, September 27.

145. ———, *Variables election in cluster analysis using resampling techniques*, British Classification Society Meeting 2013, November 8–9, University College London, Department of Statistical Science, UK, November 8.

146. H. Neidhardt, *Sturm–Liouville boundary value problems with operator potentials*, System and Operator Realizations of Analytic Functions, February 18–22, Lorentz Center, Leiden, The Netherlands, February 22.

147. ———, *Boundary triplets and tunnel junction formula with applications*, Mathematical Challenge of Quantum Transport in Nanosystems, March 12–15, Saint Petersburg National Research University of Informational Technologies, Mechanics, and Optics, Russia, March 14.

148. ———, *Perturbation determinants for singular perturbations*, Séminaire Analyse et Géometrie, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, Marseille, France, May 13.

149. St. Neukamm, *Quantitative results in stochastic homogenization*, Oberseminar Analysis, Technische Universität Dresden, Fakultät Mathematik und Naturwissenschaften, June 13.

150. ———, *Quantitative results in stochastic homogenization*, Matheon Multiscale Seminar, Technische Universität Berlin, Institut für Mathematik, June 27.

151. ———, *Optimal decay estimate on the semigroup associated with a random walk among random conductances*, Dirichlet Forms and Applications, German-Japanese Meeting on Stochastic Analysis, September 9–13, Universität Leipzig, Mathematisches Institut, September 9.

152. O. Omel'chenko, *Thermodynamic limit approach for bifurcation analysis of chimera states*, Forschungsseminar "Dynamische Systeme", Freie Universität Berlin, January 10.

153. ———, *Nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, XXXIII Dynamics Days Europe, Minisymposium MS6 "Collective Behavior in Networks of Oscillators", June 3–7, Madrid, Spain, June 4.

154. ———, *Synchronization phenomena in large size systems of coupled oscillators*, Bogolyubov Readings DIF-2013 "Differential Equations, Theory of Functions and Their Applications", June 23–30, Sevastopol, Ukraine, June 24.

155. O. Omel'chenko, M. Wolfrum, *Generalizing the Ott–Antonsen method for coupled phase oscillators*, Dynamics Days Berlin-Brandenburg, October 1–2, Technische Universität Berlin, October 2.

156. R.I. Patterson, *Monte Carlo simulation of nano-particle formation*, University of Technology Eindhoven, Institute for Complex Molecular Systems, The Netherlands, September 5.

157. R.I.A. Patterson, *Stochastic methods for particle coagulation problems in flows with boundaries*, 5th Workshop "Theory and Numerics of Kinetic Equations", May 13–15, Universität des Saarlandes, Saarbrücken, May 14.

158. ———, *Convergence of stochastic numerical methods for coagulation and advection*, German-Polish Joint Conference on Probability and Mathematical Statistics, June 6–9, Nicolaus Copernicus University, Torun, Poland, June 6.

159. Th. Petzold, *Modelling and simulation of multi-frequency induction hardening of steel parts*, Matheon Multiscale Seminar, Technische Universität Berlin, Institut für Mathematik, January 24.

160. ———, *On the sharp interface limit of a phase field model with mechanical effects applied to phase transitions in steel*, Universität Bremen, Zentrum für Technomathematik, May 22.

161. A. Pimenov, *Modelling permanent effects of a temporary stimulus (PETS) in predator-prey and SIR systems*, Equadiff13, MS20 – Slow-fast and Hysteretic Models of Population Dynamics, August 26–30, Prague, Czech Republic, August 26.

162. J. Polzehl, *Diffusion weighted magnetic resonance imaging – Data, models and problems*, Statistics Seminar, University of Minnesota, School of Statistics, USA, June 6.

163. ———, *dMRI modeling: An intermediate step to fiber tracking and connectivity*, Neuroimaging Data Analysis, June 9–14, Statistical and Applied Mathematical Sciences Institute (SAMSI), Durham (NC), USA, June 9.

164. ———, *Position-orientation adaptive smoothing (POAS) in diffusion weighted imaging*, Neuroimaging Data Analysis, June 9–14, Statistical and Applied Mathematical Sciences Institute (SAMSI), Durham (NC), USA, June 9.

165. ———, *Position-orientation adaptive smoothing – Noise reduction in dMRI*, Strukturelle MR-Bildgebung in der Neuropsychiatrischen Forschung, September 13–14, Philipps-Universität Marburg, Klinik für Psychiatrie und Psychotherapie, Zentrum für Psychische Gesundheit, September 14.

166. P.N. Racec, *Quantum modeling for semiconductor nanowires with embedded subsystems*, Interdisciplinary Workshop on Quantum Device – through Mathematical Structure – 2013, National Institute of Informatics/Okayama University, Tokyo, Japan, January 15.

167. P.N. Racec, *Transport in semiconductor nanowires with constrictions: Cylindrical quantum point contact*, 3èmes Journées Modélisation et Calcul, March 21–22, Université de Reims Champagne-Ardenne, Laboratoire de Mathématiques, France, March 21.

168. M. Radziunas, *Nonlinear dynamics in mode-locked lasers: Modeling, simulations and analysis*, 2013 International Nano-Optoelectronics Workshop (iNOW'2013), August 19–31, Cargèse, France, August 28.

169. ———, *Modeling and simulations of beam stabilization in edge-emitting broad-area semiconductor devices*, Parallel Processing and Applied Mathematics (PPAM 2013), September 8–11, Warsaw, Poland, September 11.

170. ———, *LDSL-tool: A software for simulation and analysis of longitudinal dynamics in semiconductor lasers*, Technical University of Moldova, Department of Physics, Chisinau, October 22.

171. J. Rehberg, *Sobolev extention and analysis on non-Lipschitz domain*, Oberseminar Angewandte Analysis, Universität Darmstadt, Fachbereich Mathematik, May 14.

172. S. Reichelt, *Introduction to homogenization concepts*, Freie Universität Berlin, Institut für Mathematik, April 11.

173. G. Schmidt, *On an integral equation formulation for scattering by biperiodic structures*, Analysis of Partial Differential Equations, A Symposium in honour of Prof. Vladimir Maz'ya on the occasion of his 75th birthday, December 16–17, University of Liverpool, UK, December 17.

174. J.G.M. Schoenmakers, *Simulation of conditional diffusions via forward-reverse stochastic representations*, Summer School "Numerical Methods for Stochastic Differential Equations", September 2–4, Vienna University of Technology, Institute for Analysis and Scientific Computing, Austria, September 2.

175. S. Schyschlowa, *Reduced-order modeling based on POD for incompressible flow problems*, Virginia Tech, Department of Mathematics, Blacksburg, USA, October 3.

176. V. Spokoiny, *Identification and critical dimension in semiparametric estimation*, Workshop "Mathematical Statistics of Partially Identified Objects", April 21–27, Mathematisches Forschungsinstitut Oberwolfach, April 21.

177. ———, *Robust clustering using adaptive weights*, International Workshop on Statistical Learning, June 26–28, Moscow Institute of Physics and Technology, PreMoLab, Russia, June 27.

178. ———, *A new approach to estimation of hidden Markov models*, Workshop "Statistical Inference for Complex Time Series Data", September 23–26, Mathematisches Forschungsinstitut Oberwolfach, September 23.

179. ———, *Some topics in predictive modeling*, Premolab, Russian Academy of Sciences, Institute for Information Transmission Problems, December 26.

180. J. Sprekels, *Prandtl–Ishlinskii operators and elastoplasticity*, 3 talks, Spring School on "Rate-independent Evolutions and Hysteresis Modelling", May 27–31, Politecnico di Milano, Università degli Studi di Milano, Italy, May 27–28.

181. ———, *Optimal control of Allen–Cahn equations with singular potentials and dynamic boundary conditions*, DIMO2013 – Diffuse Interface Models, September 10–13, Levico Terme, Italy, September 11.

182. ———, *Optimal control of the Allen–Cahn equation with dynamic boundary condition and double obstacle potentials: A "deep quench" approach*, Applied Mathematics Seminar, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, September 17.

183. K. Tabelow, *Noise in diffusion MRI – Impact and treatment*, Strukturelle MR-Bildgebung in der neuropsychiatrischen Forschung, September 13–14, Philipps Universität Marburg, September 13.

184. ———, *Advanced statistical methods for noisy and high-dimensional medical (and non-medical) data*, Innovation Days 2013, December 9–10, Helmholtz-Gemeinschaft, Geschäftsstelle Berlin, December 9.

185. M. Thomas, *Rate-independent damage models with spatial BV-regularization – Existence & fine properties of solutions*, Oberseminar zur Analysis, Universität Duisburg-Essen, Fachbereich Mathematik, Essen, January 24.

186. ———, *Local versus energetic solutions in rate-independent brittle delamination*, DIMO2013 – Diffuse Interface Models, September 10–13, Levico Terme, Italy, September 13.

187. ———, *A stress-driven local solution approach to quasistatic brittle delamination*, Seminar on Functional Analysis and Applications, International School of Advanced Studies (SISSA), Trieste, Italy, November 12.

188. E. Valdinoci, *Non local equations of elliptic type*, 11 talks, Summer Course "Non Local Equations of Elliptic Type", July 15–27, Cortona, Italy, July 15–27.

189. ———, *Bernstein's theorem for fractional minimal surfaces*, Universidad de Chile, Centro de Modelamiento Matemático, Santiago de Chile, August 14.

190. ———, *Allen–Cahn equations in periodic media*, 6 talks, International Summer School "Periodic Structures in Applied Mathematics", August 18–31, Georg-August-Universität Göttingen, Mathematisches Institut, August 19–23.

191. ———, *Nonlocal minimal surfaces in the plane*, Pontificia Universidad Católica de Chile, Facultad de Matemáticas, Santiago de Chile, August 21.

192. ———, *Concentration phenomena for nonlocal equations*, Seminario di Analisi & Sistemi Dinamici, Università di Roma Tre, Italy, September 18.

193. ———, *Nonlocal phase transitions and minimal surfaces*, 3 talks, Dispersive PDEs: Models and Dynamics, September 18–20, Università degli Studi di Pisa, Italy, September 19–20.

194. ———, *Phase separation and minimal surfaces, from local to nonlocal*, Working Seminar VARIOGEO, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, October 10.

195. ———, *Regularity results for fractional perimeters*, Workshop on Nonlinear Equations, October 17–20, Madrid, Spain, October 18.

196. ———, *Local and nonlocal features of some differential equations*, African Institute for Mathematical Sciences, Dakar, Senegal, November 19.

197. ———, *Phase separation and minimal surfaces, from local to nonlocal*, Oberseminar Dynamische Systeme, Ruhr-Universität Bochum, November 26.

198. ———, *Regularity of nonlocal minimal surfaces in low dimension*, University of Pisa, Department of Mathematics, Italy, December 18.

199. A.G. Vladimirov, *Interaction of oscillating dissipative optical solitons*, International Conference "Dynamics, Bifurcations, and Strange Attractors", July 1–5, Nizhny Novgorod State University, Russia, July 5.

200. ———, *Weak interaction of localized structures of light*, Dynamical Systems and PDEs Seminar, July 1–5, University of Surrey, UK, July 5.

201. B. Wagner, *On effective slip for an upper convected Maxwell fluid*, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, May 30.

202. ———, *Multiple scales in thin liquid films*, 2 talks, Summer School of the DFG-SPP 1506 "Transport Processes at Fluidic Interfaces", July 16–17, RWTH Aachen, July 16.

203. ———, *On apparent slip of a liquid polymer*, University of California, Department of Mathematics, Los Angeles, USA, November 13.

204. W. Wagner, *Stochastic particle methods for population balance equations*, 5th Workshop "Theory and Numerics of Kinetic Equations", May 13–15, Universität des Saarlandes, Saarbrücken, May 13.

205. T. Wolff, *Annealed asymptotics for occupation time measures of a random walk among random conductances*, "Young European Probabilists 2013 (YEP X)" and "School on Random Polymers", January 8–12, EURANDOM, Eindhoven, The Netherlands, January 10.

206. M. Wolfrum, *The Turing bifurcation on networks: Collective patterns and differentiated nodes*, Kolloquium SFB 910, Technische Universität Berlin, Berlin, January 11.

207. ———, *The Turing bifurcation on networks: Collective patterns and single differentiated nodes*, Applied Dynamics Seminar, University of Maryland, Washington, USA, March 7.

208. ———, *Chimera states: Patterns of coherence and incoherence in coupled oscillator systems*, Dynamical Systems and Mathematical Biology Seminar, Georgia State University, Atlanta, USA, March 12.

209. ———, *The Turing bifurcation on networks: Collective patterns and single differentiated nodes*, International Conference on Dynamics of Differential Equations, March 16–20, Georgia Institute of Technology, Atlanta, USA, March 18.

210. J. Zhang, *Backward stochastic differential equations and related control problems*, Universität Bonn, Hausdorff-Zentrum, February 5.

A.8.3 Talks for a More General Public

1. S. Amiranashvili, *Monsterwellen*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2013, WIAS Berlin, June 8.

2. U. Bandelow, *Presentation of WIAS – Applied Mathematical Research in Photonics*, Corning Technologie Zentrum, Berlin Adlershof, July 10.

3. W. Dreyer, C. Guhlke, *Luftballons, Lithium-Ionen-Batterien und Wasserstoffautos – Ein Fall für die Mathematik*, MathInside – Mathematik ist überall, Urania, Berlin, March 5.

4. C. Guhlke, *Luftballons, Lithium-Ionen-Batterien und Wasserstoffautos — Ein Fall für die Mathematik!*, Matheon Rent the Center, Herder-Gymnasium, Berlin, October 17.

5. R. Henrion, *Optimierung und Zufall in Planungsproblemen der Stromwirtschaft*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2013, WIAS Berlin, June 8.

6. R. Huth, *Luftballons, Wasserstoffautos und Lithium-Ionen-Batterien – Unmögliches zusammenbringen, das kann nur die Mathematik!*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.

7. W. König, *Streifzüge durch die Entwicklung der Wahrscheinlichkeitstheorie*, MathInside – Mathematik ist überall, Urania, Berlin, March 5.

8. ———, *Die Anfänge der Wahrscheinlichkeitsrechnung als Wissenschaft*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.

9. ———, *Was ist Zufall, und wie kam er in die Mathematik?*, Leipziger Gespräche zur Mathematik, Städtischen Kaufhaus am Neumarkt, Leipzig, May 29.

10. ———, *Bevölkerungen in zufälligen Umgebungen: Umziehen von Megacity zu Megacity?*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2013, WIAS Berlin, June 8.

11. Ch. Landry, *Zeit ist Geld: Optimale Bewegung von Industrierobotern*, MathInside – Mathematik ist überall, Urania, Berlin, January 15.

12. M. Landstorfer, *Mathematische Modellierung von Li-Batterien*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2013, WIAS Berlin, June 8.

13. A. Lehmann, *Mit Funktionsauswertungen zu qualitativen Zusammenhängen verschiedener Funktionen, Part II*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.

14. M. Liero, *What is Wasserstein distance?*, The "What is...?" Seminar Series, Berlin Mathematical School, Berlin, November 29.

15. H. Mai, *Mathematische Modellierung von Tierbewegungen*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2013, WIAS Berlin, June 8.

16. J. Rehberg, *Wozu braucht man reelle Zahlen, und wie gelangt man zu ihnen?*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.

17. G. Reinhardt, *Mit Funktionsauswertungen zu qualitativen Zusammenhängen verschiedener Funktionen, Part I*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.

18. H. Stephan, *Gleichungen dritten und vierten Grades und Konstruktionen mit mehr als Zirkel und Lineal*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.
19. ———, *Gleichungen höheren Grades und Konstruktionen mit Zirkel und Lineal als Motivation für komplexe Zahlen*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.
20. J. Wittke, *Mit Funktionsauswertungen zu qualitativen Zusammenhängen verschiedener Funktionen, Part III*, 18. Berliner Tag der Mathematik (18th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 27.

A.8.4 Posters

1. R.M. Arkhipov, *Theoretical analysis of periodically forced semiconductor mode-locked lasers*, 2013 International Nano-Optoelectronics Workshop (iNOW'2013), Cargèse, France, August 19–30.
2. ———, *Transient Cherenkov radiation from an inhomogeneous resonant string excited at superluminal velocity*, Extreme Nonlinear Optics & Solitons, Berlin, October 28–30.
3. R.M. Arkhipov, M. Radziunas, A.G. Vladimirov, *Numerical simulation of passively mode-locked semiconductor lasers under dual mode optical injection regime*, ICONO/LAT 2013 Conference, Russian Academy of Sciences, Moscow, June 17–22.
4. K. Disser, *Entropic gradient structures for reversible Markov chains and the passage to Wasserstein Fokker–Planck*, Workshop for the Initiation of the GAMM Activity Group "Analysis of Partial Differential Equations", Regensburg, October 1–2.
5. A. Fiebach, A. Glitzky, K. Gärtner, A. Linke, *Voronoi finite volume methods for reaction-diffusion systems*, MoMaS Multiphase Seminar Days — Journées MoMaS Multiphasiques, Bures-sur-Yvette, France, October 7–9.
6. K. Gärtner, *Semiconductor device simulation for silicon detectors in astro physics and generalization of the Scharfetter–Gummel scheme to "non Boltzmann" state equations*, 16th International Workshop on Computational Electronics (IWCE 2013), Nara, Japan, June 4–7.
7. J. Giesselmann, *An energy consistent discretization of the Navier–Stokes–Korteweg system*, 84th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2013), Novi Sad, Serbia, March 18–22.
8. Ch. Heinemann, *Analysis of degenerating Cahn–Hilliard systems coupled with complete damage processes*, 2013 CNA Summer School, Center for Nonlinear Analysis, Carnegie Mellon University, Pittsburgh, USA, May 30 – June 7.
9. ———, *Degenerating Cahn–Hilliard systems coupled with complete damage processes*, DIMO2013 – Diffuse Interface Models, Levico Terme, Italy, September 10–13.
10. M. Hofmann, *Probing the transient optical response in femtosecond filaments*, Extreme Nonlinear Optics & Solitons, Berlin, October 28–30.
11. D. Hömberg, Th. Petzold, *MeFreSim — Modellierung, Simulation und Optimierung des Mehrfrequenzverfahrens für die induktive Wärmebehandlung als Bestandteil der modernen Fertigung*, BMBF Status Seminar "Mathematik für Innovationen in Industrie und Dienstleistung", Bonn, June 20–21.
12. S. Jachalski, *Structure formation in thin liquid-liquid films*, Mathematical Approaches to Complex Fluids – A Two Week Summer School, Cambridge, UK, July 22 – August 2.
13. V. John, O. Suciu, *Direct discretizations of bi-variate population balance systems on tensor-product meshes*, The 5th International Conference on Population Balance Modeling (PBM 2013), Bangalore, India, September 11–13.

14. H. Abels, J. Daube, Ch. Kraus, D. Kröner, *Sharp interface limit for the Navier–Stokes–Korteweg model*, DIMO2013 – Diffuse Interface Models, Levico Terme, Italy, September 10–13.
15. A. Pérez-Serrano, *Emission wavelength multistability in semiconductor ring lasers*, CLEO/EUROPE – IQEC 2013, München, May 12–16.
16. D. Peschka, *Gradient formulation of thin-film equations with triple-junctions*, Mathematical Approaches to Complex Fluids – A Two Week Summer School, Cambridge, UK, July 22 – August 2.
17. A. Pimenov, *Theoretical analysis of delayed feedback control of solitons in semiconductor cavity*, Extreme Nonlinear Optics & Solitons, Berlin, October 28–30.
18. A. Pimenov, N. Rebrova, D. Rachinksii, A.G. Vladimirov, *Theoretical analysis of timing jitter in two-section passively mode-locked semiconductor lasers*, CLEO/EUROPE – IQEC 2013, München, May 12–13.
19. M. Radziunas, *Theoretical study of beam quality improvement in spatially modulated broad area edge-emitting devices*, CLEO/EUROPE – IQEC 2013, München, May 12–16.
20. ———, *Traveling wave modeling and mode analysis of semiconductor ring lasers*, CLEO/EUROPE – IQEC 2013, München, May 12–16.
21. S. Reichelt, *Homogenization of degenerated reaction-diffusion equations*, Doktorandenforum der Leibniz-Gemeinschaft, Sektion D, Berlin, June 6–7.
22. H. Si, *TetGen: A quality tetrahedral mesh generator*, Fourth Tetrahedron Workshop on Grid Generation for Numerical Computations (Tetrahedron IV), Verbania, Italy, July 1–3.
23. M. Welvaert, K. Tabelow, R. Seurinck, Y. Rosseel, *Defining ROIs based on localizer studies: More specific localization using adaptive smoothing*, 19th Annual Meeting of the Organization for Human Brain Mapping, Seattle, USA, June 16–20.
24. K. Tabelow, S. Becker, S. Mohammadi, N. Weiskopf, J. Polzehl, *Multi-shell position-orientation adaptive smoothing (msPOAS)*, 19th Annual Meeting of the Organization for Human Brain Mapping, Seattle, USA, June 16–20.
25. S. Mohammadi, K. Tabelow, Th. Feiweier, J. Polzehl, N. Weiskopf, *High-resolution diffusion kurtosis imaging (DKI) improves detection of gray-white matter boundaries*, 19th Annual Meeting of the Organization for Human Brain Mapping, Seattle, USA, June 16–20.
26. K. Tabelow, H.U. Voss, J. Polzehl, *Analyzing fMRI and dMRI experiments with R*, 19th Annual Meeting of the Organization for Human Brain Mapping, Seattle, USA, June 16–20.
27. M. Thomas, *Fine properties of solutions for rate-independent brittle damage models*, XXIII Convegno Nazionale di Calcolo delle Variazioni, Levico Terme, Italy, February 3–8.
28. ———, *Existence & fine properties of solutions for rate-independent brittle damage models*, 84th Annual Meeting of the International Association of Applied Mathematics and Mechanics, GAMM Juniors Poster Exhibition, Novi Sad, Serbia, March 18–22.
29. ———, *Existence & fine properties of solutions for rate-independent brittle damage models*, Workshop for the Initiation of the GAMM Activity Group “Analysis of Partial Differential Equations”, Regensburg, October 1–2.
30. E. Averlant, A.G. Vladimirov, K. Panajotov, H. Tienpont, M. Tlidi, *Delay feedback induces drift of multi-peaks cavity solitons in VCSEL devices*, CLEO/EUROPE – IQEC 2013, München, May 11–17.
31. S. Slepneva, B. O’Shuaghnessy, B. Kelleher, S.P. Hegarty, A.G. Vladimirov, G. Huyet, *Dynamics of Fourier domain mode locked lasers*, CLEO/EUROPE – IQEC 2013, München, May 11–17.
32. M. Tlidi, A.G. Vladimirov, A. Pimenov, K. Panajotov, D. Puzyrev, S.M. Yanchuk, S.M. Gurevich, *Delay induced instabilities of cavity solitons in passive and active laser systems*, CLEO/EUROPE – IQEC 2013, München, May 11–17.

A.9 Visits to other Institutions[6]

1. G. Hu, South University of Science and Technology of China, Department of Financial Mathematics and Financial Engineering, Shenzhen, June 27–30.
2. ———, Chinese Academy of Sciences, Laboratory of Scientific and Engineering Computing and Institute of Applied Mathematics, Beijing, China, July 6–16.
3. ———, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, November 18 – December 15.
4. ———, University of Tokyo, Graduate School of Mathematical Sciences, Japan, December 16–26.
5. R. Allez, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, September 20–23.
6. ———, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, September 27 – October 13.
7. ———, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, October 25–29.
8. ———, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, November 23 – December 2.
9. R.M. Arkhipov, Tyndall National Institute, Cork, Ireland, April 18 – May 11.
10. L. Avena, Université Paris Diderot, Laboratoire de Probabilités et Modèles Aléatoires, France, June 10–15.
11. ———, Università degli Studi di Roma “La Sapienza”, Dipartimento di Matematica, Italy, September 2–6.
12. ———, Aix-Marseille Université, Centre de Mathématiques et Informatique, France, September 9–14.
13. ———, Università degli Studi di Roma “La Sapienza”, Dipartimento di Matematica, Italy, December 16, 2013 – January 7, 2014.
14. U. Bandelow, Technische Universität Wien, Institut für Photonik and Institut für Theoretische Physik, Austria, June 3–8.
15. ———, The Russell Berrie Nanotechnology Institute, Haifa, Israel, November 17–21.
16. ———, Weizmann Institute of Science, Department of the Physics of Complex Systems, Rehovot, Israel, November 22–30.
17. ———, National University of Mar de Plata, Department of Physics, Argentina, December 14–23.
18. Ch. Bayer, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, February 13–22.
19. ———, National University of Singapore, Department of Economics, February 28 – March 9.
20. ———, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, October 2–13.
21. A. Caiazzo, Universitá di Trento, Dipartimento di Ingegneria Civile e Ambientale, Italy, May 14, 2012 – February 15, 2013.
22. ———, Pontificia Universidad Católica de Valparaíso, Civil Engineering, Santiago, Chile, March 11–28.
23. ———, Universidad de Castilla-La Mancha, Departamento de Matematica, Cuenca, Spain, September 20–25.

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

24. M. Eigel, Eidgenössische Technische Hochschule Zürich, Seminar für Angewandte Mathematik, Switzerland, September 24–27.
25. J. Elschner, University of Tokyo, Graduate School of Mathematical Sciences, Japan, February 18 – March 1.
26. G. Faraud, Université Paris Diderot, Laboratoire de Probabilités et Modèles Aléatoires, France, June 25 – July 5.
27. M.H. Farshbaf Shaker, Universität Regensburg, Fakultät für Mathematik, February 6–9.
28. ———, Universität Regensburg, Fakultät für Mathematik, June 25–28.
29. ———, Universität Regensburg, Fakultät für Mathematik, July 22–26.
30. K. Gärtner, University of Massachusetts, Electrical and Computer Engineering, Amherst, USA, July 18–21.
31. ———, University of Lugano, Institute of Computational Science, Switzerland, September 15–22.
32. J. Giesselmann, University of Crete, Department of Applied Mathematics, Archimedes Center for Modeling, Analysis and Computation (ACMAC), Heraklion, Greece, April 1 – June 30.
33. S. Heinz, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, August 18–23.
34. M. Hesse, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, November 21–24.
35. ———, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, November 28 – December 2.
36. R. Hildebrand, Université de Grenoble, Laboratoire Jean Kuntzmann, France, June 20–29.
37. D. Hömberg, Université Paris-Sud, Département de Mathématiques, France, January 15–18.
38. ———, Fudan University, School of Mathematical Sciences, Shanghai, China, February 27 – March 12.
39. ———, University of Bath, Department of Mathematical Sciences, UK, May 7–10.
40. ———, University of Bath, Department of Mathematical Sciences, UK, September 30 – October 4.
41. V. John, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, March 11–15.
42. ———, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, May 21–24.
43. ———, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, September 13–18.
44. ———, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, October 15 – November 14.
45. L. Kamenski, University of Kansas, Department of Mathematics, USA, October 17–28.
46. ———, University of Kansas, Department of Mathematics, USA, November 4–9.
47. O. Klein, Politecnico di Torino, DISMA Dipartimento di Scienze Matematiche “Giuseppe Luigi Lagrange”, Italy, April 22–25.
48. D. Knees, Universität Duisburg-Essen, Fakultät für Mathematik, March 13–16.
49. ———, University of Brescia, Department of Mathematics, Italy, April 8–12.
50. ———, University of Pavia, Department of Mathematics, Italy, June 24–28.
51. ———, Keio University of Science, Yokohama, Japan, October 7–11.
52. ———, Universität Köln, Mathematisches Institut, October 28 – November 29.
53. W. König, Kyoto University, Research Institute for Mathematical Sciences, Japan, April 2–17.

54. ———, University of Warwick, Mathematics Institute, Coventry, UK, June 10–15.
55. ———, Kyoto University, Research Institute for Mathematical Sciences, Japan, November 17–20.
56. ———, Kyoto University, Research Institute for Mathematical Sciences, Japan, November 23 – December 4.
57. Ch. Kraus, Università di Pavia, Dipartimento di Matematica, Italy, January 21 – March 25.
58. Ch. Landry, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, May 6–17.
59. A. Linke, Clemson University, Department of Mathematical Sciences, South Carolina, USA, July 1–7.
60. H. Mai, École Nationale de la Statistique et de l'Administration Économique, Centre de Recherche en Économie et Statistique, Paris, France, February 16–21.
61. P. Mathé, Technische Universtiät Chemnitz, Fakultät für Mathematik, September 2–6.
62. ———, Fudan University, School of Mathematical Sciences, Shanghai, China, September 14–30.
63. A. Mielke, Eindhoven University of Technology, Institute for Complex Molecular Systems, The Netherlands, February 19–22.
64. ———, University of Bath, Department of Mathematical Sciences, UK, May 19–24.
65. ———, Charles University, Mathematical Institute, Prague, Czech Republic, August 19–23.
66. R. Müller, Urgench State University, Faculty of Physics and Mathematics, Uzbekistan, December 1–20.
67. H. Neidhardt, Centre International de Rencontres Mathématiques, Marseille, France, May 5–24.
68. St. Neukamm, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, August 19–23.
69. ———, Université Libre de Bruxelles, Département de Mathématique, Belgium, August 26–30.
70. J. Polzehl, University of Minnesota, School of Statistics, USA, May 24 – June 7.
71. ———, University of Minnesota, School of Statistics, USA, June 22 – July 8.
72. M. Radziunas, Technical University of Moldova, Department of Physics, Chisinau, Moldova, October 21–26.
73. J. Rehberg, Universität Darmstadt, Fachbereich Mathematik, May 13–17.
74. S. Schyschlowa, Virginia Tech, Department of Mathematics, Blacksburg, USA, September 23 – October 4.
75. V. Spokoiny, Moscow Institute of Physics and Technology, PreMoLab, Russia, February 12–21.
76. ———, Moscow Institute of Physics and Technology, PreMoLab, Russia, June 10–29.
77. J. Sprekels, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, September 13–20.
78. M. Thomas, International School of Advanced Studies (SISSA), Trieste, Italy, November 10–21.
79. E. Valdinoci, Johann Wolfgang Goethe-Universität Frankfurt, Institut für Mathematik, June 30 – July 7.
80. ———, Università di Padova, Dipartimento di Matematica, Italy, July 8–14.
81. ———, Universidad de Chile, Departamento de Ingenieria Matemática and Centro de Modelamiento Matemático; Pontificia Universidad Católica de Chile, Departamento de Matemáticas, Santiago de Chile, July 29 – August 23.
82. ———, African Institute for Mathematical Sciences, Dakar, Senegal, November 17–23.
83. ———, Ruhr-Universität Bochum, Fakultät für Mathematik, November 25–28.
84. ———, Universidad Autonoma de Madrid, Departamento de Matemáticas, Spain, December 9–15.
85. ———, Università di Pisa, Dipartimento di Matematica, Italy, December 15–23.

86. B. Wagner, University of California, Department of Mathematics, Los Angeles, USA, November 8–22.
87. M. Wolfrum, University of Maryland, Department of Physics, Washington, USA, March 4–9.
88. ———, Georgia State University, Department of Mathematics & Statistics, Atlanta, USA, March 10–16.
89. J. Zhang, Universität Bonn, Hausdorff-Zentrum, February 4–8.
90. M. Zhilova, Moscow Institute of Physics and Technology, PreMoLab, Russia, June 24 – July 12.

A.10 Academic Teaching[7]

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. V. John, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
8. C. Carstensen, P. Deuflhard, H. Gajewski, V. John, R. Klein, R. Kornhuber, J. Sprekels, others, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
9. D. Knees, *Gewöhnliche Differentialgleichungen* (lecture), Universität Duisburg-Essen, 4 SWS.
10. ———, *Gewöhnliche Differentialgleichungen* (practice), Universität Duisburg-Essen, 2 SWS.
11. W. König, *Wahrscheinlichkeitstheorie II* (lecture), Technische Universität Berlin, 4 SWS.
12. D. Becherer, J. Blath, P. Friz, W. König, others, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
13. A. Mielke, *Mehrdimensionale Variationsrechnung/BMS Advanced Course on Multidimensional Calculus of Variations* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
14. ———, *Mehrdimensionale Variationsrechnung* (practice), Humboldt-Universität zu Berlin, 2 SWS.
15. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
16. R. Müller, *Numerische Verfahren für Erhaltungsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. R.I.A. Patterson, *Lineare Algebra I für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
18. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
19. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. H. Stephan, *Additive Zahlentheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
21. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
22. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

[7] SWS = semester periods per week

Summer Semester 2013

1. P. Friz, *Applied Probability and Financial Mathematics* (seminar), Technische Universität Berlin, 2 SWS.
2. ———, *Further Topics in Finance* (seminar), Technische Universität Berlin, 2 SWS.
3. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
4. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
5. W. Dreyer, *Nichtlineare Kontinuumsmechanik* (lecture), Technische Universität Berlin, 4 SWS.
6. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
7. D. Hömberg, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
8. V. John, *Numerik III: Numerical Methods for Partial Differential Equations* (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. Becherer, J. Blath, P. Friz, W. König, others, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
11. J. Blath, W. König, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
12. A. Mielke, *Ausgewählte Kapitel der Variationsrechnung* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
14. R. Müller, *Iterative Verfahren für große Gleichungssysteme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
15. J.G.M. Schoenmakers, *Berechnungs- und Simulationsmethoden in der Finanzmathematik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
16. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
17. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
18. H. Stephan, *Additive Zahlentheorie II* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
19. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
20. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

Winter Semester 2013/2014

1. P. Friz, *Hairer's Regularity Structures* (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. A. Caiazzo, *Analysis I (lehramtsbezogen)* (seminar), Freie Universität Berlin, 2 SWS.

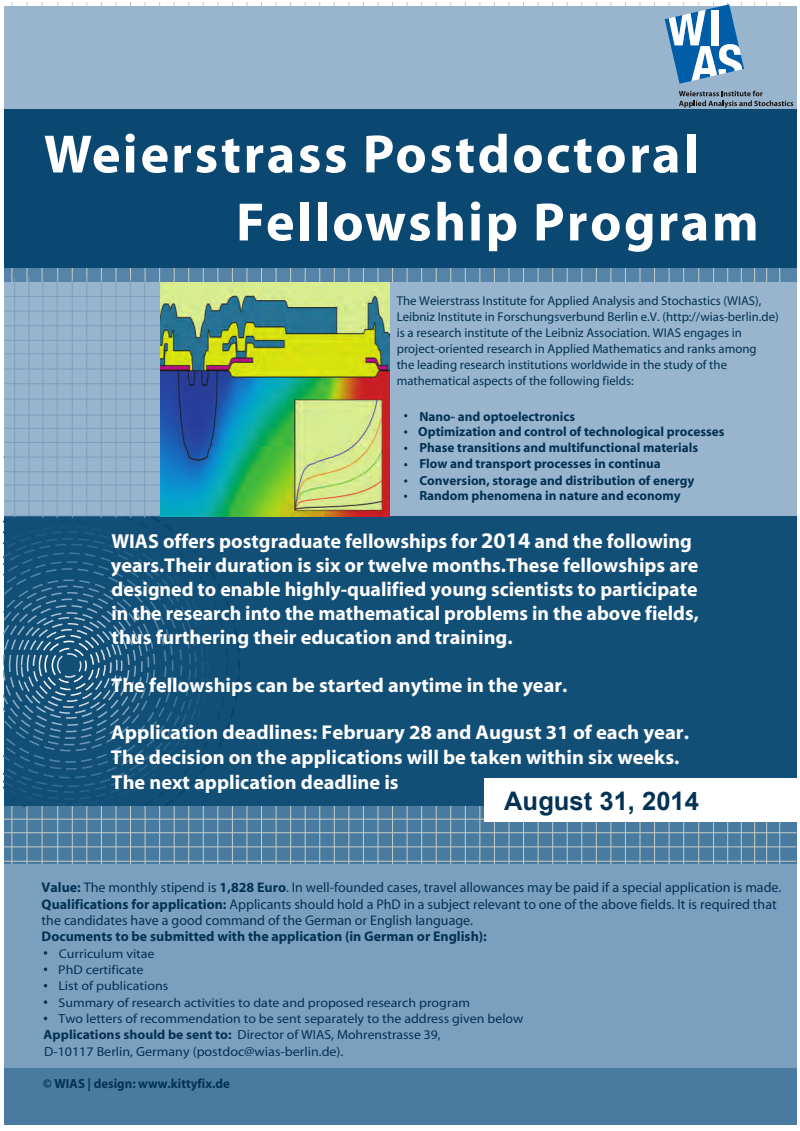
5. W. Dreyer, *Grundlagen der Kontinuumstheorie II* (lecture), Technische Universität Berlin, 4 SWS.
6. M. Eigel, *Lineare Algebra für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
7. A. Glitzky, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
8. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
9. D. Hömberg, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
10. V. John, *Numerik IV* (lecture), Freie Universität Berlin, 4 SWS.
11. C. Carstensen, P. Deuflhard, H. Gajewski, V. John, R. Klein, R. Kornhuber, J. Sprekels, others, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
12. D. Becherer, J. Blath, P. Friz, W. König, others, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
13. J. Blath, W. König, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
14. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
15. R. Müller, *Numerical Methods for Partial Differential Equations* (lecture), Urgench State University, Faculty of Physics and Mathematics, Usbekistan, 4 SWS.
16. St. Neukamm, *Partielle Differentialgleichungen* (lecture), Ruprecht-Karls-Universität Heidelberg, 4 SWS.
17. ———, *Stochastic Homogenization* (lecture), Ruprecht-Karls-Universität Heidelberg, 2 SWS.
18. ———, *Homogenisierung* (seminar), Ruprecht-Karls-Universität Heidelberg, 2 SWS.
19. D. Peschka, *Numerische Mathematik II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
20. V. Spokoiny, *Methoden der Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
21. ———, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
22. ———, *Methoden der Statistik* (practice), Humboldt-Universität zu Berlin, 2 SWS.
23. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
24. J. Sprekels, *Höhere Analysis I (Funktionalanalysis)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
25. H. Stephan, *Mathematische Modellierung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
26. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
27. 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 2013, Dr. Emmanuel Boissard (Université Paul Sabatier, Institut de Mathématiques de Toulouse, France) worked as fellowship holder at WIAS.



A.12 Visiting Scientists[8]

A.12.1 Guests

1. L. Adam, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, November 7–21.
2. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, May 21–29.
3. M. Arias-Chao, Alstom Power Ltd., Baden, Switzerland, June 30 – July 5.
4. L. Avena, Universität Zürich, Institut für Mathematik, Switzerland, March 4–9.
5. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, February 2–13.
6. D. Belomestny, Universität Duisburg-Essen, Fachbereich Mathematik, May 13–17.
7. M. Belyaev, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
8. A. Bernsteyn, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
9. M. Bessemoulin-Chatard, Université Blaise Pascal, Clermont-Ferrand II, Laboratoire de Mathématiques, Aubière, France, January 29 – February 1.
10. A. Boitsev, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russia, November 30 – December 7.
11. A. Bradji, University of Badji Mokhtar Annaba, Department of Mathematics, Algeria, August 31 – September 9.
12. V.-E. Brunel, École Nationale de la Statistique et de l'Administration Économique (ENSAE ParisTech), Groupe de Statistique Appliquée, France, November 16–24.
13. E. Burnaev, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
14. ———, September 16–22.
15. I. Castillo, Université Pierre et Marie Curie, Laboratoire de Probabilités et Modèles Aléatoires, Paris, France, May 21–25.
16. C. Cavaterra, Università degli Studi di Milano, Dipartimento di Matematica, Italy, November 20–27.
17. E. Chernousova, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
18. A.B. Cibik, Gazi University, Faculty of Science, Teknikokullar/Ankara, Turkey, June 11, 2012 – June 10, 2013.
19. R. Ciegis, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, June 18–22.
20. ———, November 27 – December 6.
21. A. Cipriani, Universität Zürich, Institut für Mathematik, Switzerland, October 24–29.
22. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, April 18–26.
23. E. Creusen, Eindhoven University of Technology, Biomedical Engineering, Biomedical Image Analysis, The Netherlands, October 27 – November 2.
24. F. Dassi, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, July 5 – September 30.

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

25. ———, November 4–15.
26. T. Dela Haije, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands, April 14–20.
27. A. Derendyaev, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, September 8–14.
28. E. Diederichs, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 27–31.
29. Y. Dorn, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
30. L. Dumaz, University of Cambridge, Centre for Mathematical Sciences, UK, December 10–19.
31. P. Dvurechenskiy, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
32. K. Efimov, Moscow Institute of Physics and Technology, PreMoLab, Russia, September 16, 2013 – August 31, 2014.
33. R. Ellwanger, European University Institute, Department of Economics, Florence, Italy, August 5–31.
34. P. Erofeev, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
35. M.M. Fall, African Institute for Mathematical Sciences, Endowed Chair in Mathematics and Applications, Mbour, Senegal, June 3–9.
36. J. Feng, University of Kansas, Department of Mathematics, USA, July 9–13.
37. A. Figalli, University of Texas at Austin, Department of Mathematics, USA, June 24–29.
38. R. Fukushima, Kyoto University, Research Institute for Mathematical Sciences, Japan, September 14–21.
39. A. Gagloev, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
40. Th. Gallay, Université de Grenoble I, Institut Fourier, Saint-Martin-d'Hères, France, June 1–7.
41. A. Gasnikov, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
42. ———, May 21–29.
43. A. Gaudillière, Aix-Marseille Université, Centre de Mathématiques et Informatique, Laboratoire d'Analyse, Topologie, Probabilités, France, June 16–20.
44. M. Gerdts, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, December 16–19.
45. A. Goldenschluger, University of Haifa, Department of Statistics, Israel, April 29 – May 4.
46. S. Gurevich, Wilhelms-Universität Münster, Institut für theoretische Physik, January 7–12.
47. ———, July 27 – August 1.
48. U. Hämarik, University of Tartu, Institute of Mathematics, Estonia, April 22 – May 21.
49. J. Häppölä, King Abdullah University of Science and Technology (KAUST), Department of Computer, Electrical and Mathematical Sciences & Engineering (CEMSE), Jeddah, Saudi Arabia, June 10 – July 15.
50. M. Heida, Universität Dortmund, Fakultät für Mathematik, January 28–31.
51. M. Hesse, University of Bath, Department of Mathematical Sciences, UK, August 26–29.
52. D. Hilhorst, Université Paris-Sud, Laboratoire d'Analyse Numérique, Orsay, France, October 14–17.
53. M. Hirokawa, Okayama University, Graduate School of Natural Sciences and Technology, Department of Mathematics, Japan, August 25 – September 12.
54. G.C. Hsiao, University of Delaware, Department of Mathematical Sciences, Newark, USA, August 31 – September 14.

55. T. Ichinose, Kanazawa University, Faculty of Science, Department of Mathematics, Japan, August 2–19.
56. S. Käbisch, University of Surrey, Department of Mathematics, Guildford, UK, October 16–22.
57. L. Kamenski, University of Kansas, Department of Mathematics, Lawrence, USA, February 11–15.
58. U. Kangro, University of Tartu, Institute of Mathematics, Estonia, April 22 – May 7.
59. ———, May 10–21.
60. I. Kashchenko, Yaroslavl Demidov State University, Department of Mathematical Modeling, Russia, November 10–17.
61. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, February 2–8.
62. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, July 15 – August 15.
63. M. Kružik, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, May 13–17.
64. E. Krymova, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
65. G. Lazzaroni, Universität Würzburg, Institut für Mathematik, May 12–16.
66. A. Lechleiter, Universität Bremen, Zentrum für Technomathematik, September 16–20.
67. V. Lotoreichik, Technische Universität Graz, Institut für Numerische Mathematik, Austria, January 13–20.
68. J. Maas, Universität Bonn, Institut für Angewandte Mathematik, May 26 – June 4.
69. M.M. Malamud, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Donetsk, Ukraine, April 2–30.
70. Y. Maximov, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
71. M. Meyries, Martin-Luther-Universität Halle-Wittenberg, Institut für Mathematik, Halle, March 4–28.
72. G. Milshteyn, Ural Federal University, Institute of Physics and Applied Mathematics, Ekaterinburg, Russia, October 1 – November 29.
73. P. Mishchenko, Moscow Institute of Physics and Technology, PreMoLab, Russia, January 17–27.
74. ———, May 13–17.
75. V. Moldoveanu, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, July 28 – August 11.
76. E. Montbrio, Universitat Pompeu Fabra, Department of Information and Communication Technologies, Barcelona, Spain, August 10–25.
77. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, July 28 – August 9.
78. A. Nazin, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
79. R. Nickl, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, March 18–28.
80. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, November 7–21.
81. M. Panov, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
82. ———, August 1 – December 31.
83. V. Panov, Universität Duisburg-Essen, Fachbereich Mathematik, May 13–17.

84. F.S. Patacchini, University of Bath, Department of Mathematical Sciences, UK, August 19–23.
85. C. Patz, Robert Bosch GmbH, Stuttgart, January 30 – February 6.
86. ———, April 17–21.
87. ———, September 26–30.
88. M.A. Peletier, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), Department of Mathematics and Computer Science, The Netherlands, November 18–22.
89. P. Perlikowski, Lodz University of Technology, Division of Dynamics, Poland, May 12–27.
90. B. Polyak, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
91. P. Prikhodko, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
92. T. Pryer, University of Kent, School of Mathematics, Statistics and Actuarial Science, Canterbury, UK, August 5–9.
93. D.R.M. Renger, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), Department of Mathematics and Computer Science, The Netherlands, January 13–17.
94. F. Rindler, University of Warwick, Mathematics Institute, UK, November 26–30.
95. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, July 3–11.
96. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, January 28 – February 28.
97. ———, April 15 – May 15.
98. ———, September 4 – October 4.
99. ———, November 11 – December 11.
100. T. Sadeev, Technische Universität Berlin, Institut für Festkörperphysik, January 21 – February 1.
101. M. Sart, Université Sophia Antipolis, Laboratoire Jean-Alexandre Dieudonné, Nice, France, November 11–14.
102. M. Schmuck, Imperial College London, Departments of Chemical Engineering and Mathematics, UK, April 1–30.
103. M. Schonbek, University of California, Department of Mathematics, Santa Cruz, USA, October 2–11.
104. H. Schwetlick, University of Bath, Department of Mathematical Sciences, UK, June 9–12.
105. J. Seidel, Technische Universität Chemnitz, Fakultät für Mathematik, December 2–5.
106. B. Sengul, University of Cambridge, Centre for Mathematical Sciences, UK, December 10–20.
107. J. Serra Montolí, Universitat Politecnica de Catalunia, Departament de Matemàtica Aplicada I, Barcelona, Spain, June 10–14.
108. G. Shaw, University of Cambridge, Faculty of Mathematics, UK, November 26–29.
109. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, July 7–31.
110. A. Shilnikov, Georgia State University, Neuroscience Institute, Atlanta, USA, January 6–13.
111. S. Shpirko, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
112. E. Sidorova, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
113. J. Sieber, University of Exeter, Mathematics, UK, January 6–11.
114. ———, June 16–22.

115. ———, December 16, 2013 – January 8, 2014.
116. D. Skryabin, University of Bath, Department of Physics, UK, January 15 – April 16.
117. St. Sperlich, Université de Genève, Département des Sciences Économiques, Switzerland, October 9–14.
118. E. Spodarev, Universität Ulm, Institut für Stochastik, January 22–25.
119. U. Stefanelli, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nationale delle Ricerche (IMATI-CNR), Pavia, Italy, April 15–19.
120. A. Suvorikova, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
121. ———, October 1 – December 31.
122. A.F.M. ter Elst, The University of Auckland, Department of Mathematics, New Zealand, July 28 – August 24.
123. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, October 25–29.
124. M. Tretyakov, University of Nottingham, School of Mathematical Sciences, UK, November 10–14.
125. A. Trifanov, St. Petersburg National University of Information Technologies, Mechanics and Optics, Quantum Optics, Russia, November 30 – December 7.
126. A. Tsimbalyk, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
127. D. Turaev, Imperial College London, Department of Mathematics, UK, July 24–31.
128. S. Ullmann, Technische Universität Darmstadt, Fachbereich Mathematik, January 20–25.
129. H. Wu, Fudan University, School of Mathematical Sciences, Shanghai, China, November 24–30.
130. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 9–29.
131. ———, September 14 – October 2.
132. Y. Yanovich, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 13–17.
133. A. Yilmaz, Bogazici University, Department of Mathematics, Bebek-Istanbul, Turkey, October 14–18.
134. T. Yin, Chongqing University, College of Mathematics and Statistics, China, October 28, 2013 – October 25, 2014.
135. V. Zagrebnov, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, France, August 4–16.
136. O. Zaitsev, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, September 16–22.
137. Ch. Zanini, Politechnic University of Turin, Department of Mathematics, Italy, July 3–12.
138. N. Zhivotovskiy, Moscow Institute of Physics and Technology, PreMoLab, Russia, October 20 – November 1.
139. J. Zimmer, University of Bath, Department of Mathematical Sciences, UK, January 22–25.

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. P. Friz, Technische Universität Berlin, Institut für Mathematik, WIAS, June 12, 2009 – June 11, 2014.
4. Ž. Tomovski, Sts. Cyril and Methodius University, Institute of Mathematics, Skopje, Republic of Macedonia, IMU Berlin Einstein Foundation Program, January 7 – February 6.
5. Ž. Tomovski, Sts. Cyril and Methodius University, Institute of Mathematics, Skopje, Republic of Macedonia, IMU Berlin Einstein Foundation Program, July 1 – August 31.

A.12.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. B. Bugert, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
2. M. Panov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, doctoral candidate, August 1 – December 31.
3. C. Patz, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, January 1 – December 31.
4. B. Rehle, Technische Universität Berlin, Institut für Mathematik, Research Training Group 1845 "Stochastic Analysis with Applications in Biology, Finance and Physics", doctoral candidate, October 1 – December 31.
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, January 1 – March 31.
6. K. Schildknecht, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, February 1 – December 31.
7. O. Sekulovic, Berlin Mathematical School, Einstein Foundation, doctoral candidate, January 1 – August 24.
8. J. Stange, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, January 1 – December 31.
9. A. Suvorikova, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group 1792 "High Dimensional Non Stationary Time Series Analysis", doctoral candidate, October 1 – December 31.
10. W. van 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, January 1 – December 31.
11. U. Wilbrandt, Freie Universität Berlin, Institut für Mathematik, Helmholtz-Kolleg GEOSIM, doctoral candidate, January 1 – November 30.

A.13 Guest Talks

1. L. Adam, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *Analysis of the solution map governed by a parametrized differential inclusion*, November 12.
2. V. Agostiniani, University of Oxford, Mathematical Institute, UK, *Minimum problems for a class of non-quasiconvex energy densities*, December 10.
3. B. Andreianov, Université de Franche-Comté, Besançon, France, *Structural stability and well-posedness for scalar degenerate parabolic equations*, December 11.
4. M. Arias-Chao, Alstom Power Ltd., Baden, Switzerland, *Calibration and uncertainty quantification for gas turbines models*, July 2.
5. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Eigenvalue enclosures for the Maxwell operator*, February 7.
6. J. Behrndt, Technische Universität Graz, Institut für Numerische Mathematik, Austria, *Titchmarsh–Weyl theory for elliptic differential operators on unbounded domains*, May 29.
7. D. Belomestny, Universität Duisburg-Essen, Fachbereich Mathematik, *On one inverse problem of nancial mathematics with error in the operator*, October 30.
8. M. Bessemoulin-Chatard, Université Blaise Pascal, Clermont-Ferrand II, Laboratoire de Mathématiques, Aubière, France, *A finite volume scheme for a Patlak–Keller–Segel model with cross-diffusion*, January 31.
9. M. Blum, Universität Siegen, Fachgruppe Angewandte Analysis und Numerik, *A short introduction into a few aspects of environmental physics and geomathematics*, April 3.
10. O. Bodnar, Universität Frankfurt (Oder), Institut für Mathematik, *Bayesian analysis of inconsistent key comparison data*, January 15.
11. A. Boitsev, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russia, *Boundary triplets for sum of tensor products of operators*, December 5.
12. D. Bontemps, Université Paul Sabatier, Institut de Mathématiques de Toulouse, France, *Bayesian posterior consistency and contraction rates in the shape invariant model*, October 23.
13. A. Böttcher, Technische Universität Darmstadt, Fachbereich Mathematik, *The hybrid phase field model – Introduction and numerical examples*, September 24.
14. A. Bradji, University of Badji Mokhtar Annaba, Department of Mathematics, Algeria, *Some recent results on the convergence order of finite volume methods for evolution equations on general nonconforming multidimensional spatial meshes*, September 5.
15. Th.J. Bridges, University of Surrey, Department of Mathematics, Guildford, UK, *Reappraisal of 2+ myths in the theory of nonlinear waves*, March 5.
16. V.-E. Brunel, École Nationale de la Statistique et de l'Administration Économique (ENSAE ParisTech), Groupe de Statistique Appliquée, France, *Adaptive estimation of convex polytopes*, November 16.
17. B. Bugert, Technische Universität Berlin, Berlin Mathematical School, *On an integral equation method for electromagnetic scattering by biperiodic structures*, January 8.
18. A. Caboussat, Haute École de Gestion de Genève, Economie d'Entreprise, Carouge, Switzerland, *Numerical solution of fully nonlinear elliptic equations: Least-squares methods and nonlinear optimization*, February 5.
19. I. Castillo, Université Pierre et Marie Curie, Laboratoire de Probabilités et Modèles Aléatoires, Paris, France, *Some results on frequentist analysis of Bayesian posterior distributions*, May 22.

20. C. Cavaterra, Università degli Studi di Milano, Dipartimento di Matematica, Italy, *Global weak solution and blow-up criterium of the general Ericson–Leslie system for nematic crystal flows*, November 26.
21. I. Chuesov, Karazin Kharkov National University, Department of Mathematical Physics and Computational Mathematics, Ukraine, *Dynamics in the random kick model generated by 3D viscous primitive equations for ocean circulation*, June 12.
22. R. Ciegis, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, *On comparison of numerical methods for generalized nonlinear Schrödinger equations*, December 5.
23. A. Cipriani, Universität Zürich, Institut für Mathematik, Switzerland, *High points for a discrete and a continuum random interface*, October 28.
24. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, *A phase-field model for the Willmore flow with constraints*, April 24.
25. E. Creusen, Eindhoven University of Technology, Biomedical Engineering, Biomedical Image Analysis, The Netherlands, *Diffusion weighted MRI: Enhancement and analysis*, October 29.
26. J. Dannberg, Helmholtz-Zentrum Potsdam, Geodynamische Modellierung, *Modelling mantle plumes with ASPECT: An advanced solver for problems in earth's convection*, July 4.
27. F. Dassi, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, *Anisotropic error estimates for PDE defined on surfaces*, August 20.
28. ———, *A curvature-adapted anisotropic surface remeshing method*, September 24.
29. ———, *Surface mesh simplification strategy for saptial regression analysis of cortical surface data*, November 7.
30. Th. Dickhaus, Humboldt-Universität zu Berlin, Institut für Mathematik, *Structural simultaneous statistical inference*, January 15.
31. E. Diederichs, Moscow Institute of Physics and Technology, PreMoLab, Russia, *Identifying enterotypes by high dimensional clustering*, May 28.
32. A. Dörre, Otto-von-Guericke-Universität Magdeburg, Fakultät für Mathematik, *Bernstein-Copulas als nichtparametrische Copula-Schätzer im Vergleich zu modifizierten Kernschätzern*, April 26.
33. C. dos Reis, Technische Universität Berlin, Institut für Mathematik, *Root's barrier, viscosity solutions of obstacle problems and reflected FBSD*, February 12.
34. L. Dumaz, University of Cambridge, Centre for Mathematical Sciences, UK, *Some properties of the true selfrepelling motion*, December 13.
35. M. Eigel, Humboldt-Universität zu Berlin, Institut für Mathematik, *Adaptive stochastic Galerkin FEM*, January 9.
36. R. Ellwanger, European University Institute, Department of Economics, Florence, Italy, *The term structure of volatility in commodity futures markets*, August 27.
37. H.-J. Engelbert, Friedrich-Schiller-Universität Jena, Institut für Stochastik, *On the martingale property of stochastic exponentials for continuous local martingales: A new approach*, January 23.
38. A. Evgrafov, Technical University of Denmark, Department of Applied Mathematics and Computer Science, Kgs. Lyngby, *An inexpensive locally quadratically convergent algorithm for topology optimization of flow domains*, November 19.
39. J. Feng, University of Kansas, Department of Mathematics, USA, *A Hamilton–Jacobi equation in space of probability measures, in connection with the Onsager–Joyce–Montgomery theory*, July 10.
40. A. Figalli, The University of Texas at Austin, Department of Mathematics, USA, *Stability results for sum of sets in* R^n, June 26.

41. R. Fukushima, Kyoto University, Research Institute for Mathematical Sciences, Japan, *Quenched large deviations for multidimensional random walk in random environment with holding times*, September 18.
42. A. Fuster, Technische Universiteit Eindhoven, Department of Biomedical Engineering, The Netherlands, *Riemannian framework for brain diffusion MRI*, April 15.
43. St. Gaïffas, École Polytechnique, Centre de Mathématiques Appliquées, Palaiseau, France, *Link prediction in graphs with time-evolving features*, November 6.
44. V.A. Galkin, Surgut State University, Polytechnical Institute, Russia, *Generalized solutions of the Smolukhovskii semilinear system of equations and their approximations*, October 24.
45. Th. Gallay, Université de Grenoble I, Institut Fourier, Saint-Martin-d'Hères, France, *Distribution of energy and convergence to equilibria in extended dissipative systems*, June 5.
46. A. Gasnikov, Moscow Institute of Physics and Technology, PreMoLab, Russia, *Sparsity page rank*, May 21.
47. A. Gaudillière, Aix-Marseille Université, Centre de Mathématiques et Informatique, Laboratoire d'Analyse, Topologie, Probabilités, France, *Looking for large cliques through spin glasses*, June 17.
48. A. Goldenschluger, University of Haifa, Department of Statistics, Israel, *A unified framework for change point detection and other related problems*, April 30.
49. St. Grützner, Bundesanstalt für Materialforschung und -prüfung (BAM), Fachbereich 5.2, Experimentelle und modellbasierte Werkstoffmechanik, Berlin, *Problematik der Bestimmung der Parameter von viskoplastischen Verformungsmodellen über einem Temperaturbereich*, July 18.
50. P. Gurevich, S. Tikhomirov, Freie Universität Berlin, Institut für Mathematik, *Reaction-diffusion equations with spatially distributed hysteresis*, January 22.
51. S. Gurevich, Wilhelms-Universität Münster, Institut für theoretische Physik, *Instabilities of localized structures in reaction-diffusion systems with delayed feedback*, January 8.
52. M. Hairer, The University of Warwick, Department of Mathematics, UK, *Dynamics near criticality*, April 22.
53. M. Heida, Universität Dortmund, Fakultät für Mathematik, *Modeling multiphase flow within rational thermodynamics*, January 30.
54. R. Hildebrand, Université Joseph Fourier, Laboratoire Jean Kuntzmann, Grenoble, France, *Konvexe Optimierung und semi-definite Relaxierungen*, April 3.
55. D. Hilhorst, Université Paris-Sud, Laboratoire d'Analyse Numérique, Orsay, France, *A fast precipitation and dissolution limit for a reaction-diffusion system arising in porous medium*, October 16.
56. F. Hoecker-Escuti, Technische Universität Chemnitz, Fakultät für Mathematik, *Sharp Lifshitz tails in a weak coupling constant regime*, July 1.
57. M. Hoffmann, Université Paris Dauphine, Département Mathématiques et Informatique, France, *Statistical estimation of a growth-fragmentation model observed on a genealogical tree*, November 27.
58. M. Hoffmann, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Das Navier-Stokes-Darcy-Problem*, December 19.
59. J. Höntschel, GLOBALFOUNDRIES Dresden Module One Limited Liability Company & Co. KG, *Advanced VLSI CMOS technology scaling – The industry approach from classical scaling towards 3D device integration*, April 29.
60. S. Hörmann, Université Libre de Bruxelles, Département de Mathématique, Belgium, *PCA for functional time series: Basics, applications and extensions*, January 30.
61. J. Höwing, Universität Hamburg, Fachbereich Mathematik, *Stability of solitary waves in generalized KdV, Boussinesq, and Euler–Korteweg equations*, July 2.

62. G.C. Hsiao, University of Delaware, Department of Mathematical Sciences, Newark, USA, *Time dependent fluid-structure interactions*, September 3.

63. S. Käbisch, University of Surrey, Department of Mathematics, Guildford, UK, *Phasenfeldmethode mit Hindernispotential und ihre Anwendung in der Formoptimierung*, August 15.

64. M. Kachanovska, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Fast Runge–Kutta convolution quadrature for the wave equation in three dimensions*, May 16.

65. L. Kamenski, University of Kansas, Department of Mathematics, Lawrence, USA, *Adaptive finite elements with anisotropic meshes*, February 14.

66. ———, *Anisotrope Gitter: Den Zusammenhang zwischen Gittern und Eigenschaften der Diskretisierungsverfahren richtig verstehen*, April 18.

67. V. Kapoor, Universität Rostock, Institut für Physik, *Exact exchange-correlation potentials for worst case-TDDFT scenarios*, May 28.

68. I. Kashchenko, Yaroslavl Demidov State University, Department of Mathematical Modeling, Russia, *Dynamics of Lang–Kobayashi equations with large control coefficient*, November 14.

69. S.A. Kashchenko, Yaroslavl Demidov State University, Department of Mathematical Modelling, Russia, *Relaxation oscillations in autogenerators with different delay feedbacks*, January 16.

70. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, *Mesh optimization for convection-diffusion problems*, February 7.

71. O. Knoth, Leibniz-Institut für Troposphärenforschung e.V. (TROPOS), Leipzig, *Multirate time integration methods for the simulation of the atmosphere*, December 12.

72. C. Köstler, University College Cork, School of Mathematical Sciences, Ireland, *Symmetrien in der nichtkommutativen Wahrscheinlichkeitstheorie*, January 18.

73. K. Krause, Technische Universität Berlin, Institut für Mathematik, *Statistische Physik wechselwirkender N -Teilchen-Systeme*, April 26.

74. K. Krischer, Technische Universität München, Physik-Department, *Cooperative phenomena during electrochemical reactions*, October 8.

75. H. Kröner, Eberhard Karls Universität Tübingen, Mathematisches Institut, *Finite element approximation of power mean curvature flow*, October 30.

76. M. Kružik, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *Thermodynamically-consistent mesoscopic model of the ferro/paramagnetic transition*, May 16.

77. A. Kulik, Taras Shevchenko University, Faculty of Mechanics and Mathematics, Kiev, Ukraine, *Limit theorems and statistical inference in Markov models*, May 8.

78. T. Kutzker, Technische Universität Dresden, Institut für Mathematische Stochastik, *Semikonvergenz in Verteilung abgeschlossener Zufallsmengen in topologischen Räumen*, April 26.

79. G. Lazzaroni, Universität Würzburg, Institut für Mathematik, *Dislocations in nanowire heterostructures: From discrete to continuum*, May 16.

80. A. Lechleiter, Universität Bremen, Zentrum für Technomathematik, *Inside-outside duality for scattering problems*, September 19.

81. F. Litzinger, Freie Universität Berlin, Institut für Mathematik, *Diskretisierung der stationären inkompressiblen Navier-Stokes-Gleichungen in 3D auf unstrukturierten Tetraedergittern*, December 19.

82. V. Lotoreichik, Technische Universität Graz, Institut für Numerische Mathematik, Austria, *Self-adjoint Laplacians on partitions of Euclidean spaces with δ and δ' -couplings*, January 16.

83. E. Luçon, Technische Universität Berlin, Institut für Mathematik, *On the fluctuations of the weakly asymmetric exclusion process and KPZ equation*, February 19.

84. R. Luke, Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *Nonconvex regularity and convergence of fundamental algorithms for feasibility problems*, April 23.

85. J. Maas, Universität Bonn, Institut für Angewandte Mathematik, *Optimal transport in discrete and noncommutative analysis*, May 29.

86. H.S. Mahato, Universität Bremen, Zentrum für Technomathematik, *Homogenization in $W^{1,p}$ for a highly nonlinear coupled system of reaction-diffusion equations*, March 13.

87. M.M. Malamud, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Donetsk, Ukraine, *To the spectral theory of Dirac operators with point interactions*, April 24.

88. Ch. Merdon, Humboldt-Universität zu Berlin, Institut für Mathematik, *Garantierte Fehlerkontrolle bei PDGLen mit aktuellen Equilibrierungstechniken*, April 2.

89. ———, *Aspects of guaranteed error control for finite element approximations in computations for PDEs*, July 10.

90. M. Meyries, Universität Halle, Arbeitsgruppe Analysis, *Weighted function spaces, Hardy's inequality, and a free boundary problem*, March 20.

91. P. Micha, Charles University, Faculty of Mathematics, Prague, Czech Republic, *Limit theorems and statistical inference in Markov models*, April 24.

92. A. Mihoci, Humboldt-Universität zu Berlin, C. A. S. E., *Local adaptive multiplicative error models for high-frequency forecasts*, April 17.

93. V. Moldoveanu, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, *Exciton dynamics in optically active quantum dots*, July 31.

94. St. Moore, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics, Linz, *Discontinuous Galerkin isogeometric analysis for elliptic PDEs on manifolds*, June 27.

95. G. Müller, Technische Universität Berlin, Institut für Mathematik, *Beispiele numerischer Verfahren für PDEs und Optimalsteuerungsprobleme*, April 2.

96. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, *Coupled quantum-classical transport in silicon nanowires*, July 31.

97. A. Myśliński, Systems Research Institute, Warsaw, Poland, *Topology optimization of variational inequalities based on modified level set approach*, October 29.

98. H. Oberhauser, Technische Universität Berlin, Institut für Mathematik, *An extension of the functional Ito formula*, February 19.

99. F. Otto, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *A quantitative theory in stochastic homogenization*, February 6.

100. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *Second-order chain rules and their applications in stability and numerics*, November 12.

101. O. Pajonk, SPT Group GmbH, Hamburg, *A sampling-free method for linear Bayesian updating with application to spectral representations*, June 4.

102. M. Panov, Moscow Institute of Physics and Technology, PreMoLab, Russia, *The (non-)asymptotic posterior properties of hidden Markov models and Bernstein–von Mises theorem*, September 10.

103. F.S. Patacchini, University of Bath, Department of Mathematical Sciences, UK, *Numerical simulation of the evolution of grain size distribution in steel*, August 20.

104. M.A. Peletier, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), Department of Mathematics and Computer Science, The Netherlands, *Upscaling dislocations in two dimensions*, November 20.

105. A. Politi, University of Aberdeen, Institute for Complex Systems and Mathematical Biology, UK, *Coarsening processes in discrete nonlinear Schrödinger-type models*, November 19.

106. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *Solution regularity and smooth dependence for abstract equations and applications to PDEs*, October 23.

107. D.R.M. Renger, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), Department of Mathematics and Computer Science, The Netherlands, *Time reversibility and entropic gradient flows*, January 16.

108. R. Richter, Bundesanstalt für Materialforschung und -prüfung, Fachbereich Akustische und elektromagnetische Verfahren, Berlin, *Numerische Verfahren für die aktive Thermografie zur Untersuchung von Rückwandgeometrien und Singularitäten einer geometrischen Evolutionsgleichung (MCF)*, April 2.

109. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, *A vanishing viscosity approach to a rate-independent model for damage*, July 8.

110. M. Rother, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *Eine Reise ins Ich und zurück in 20 Minuten*, April 23.

111. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Thermomechanics of hydrogen storage in metallic hydrides: Modeling and analysis*, February 13.

112. A. Ruziyeva, TU Bergakademie Freiberg, Fakultät für Mathematik und Informatik, *Fuzzy bilevel optimization*, January 14.

113. R. Samworth, University of Cambridge, Faculty of Mathematics, UK, *New theory and methodology*, January 30.

114. M. Sart, Université Sophia Antipolis, Laboratoire Jean-Alexandre Dieudonné, Nice, France, *Estimation of the transition density of a Markov chain*, November 13.

115. M. Scherer, Technische Universität München, Fakultät für Mathematik, *On the construction and use of factor copula models*, May 15.

116. M. Schmuck, Imperial College London, Departments of Chemical Engineering and Mathematics, UK, *Homogenized phase-field equations for interfacial dynamics in strongly heterogeneous materials*, April 17.

117. ———, *Upscaling of ionic transport equations in strongly heterogeneous media and finite element approximations*, April 18.

118. R. Scholz, Technische Universität Dresden, Institut für Angewandte Photophysik (IAPP), *Optoelektronische Bauelemente aus organischen Halbleitern: Simulation von spektroskopischen Eigenschaften und elektronischem Transport*, June 3.

119. M. Schonbek, University of California, Department of Mathematics, Santa Cruz, USA, L^2 *-asymptotic stability of mild solution to Navier–Stokes system in* R^3 , October 8.

120. L. Schumacher, Humboldt-Universität zu Berlin, Institut für Mathematik, *Isogeometric analysis for scalar convection-diffusion equations*, May 30.

121. H. Schwetlick, University of Bath, Department of Mathematical Sciences, UK, *Front propagation in nonlinear transport equations with delay*, June 11.

122. J. Seidel, Technische Universität Chemnitz, Fakultät für Mathematik, *Model reduction with POD and DEIM*, December 3.

123. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, *Fast segment insertion and incremental construction of constrained Delaunay triangulations*, July 11.

124. A. Shilnikov, Georgia State University, Neuroscience Institute, Atlanta, USA, *Symbolic toolkit for exploration of deterministic chaos*, January 8.

125. ———, *Symbolic toolkit for exploration of deterministic chaos*, January 10.

126. J. Sieber, University of Exeter, Mathematics, UK, *Periodic orbits in equations with state-dependent delay*, December 17.

127. D. Skryabin, University of Bath, Department of Physics, UK, *Polariton solitons*, January 24.

128. K. Soga, Waseda University, Department of Mathematics, Tokyo, Japan, *Numerical analysis of hyperbolic and parabolic PDEs based on the law of large numbers and the central limit theorem*, February 27.

129. E. Spodarev, Universität Ulm, Institut für Stochastik, *Limit theorems for excursion sets of stationary random fields*, January 22.

130. H.-J. Starkloff, Westsächsische Hochschule Zwickau, Fakultät Physikalische Technik/Informatik, *On some questions related to generalized polynomial chaos expansions*, May 24.

131. U. Stefanelli, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nationale delle Ricerche (IMATI-CNR), Pavia, Italy, *Regular tilings via crystallization*, April 17.

132. A.F.M. ter Elst, The University of Auckland, Department of Mathematics, New Zealand, *Diffusion determines the manifold*, August 14.

133. H. Tiesler, Fraunhofer-Institut für Bildgestützte Medizin MEVIS, Bremen, *Stochastic collocation for optimal control problems with stochastic PDE constraints*, January 15.

134. Ž. Tomovski, Sts. Cyril and Methodius University, Institute of Mathematics, Skopje, Republic of Macedonia, *Generalized Cauchy type problems for linear and nonlinear fractional differential equations with composite fractional derivative operator*, January 30.

135. M. Trabs, Humboldt-Universität zu Berlin, Institut für Mathematik, *Semiparametric efficiency for inverse problems with applications to deconvolution and Lévy models*, May 14.

136. M. Tretyakov, University of Nottingham, School of Mathematical Sciences, UK, *Numerical integration of SDEs with nonglobally Lipschitz coefficients*, November 12.

137. J. Tugaut, Universität Bielefeld, Mathematische Fakultät, *Long-time convergence of a McKean–Vlasov diffusion*, March 26.

138. D. Turaev, Imperial College London, Department of Mathematics, UK, *Bifurcations*, July 30.

139. S. Ullmann, Technische Universität Darmstadt, Fachbereich Mathematik, *POD-Galerkin reduced-order modeling of flow problems with stochastic boundary conditions*, January 24.

140. E. Valdinoci, University of Milan, Department of Mathematics, Italy, *A fractional framework for perimeters and phase transitions*, February 13.

141. M. Vetter, Ruhr-Universität Bochum, Fakultät für Mathematik, *On discriminating between long-range dependence and non stationarity*, January 16.

142. J. Wensch, Technische Universität Dresden, Institut für Wissenschaftliches Rechnen, *Efficient time integration methods for the compressible Euler equations in atmospheric dynamics*, April 23.

143. M. Wolfmayr, Johannes Kepler Universität Linz, Institut für Numerische Mathematik, Austria, *Multiharmonic finite element analysis of time-periodic parabolic optimal control problems*, May 21.

144. H. Wu, Fudan University, School of Mathematical Sciences, Shanghai, China, *Well-posedness and stability of the Ericksen–Leslie system for incompressible nematic liquid crystal flow*, November 27.

145. K. Wünnemann, D. Elbeshausen, Museum für Naturkunde, Leibniz-Institut für Evolutions- und Biodiversitätsforschung, Berlin, *Computer simulations of meteorite impact processes: A multi-material, multi-rheology CFD-approach for compressible flows*, December 2.

146. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Initial-boundary value problems for non-symmetric linear diffusion equation with multiple time-fractional derivatives and applications to some inverse problems*, March 19.

147. ———, *Mathematical analysis for some inverse problems in risk managements*, September 24.

148. M. Yor, Université Pierre et Marie Curie, Laboratoire de Probabilités et Modèles Aléatoires, Paris, France, *Convex order, peacocks, and martingales*, January 9.

149. V. Zagrebnov, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, France, *About the Trotter–Kato product formula in Banach spaces*, August 14.

150. E. Zander, Technische Universität Braunschweig, Institut für Wissenschaftliches Rechnen, *Towards a unified framework for reduced basis methods in uncertainty quantification*, March 19.

151. Ch. Zanini, Politechnic University of Turin, Department of Mathematics, Italy, *First order approximations of finite dimensional gradient flows*, July 10.

152. J. Zimmer, University of Bath, Department of Mathematical Sciences, UK, *Limit passages from particle models to entropic gradient flows*, January 23.

A.14 Software

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).

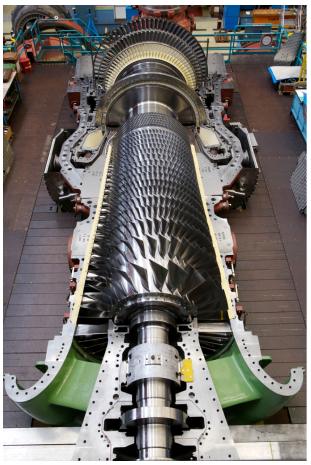
BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: juergen.borchardt@wias-berlin.de)

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



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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`.

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.

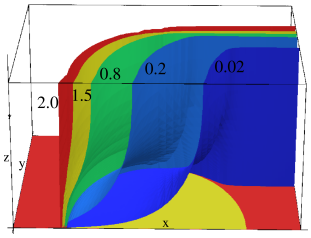
Detailed information: `http://www.wias-berlin.de/software/ldsl`

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, like population balance systems or systems coupling free flows and flows in porous media. Important features of `MooNMD` are

- the availability of more than 100 finite elements in 1D, 2D, and 3D (conforming, non-conforming, discontinuous, higher-order, vector-valued, 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,
- tools for using reduced-order models based on proper orthogonal decomposition (POD) are available.

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de)



Concentration isosurfaces in a thin-layer flow cell

`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

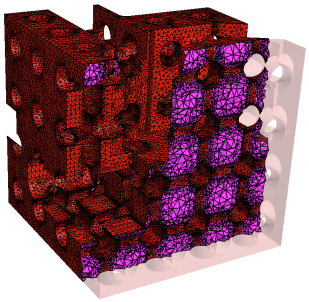
- iterative solvers for linear and nonlinear systems of equations
- sparse matrix structures with preconditioners and direct solver interfaces
- dimension-independent simplex grid handling in one, two, and three space dimensions
- finite volume based solution of coupled parabolic reaction-diffusion-convection 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`.

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 multi-band kp models it allows to treat band mixing effects, confinement effects, crystal symmetry, and the influence of mechanical strain.

In particular, WIAS–QW calculates the

- subband dispersion
- eigenfunctions
- transition matrix elements
- miniband effects in multi-quantum-well structures

In dependence on the sheet carrier densities and the temperature, WIAS–QW calculates the

- optical response function
- gain spectrum
- radiative recombination rate
- carrier density distributions

Furthermore, the calculations can be 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.

WIAS Software Collection for Imaging (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).

The AWS for AMIRA (TM) plugin implements a structural adaptive smoothing procedure for two- and three-dimensional 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/).

WIAS Software Collection for Neuroscience (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). It can be used to read dMRI data, to estimate the diffusion tensor, for the adaptive smoothing of dMRI data, the estimation of the orientation density function or its square root, the estimation of tensor mixture models, the estimation of the diffusion kurtosis model, fiber tracking, and for the two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org). The multi-shell position-orientation adaptive smoothing (msPOAS) method for dMRI data is additionally available within the ACID toolbox for SPM (http://www.diffusiontools.com).

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).