

***Intelligent solutions for complex problems***

***Annual Research Report 2014***

Cover figure: Snapshot from a numerical simulation of damage with time-dependent loading.

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The Weierstrass Institute for Applied Analysis and Stochastics, Leibniz Institute in Forschungsbund Berlin e.V. (WIAS, member of the Leibniz Association), presents its Annual Report 2014. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2014. Following a more general introduction in part one, in its second part six 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. Its eager staff, headed by the WIAS Deputy Director and IMU Treasurer Prof. Alexander Mielke, continued their work, serving mathematics and mathematicians all over the world. Meanwhile, only four years after its official opening in February 2011, the IMU Secretariat at WIAS has become a well-known and well-accepted meeting point of the worldwide mathematical community, which has increased the international visibility of WIAS tremendously.

In 2014, the main event in the mathematical world was the International Congress of Mathematicians (ICM) 2014 in Korea, in whose organization the IMU Secretariat was strongly involved. During the meeting of the General Assembly of IMU in Gyeongju, the Chair of the IMU Office Committee reported very positively on the performance of the secretariat. The General Assembly of IMU acknowledged this report and adopted on August 31 the following Resolution 3: “The General Assembly of the IMU thanks Alexander Mielke, Sylwia Markwardt, Lena Koch, and all the other staff at the IMU Secretariat in Berlin for their dedicated work and for all their multiple contributions to the IMU”.

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 2014 was a year of records for WIAS. Among other things, fourteen doctoral theses, the largest number ever, were successfully defended, 138 research papers authored by WIAS members appeared in refereed scientific journals, and 164 preprints were written. The third-party funding reached 2.7 million euros.

The scientific excellence of WIAS is best reflected by the fact that the institute is now hosting three ERC Starting Grants (Profs. Peter Friz, Elisabetta Rocca, and Enrico Valdinoci) and one ERC Advanced Grant (Prof. Alexander Mielke). Moreover, the “mega-grant” of the Russian government for Prof. Vladimir Spokoiny, which was prolonged in 2013, is 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. Further evidence for the excellent work done at WIAS is the fact that the International Society for the Interaction of Mechanics and Mathematics (ISIMM) awarded the ISIMM Junior Prize 2014 at equal parts to two members of WIAS, namely to Dr. Stefan Neukamm and to Prof. Elisabetta Rocca.

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 2014: Dr. Thorsten Dickhaus received calls for a W2 professorship at the Technical University of Applied Sciences in Wildau and for a W3 professorship at the University of Bremen, Dr. Stefan



*Prof. Dr. Jürgen Sprekels,  
Director*

Neukamm for a W2 professorship at the Technical University of Dresden and Dr. Christian Bayer for a senior lectureship at Linköping University.

Since the institute's foundation in 1992, a total of 52 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.

The Young Scientists' Group *Modeling of Damage Processes* under the leadership of 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 2014, the institute defended the "audit berufundfamilie" (audit job and family) quality seal that it received in December 2013.

Besides these important events of the year 2014, 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 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, 49 additional co-workers (+ two outside WIAS; Dec. 31, 2014) could be financed from grants.

Fourteen international workshops and a summer school 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 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 2014,

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 2014 the joint operation of the Research Center MATHEON “Mathematics for key technologies” located at the Technische Universität Berlin. The DFG funding of MATHEON terminated on May 31, 2014. Since June 1, funds for MATHEON have come from the Berlin Einstein Foundation in the framework of the “Einstein Center for Mathematics (ECMath)”. From these funds, seven new MATHEON subprojects managed by WIAS staff were begun, in which seven scientific collaborators were employed at WIAS.

WIAS is committed to the success of the center by providing considerable financial and personal resources: the deputy director of WIAS, Prof. Alexander Mielke, and Dr. Dorothee Knees were members of MATHEON’s Executive Board, Prof. Barbara Wagner was deputy chair of the MATHEON Council, and several members of WIAS served as *Scientists in Charge* of the center’s mathematical fields or application areas.

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. Presently, the BMS hosts more than two hundred students. 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. A special highlight of 2014 was the fact that Prof. Wolfgang König, Second Deputy Director of WIAS and Head of the Research Group *Interacting Random Systems*, was the main organizer of the 2014 Summer School “Applied Analysis for Materials” of the Berlin Mathematical School, in which several lecturers were members of the WIAS staff.

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 2015

J. Sprekels

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# 1 WIAS in 2014

- 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 transregional 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 stochastic 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.

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 to the preparation of two trainees to become “mathematical technical software developers”.

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 2014, 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 2014 organized into the departments for technical services, the Secretariat of the International Mathematical Union (IMU, see page 58), the seven scientific re-



search groups, the Young Scientists' Group, two Leibniz and two ERC groups<sup>1</sup>:

**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**

**LG 4. Probabilistic Methods for Mobile Ad-hoc Networks**

**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 2014.

### 1.2.2 Main Application Areas

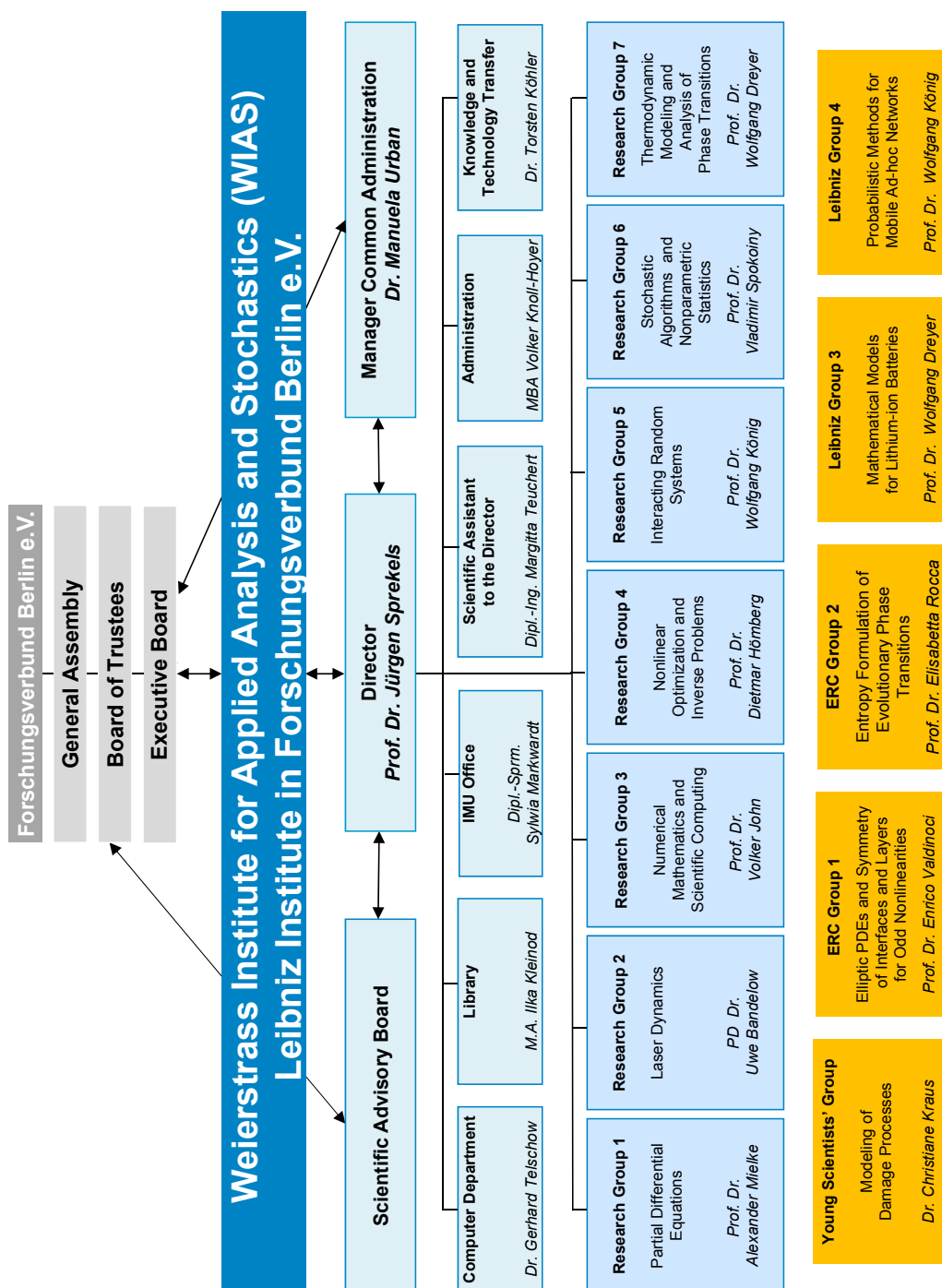
The research at WIAS focused in 2014 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

- **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 fuel cells, lithium batteries, hydrogen storage, photovoltaics)

<sup>1</sup>In the following, the terms “research group” will often be abbreviated by “RG”, Young Scientists' Group by “YSG”, and “Leibniz group” by “LG”.



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

The seven research groups, the Young Scientists' group, the two Leibniz groups, 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, calling for 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 2014 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	LG 4	ERC 1	ERC 2
Nano- and optoelectronics	X	X	X	X								
Optimization & control of technological processes	X		X	X		X	X			X		X
Phase transitions & multi-functional materials	X			X	X		X	X	X		X	X
Flow and transport processes in continua	X		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	X	

In the following, special research topics are listed that were addressed in 2014 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 and their dynamics (multisection lasers, VCSELs, quantum dots; in RG 1 and RG 2)
- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in RG 2)

- Photovoltaics (in RG 1)

## **2. Optimization and control of technological processes**

- Simulation and control in process engineering (in RG 3, RG 4, and RG 6)
- Problems of optimal shape and topology design (in RG 4 and RG 7)
- Optimal control of multifield problems in continuum mechanics and biology (in RG 3, RG 4, RG 7, and ERC 2)
- Evaluation of the quality of mobile ad-hoc communication systems (in LG 4)

## **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, RG 7, and ERC 2)
- Modeling of damage and crack processes (phase field systems and sharp interface problems, multiscale transitions; in YSG, RG 1, RG 7, and ERC 2)
- 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, YSG, and ERC 2; 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 5)
- Trajectories of message flow in mobile ad-hoc communication systems (in LG 4)

### 5. Conversion, storage and distribution of energy

- Photovoltaics (in RG 1)
- 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 and LG 4)
- 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 2014, having raised a total of 2.7 million euros, from which 49 additional researchers (+ 2 outside WIAS; Dec. 31, 2014) have been financed. In total in 2014, 22.8 percent of the total budget of WIAS and 41.5 percent 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<sup>2</sup>.

### 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 has been funded by the European Research Council since April 2011 and lasts for 5 years. The research topics include the modeling

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



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.

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

The project ERC-2010-StG no. 258237 takes part in RG 6 and has been 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, in particular, Lions' *viscosity approach* was pursued, 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 has been funded by the European Research Council since January 2012 and lasts for 5 years. The research topics include partial differential equations, non-local 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 has been 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 has been 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.

### 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 Safety (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.



### Research Center MATHEON

The highlight of the cooperation with the mathematical institutions in Berlin was again the joint operation of the 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 the end of May 2014. DFG funds exceeding 5.5 million euros per full year flowed into Berlin for MATHEON. Starting from June 1, 2014, the funding of MATHEON is about 2 million euros per year through the Einstein Center for Mathematics (ECMath), which is funded by the Einstein Foundation Berlin.



In 2014, WIAS again 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”, Priv.-Doz. Dr. U. Bandelow (RG 2), Scientist in Charge of the Application Area D “Electronic and Photonic Devices”; and WIAS members participated until May in the management of 15 and from June in seven of its subprojects.

### 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 has been 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. The annual Summer School 2014 was predominantly taught by WIAS members and was devoted to the subject “Applied Analysis for Materials”.



### 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 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, GeoForschungs-Zentrum 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. One student was supervised by Volker John (RG 3), working at the simulation of mantle convection. 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 center, 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. The review process in 2014 for the second four-year period 2015–2018 was successful.



### DFG Collaborative Research Center (SFB) 1114 *Scaling Cascades in Complex Systems*

The center began its work on October 1, 2014 (funding period until June 30, 2018). It is located at the Freie Universität Berlin. WIAS participates in the three subprojects “Fault networks and scaling properties of deformation accumulation” (RG 1), “Effective models for interfaces with microstructure” (RG 1 and YSG), and “Stochastic spatial coagulation particle processes” (RG 5).

### DFG Collaborative Research Center/Transregio (TRR) 154 *Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks*

WIAS takes part in this Collaborative Research Center/Transregio, which is located at the Friedrich Alexander Universität at Erlangen/Nürnberg (first funding period: October 1, 2014 – June 30, 2018) with the subproject “(Nonlinear) chance constraints in problems of gas transportation” (RG 4).

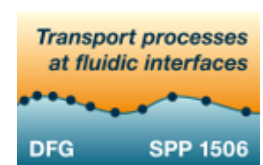
### DFG Priority Program SPP 1204 *Algorithms for Fast, Material-specific Process-chain Design and Analysis in Metal Forming*

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 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 participated for the first funding period (Oct. 2010 – Sept. 2013, principal investigators: Prof. B. Wagner and Dr. D. Peschka) and participates now 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” (RG 5).



### DFG Priority Program SPP 1679 *Dyn-Sim-FP – Dynamic Simulation of Interconnected Solids Processes*

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 population balance systems. In the first phase, direct discretizations and operator-splitting methods for uni-variate systems were studied. 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 797 *Analysis and Computation of Microstructure in Finite Plasticity*

WIAS participated 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 it for estimation. The research group at WIAS is studying the convergence and efficiency of such algorithms (RG 6; first funding period until March 31, 2015).



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### ProFit Project “Erforschung effizienter mathematischer Methoden zur Modelkalibrierung und Unbestimmtheitsabschätzung in Umweltsituationen (MUSI)”

The project “Efficient mathematical methods for model calibration and uncertainty estimation in environmental simulations” is a cooperation between WIAS and the DHI-WASY GmbH Berlin. It is funded by the Investitionsbank Berlin in the framework of its “ProFIT” (Programm zur Förderung von Forschung, Innovationen und Technologien) funding program. The main purpose of the project is knowledge transfer on modern methods for partial differential equations with stochastic coefficients from research to industry. It focuses on the assessment of efficient methods for partial differential equations with stochastic coefficients and the selection of preferred methods to be

implemented in the software of the project partner DHI-WASY. In addition, the investigation of stochastic methods for inverse problems will be started.

### TOTAL Project

The aim of this R&D cooperation is the development of improved algorithms and software for hybrid volumetric meshing based on Voronoi diagrams for geological models. The project is planned for a period of one year with an optional prolongation for one more year.







## 2 Scientific Highlights

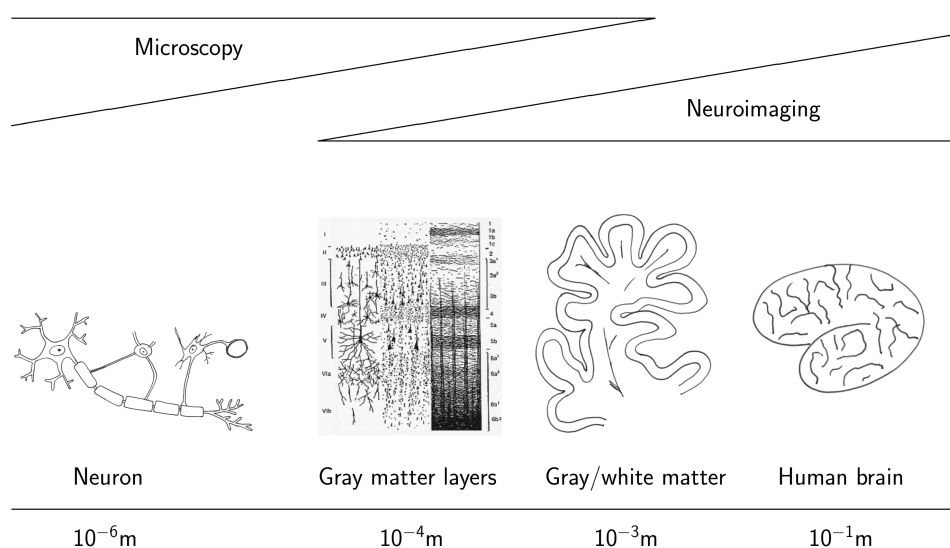
- Enabling In-vivo Histology of the Brain
- Beam-quality Improvement in Edge-emitting Broad-area Semiconductor Lasers and Amplifiers
- Multiscale Modeling and Evolutionary  $\Gamma$ -Convergence
- Probabilistic Programming with Applications to Power Management
- Population Growth on Random Fitness Landscapes
- Reduced-order Modeling for Blood Flows in the Pulmonary Artery



## 2.1 Enabling In-vivo Histology of the Brain

Jörg Polzehl and Karsten Tabelow

The brain is a key part of the human central nervous system and subject to intense research both from a pure scientific viewpoint but also increasingly from a clinical perspective. The neurosciences are of considerable importance for the society. Neurodegenerative diseases like multiple sclerosis or Alzheimer's disease cause great suffering for the persons concerned and not least huge cost for the public health care.



**Fig. 1:** Non-invasive neuroimaging techniques progress into spatial domains so far reserved for microscopy

The human brain and its structural organization can be viewed at different spatial scales; see Figure 1. At the cellular level, the brain is made of different cell types. The most prominent are the neurons, consisting of the cell body and short dendrites within the brain's gray matter, or cortex, and a single axon which, combined in bundles, forms the bulk of the white matter. Several other cell types and subdivisions of the brain tissue, like the layer organization of the gray matter, add up to a complex picture of neuroanatomy [1].

For a long time, histology of brain tissue was only possible *ex-vivo* using microscopy. With the advance in neuroimaging in the past two decades, the *in-vivo* examination of the brain became possible. However, typical image resolutions achieved by neuroimaging methods are in the order of millimeters and thus cannot compete with microscopic examinations. One of the main obstacles is the intrinsic loss of signal, which is proportional to the voxel volume, with higher resolutions. While improvements on the scanner hardware are possible, but very costly, we are now, with advanced mathematical methods, at the brink of entering the submillimeter level of resolution and enable access to structural details that have not been accessible before for in-vivo imaging. It is our intention and hope that in some near future in-vivo histology becomes possible.

## Diffusion MRI – A quantitative technique

Among the imaging methods, diffusion magnetic resonance imaging (dMRI) plays a special role, as it directly probes microscopic structure via the observation of the water diffusion process. Considering the omnipresence of water (with its hydrogen nucleus suitable for MRI) within the human brain, the observation of this diffusion process enables inference on the white/gray matter structure that constitutes natural borders for the diffusion process.

We consider the diffusion propagator  $P(\vec{r}, \vec{r}', \tau)$ , i.e., the probability density for a particle to move from position  $\vec{r}'$  to  $\vec{r}$  in time  $\tau$ . Using Fick's laws, the diffusion process can then be described by the diffusion or heat equation

$$\frac{\partial}{\partial \tau} P(\vec{r}, \vec{r}', \tau) = \nabla \cdot (\mathcal{D} \cdot \nabla P(\vec{r}, \vec{r}', \tau)). \quad (1)$$

Here,  $\mathcal{D}$  denotes a location-dependent diffusion tensor that describes the diffusion process in anisotropic media. Although anisotropic diffusion seems not realistic for the free water component in the brain, the barriers formed by the different brain tissues in fact lead to a directional dependence of the diffusion constant  $D(\vec{g})$ . It turns out that the diffusion tensor model serves as a valuable approximation for this case. In dMRI, the “observed” diffusion propagator is the spatial sum over the microscopic environments, say, in a voxel volume  $V$ . Thus, we define the ensemble-averaged propagator (EAP)

$$P(\vec{R}, \tau) = \int_{\vec{r}' \in V, \vec{R}=\vec{r}-\vec{r}'} P(\vec{r}, \vec{r}', \tau) p(\vec{r}') d\vec{r}' \quad (2)$$

with the initial particle density  $p(\vec{r}')$  and consider it henceforth.

DMRI uses the pulsed-gradient spin-echo (PGSE) sequence for image acquisition applying additional magnetic field gradients in direction  $\vec{g}$  at a  $b$ -value coding the diffusion time  $\tau$  and the gradient strength. The mathematical treatment shows that the image acquired with these gradient fields is attenuated compared to the so-called *non-diffusion-weighted image*. Specifically, for this PGSE signal attenuation  $E(\vec{q})$  we obtain a three-dimensional Fourier transform of the diffusion propagator

$$E(\vec{q}) = \int_{\mathbb{R}^3} P(\vec{R}, \tau) e^{i\vec{q}^\top \vec{R}} d\vec{R}. \quad (3)$$

Thus, the measurement of the signal attenuation  $E(\vec{q})$  for a sufficient sampling of the  $q$ -space allows a direct access to the EAP via (inverse) Fourier transform. Obviously, the full Fourier transform in three dimensions requires a large number of diffusion-weighted image volumes, such that the acquisition is not feasible for most applications. Thus, specific diffusion models, i.e., additional assumptions for the structure of  $P$  or the limitation to special features of  $P$  can reduce the number of diffusion-weighted images that have to be acquired for inference.

For example, the diffusion tensor model (DTI) assumes the EAP to be of Gaussian form with the diffusion tensor  $\mathcal{D}$  “as covariance matrix”, which leads to

$$E(\vec{q}) = e^{-b\vec{g}^\top \mathcal{D} \vec{g}}, \quad \vec{g} = \vec{q}/\|\vec{q}\|.$$

For a given diffusion gradient direction  $\vec{g}$  the quantity

$$D_{app} = \vec{g}^T \mathcal{D} \vec{g}$$

defines the apparent diffusion coefficient (ADC). The relation between the diffusion MR signal and local physical parameters (diffusion constant) makes dMRI a quantitative method.

### Artifacts in dMRI

The utilization of dMRI generally requires sufficient image quality in, especially for patients, clinically feasible settings. In addition to optimized MR sequences and image reconstruction methods, also several post-processing steps dealing with artifacts in the data are needed. The most prominent of these result from *subject motion*, *eddy currents*, *susceptibility differences*, and *image noise*. Here, we focus on the latter, image noise, its impact on the analysis and its removal from the data. Noise is one of the core obstacles on the way to in-vivo histology using brain imaging methods, since the signal-to-noise ratio (SNR) inherently deteriorates with the voxel volume and hence with increasing image resolution; see Figure 2.

MR images are acquired as complex (phase and magnitude) signals in frequency or  $k$ -space and have to be transferred to the common image domain via inverse Fourier transform. Modern MR scanning facilities use setups with multiple receiver coils for improved image quality and implement special image reconstruction methods to combine their signals. The noise present in  $k$ -space data of a single receiver coil can be modeled as additive complex Gaussian errors with zero expectation and homogeneous standard deviation  $\sigma$ . Then, in image space the distribution of the data can be well approximated by a scaled non-central  $\chi$ -distribution for most parallel image reconstruction methods. The probability density  $p_S$  for the distribution of the signal  $S_i(\vec{q})$  at some voxel  $i$  generally depends on three parameters  $\eta_i$ ,  $\sigma_i$ ,  $L_i$  and is given by

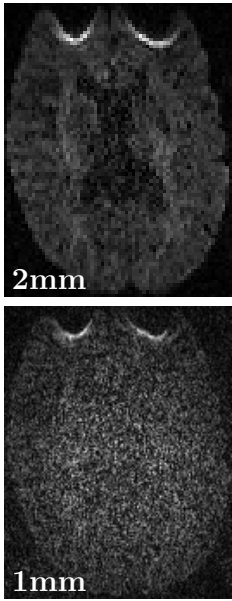
$$p_S(S_i; \eta_i, \sigma_i, L_i) = \frac{S_i^{L_i} \eta_i^{(1-L_i)}}{\sigma_i^{2L_i}} e^{-\frac{1}{2} \left( \frac{S_i^2 + \eta_i^2}{\sigma_i^2} \right)} I_{L_i-1} \left( \frac{\eta_i S_i}{\sigma_i^2} \right), \quad (4)$$

where  $I_{L_i-1}$  denotes the  $(L_i - 1)$ -th-order modified Bessel function of the first kind.  $\eta_i$  is the non-centrality parameter of the distribution and corresponds to the signal value in the noiseless situation.  $\sigma_i$  and  $L_i$  are (local) effective values for the scale parameter and the number of receiver coils, respectively. For some parallel image reconstruction algorithms  $L_i \equiv 1$ , and the distribution is Rician. Due to the reconstruction algorithms,  $\sigma_i$  varies smoothly with location.

The common approach in dMRI data analysis is to use the diffusion tensor model, to estimate the parameters of the diffusion tensor  $\mathcal{D}_i$  and the expected non-diffusion-weighted signal  $\zeta_{0,i}$  by nonlinear regression

$$(\hat{\zeta}_{0,i}, \hat{\mathcal{D}}_i) = \operatorname{argmin}_{\zeta_{0,i}, \mathcal{D}_i} \sum_{b,g} (S_i(\vec{q}) - \zeta_{0,i} \exp(-b \vec{g}^T \mathcal{D}_i \vec{g}))^2, \quad (5)$$

and to derive characteristics like the fractional anisotropy (FA) from the eigenvalues of the estimated diffusion tensor  $\hat{\mathcal{D}}_i$ . This estimate is severely biased in case of small SNR  $\zeta_{0,i}/\sigma_i$ . The



**Fig. 2:** Artifacts in dMRI. The upper bright spots caused by nonlinear image deformations are an example of susceptibility artifacts. The reduced SNR at higher resolutions below prohibits detailed structural inference.



reason is twofold.

For small SNR, i.e.  $S_i(\vec{q}, \tau) < 4\sigma_i$  for some gradient directions and b-values, the use of model (5) causes a bias, since the expected value

$$\mu_1^{L_i}(\eta_i, \sigma_i) = \mathbf{E}S_i(\vec{q}) = \sigma_i \sqrt{\frac{\pi}{2}} \mathbb{L}_{1/2}^{(L_i-1)} \left( -\frac{\zeta_{0,i}^2 \exp(-2b\vec{g}^\top \mathcal{D}_i \vec{g})}{2\sigma_i^2} \right) > \zeta_{0,i} \exp(-b\vec{g}^\top \mathcal{D}_i \vec{g}) \quad (6)$$

of the observed signal becomes significantly larger than the noiseless signal. Additionally, small SNR causes high variability in the tensor estimates and, as a consequence, biased estimates of the tensor eigenvalues and FA. The problem becomes more severe with both decreasing SNR and increasing  $b$ -value. Figure 3 illustrates bias and variability of estimated FA in dependence of the true FA for two  $b$ -values.

Adequate modeling therefore requires both to correctly assess the local scale parameter  $\sigma_i$  and to reduce the variability of the observed signal by borrowing spatial information. Approximately unbiased and less variable estimates can be obtained by

$$(\hat{\zeta}_{0,i}, \hat{\mathcal{D}}_i) = \operatorname{argmin}_{\zeta_{0,i}, \mathcal{D}_i} \sum_{b,g} \frac{(\hat{S}_i(\vec{q}) - \mu_1^{L_i}(\eta_i, \sigma_i))^2}{\mathbf{Var}\hat{S}_i(\vec{q})},$$

employing a quasi-likelihood approach.

## Characterization of noise in MRI

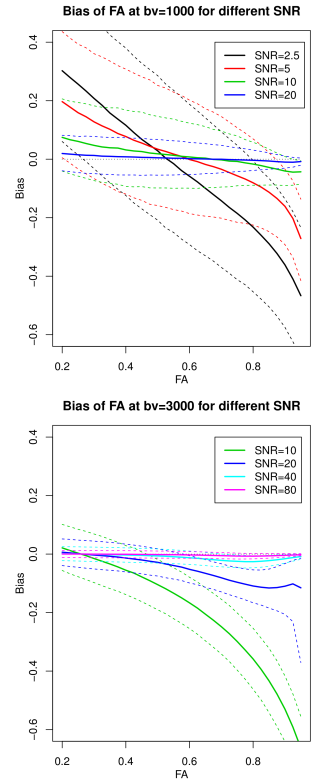
Most methods dealing with the noise component of the data require knowledge about the noise level  $\sigma_i$  for adequate consideration. Standard methods assume this parameter not to depend on the location and estimate it from the background of the image, where the true MR signal is known to vanish. These methods cannot incorporate the fact that the parameter  $\sigma_i$  is location-dependent. Additionally, they cannot determine the noise level in tissue areas.

Suppose we have multiple realizations of a local signal value. We can provide an estimate for the parameters of the distribution using maximum likelihood (ML) estimators. Since a multiple image acquisition can be typically ruled out in MRI due to time constraints, we have to use different strategies. In [2], we used the fact that MR images contain a local homogeneity structure, i.e., the non-centrality parameter  $\eta$  of the distribution is constant in local environments. Assuming we can describe this property by a suitable weighting scheme  $W_i = (w_{ij})$ , we can use a locally weighted ML estimator for inference

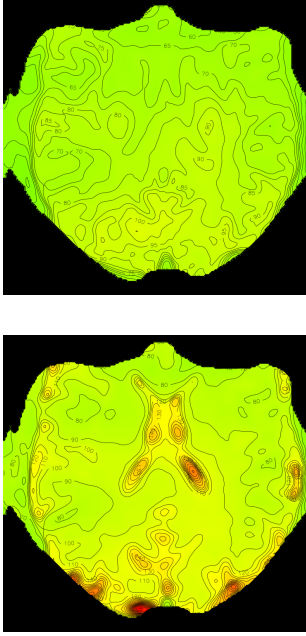
$$l(S; W_i; \eta, \sigma, L) = \sum_j w_{ij} \log p_S(S_j; \eta, \sigma, L).$$

The weighting schemes  $W_i$  can be determined using a propagation-separation approach [2].

The result of this new procedure is a characterization of the local noise parameter; see Figure 4. There, the estimated local standard deviation  $\sigma$  for a diffusion and a non-diffusion-weighted MR image are shown. The figure shows that the new method from [2] is able to quantify the noise



**Fig. 3:** Bias of FA in nonlinear regression diffusion tensor models for varying SNR. Top:  $b$ -value  $1000s/mm^2$ , bottom:  $b$ -value  $3000s/mm^2$ . Dotted lines are 0.1 and 0.9 quantiles.



**Fig. 4:** Estimated local standard deviation for an MR image with and without diffusion weighting, result from [2]

for tissue areas. This information is essential and can be used for reducing the modeling bias described above and for noise reduction.

### Towards higher resolution in dMRI

Increasing the resolution of MRI data lowers the signal-to-noise ratio. Thus, any effort to obtain a higher resolution leads to the deterioration of the image, making attempts to use current MRI techniques for quasi-microscopic images hopeless at first sight.

However, adaptive noise reduction methods have the potential to use spatial information in the data to infer on an improved version of the data. We developed a powerful method named *multi-shell position orientation adaptive smoothing (msPOAS)* [3] that infers on the true values using increasing spatial scales to define weighting schemes  $W_i = (w_{ij})$  for local parameter estimation. One important feature of the methods is its definition of locality that is considered not only in the three-dimensional space  $\mathbb{R}^3$  of individual images but in a five-dimensional orientation space  $\mathbb{R}^3 \times \mathbb{S}^2$ , where  $\mathbb{S}^2$  denotes the unit sphere of diffusion gradient orientations  $\vec{g}$ . Further, if measurements on multiple  $q$ -shells, i.e., for multiple  $b$ -values, are available, they can be used to further improve the decision on the local homogeneity structure. Thus, dMRI data representation in msPOAS is done via a function

$$\mathcal{S} : V \times G \ni (\vec{v}, \vec{g}) \mapsto (S_0(\vec{v}), S_{b_1}(\vec{v}, \vec{g}), \dots, S_{b_{\mathfrak{B}}}(\vec{v}, \vec{g}))^T \in \mathbb{R}^{\mathfrak{B}+1}, \quad (7)$$

where  $V$  is the space of voxel locations and  $G$  the space of gradient orientations. The consideration of local neighborhoods in  $\mathbb{R}^3 \times \mathbb{S}^2$  requires the definition of a suitable metric in this space via its embedding into  $SE(3)$  and an approximation for numerical feasibility. The solution to these problems was readopted in [3] from one of our previous publications. Additionally, the local characterization of the noise level from the method in [2] further improves the results of msPOAS.

MSPOAS is extremely efficient for noise reduction, see Figure 5, where the fractional anisotropy in a DTI model of the dMRI data for different settings is shown. While the upper image has an acceptable quality, the voxel resolution of 2 mm is too large for finer structural details; cf. Figure 1. The high-resolution scan in the center is practically useless due to the high noise component. The reconstruction using the new msPOAS method has a very high quality combined with a high resolution. This result also shows that the local information in the data is very strong and should be used for advanced image processing. For a broad visibility in the neuroscience community we published a corresponding msPOAS toolbox for the popular SPM software [4].

### Summary

Sophisticated mathematical and statistical methods for dMRI analysis as described in [2] and [3] enable a much more detailed inference on the structure of the human brain than available so far. Combined with the advance of ultra-high magnetic field strengths, structural images from dMRI data are now clearly entering the submillimeter domain. With this approach, imaging, e.g., the

columnar structures of the cortex, which were only accessible by microscopy until now, becomes possible. This is already very close to an in-vivo histology of the human brain.

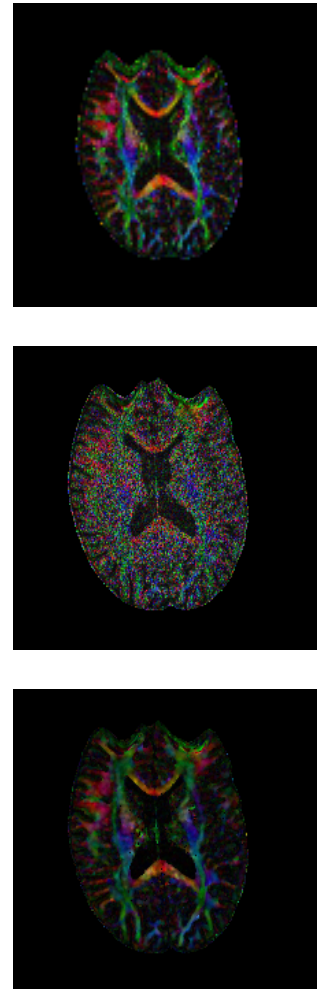
The high quality of the processed data also enables the evaluation of more complex diffusion models, like the diffusion kurtosis model, see [5], to obtain even more detailed information about the underlying tissue.

## Acknowledgments

This project was performed in close collaboration with colleagues from the Wellcome Trust Centre for Neuroimaging, UCL: Nikolaus Weiskopf and Siawoosh Mohammadi. We also particularly thank Henning U. Voss (Citigroup Biomedical Imaging Center, Weill Cornell Medical College), Alfred Anwander (Max Planck Institute for Human Cognitive and Brain Sciences), and Robin Heidemann (Siemens AG) for providing DW-MRI datasets and many helpful discussions. Parts of this project were funded as project “F10 – Image and signal processing in the biomedical sciences” of the DFG Research Center MATHEON.

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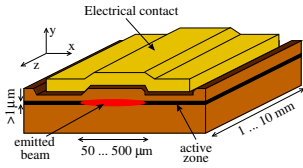
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**Fig. 5:** Increasing the resolution of dMRI data. We show the fractional anisotropy in the DTI model for a low-resolution dMRI scan (top), a high-resolution dMRI scan (center), and an msPOAS reconstruction of the high-resolution data (bottom).

## 2.2 Beam-quality Improvement in Edge-emitting Broad-area Semiconductor Lasers and Amplifiers

*Mindaugas Radziunas*



**Fig. 1:** Schematic of a BAS laser

High-power high-brightness edge-emitting broad-area semiconductor (BAS) lasers and optical amplifiers are compact, efficient, and reliable light sources playing a crucial role in different laser technologies, such as materials processing, precision metrology, medical applications, nonlinear optics, and sensor technology. BAS lasers and amplifiers have a relatively simple geometry, see Figure 1, allowing an efficient energy pumping through a broad electric contact on the top of the device and can operate at high-power (tens of watts) regimes. However, BAS devices have one serious drawback: Operated at high power, they suffer from a low beam quality due to simultaneous irregular contributions of different lateral and longitudinal optical modes. As a result, the emitted optical beam is irregular, has undesirably broad optical spectra, and a large divergence. Thus, a quality improvement of the beam amplified in BAS amplifiers or generated by BAS lasers is a critical issue of modern semiconductor laser technology.

Seeking to understand the dynamics of BAS devices, to suggest improvements of existing devices, or to propose novel device design concepts, we carry out a variety of related tasks. We perform modeling at different levels of complexity, do a mathematical analysis of the hierarchy of models, create and implement efficient and robust numerical algorithms, and perform numerical simulations of the model equations. Typically, all these steps are done within research projects in cooperation with the developers of the devices.

### Modeling and numerical algorithms

The dynamics of BAS devices can be described in different ways. The most comprehensive approach resolving the spatio-temporal evolution of full semiconductor equations self-consistently coupled to the optical fields is given by 3 (space) + 1 (time)-dimensional nonlinear partial differential equations (PDEs). Since the *height* of the active zone, where the optical beam is generated and amplified ( $y$ -dimension), is considerably smaller than the longitudinal ( $z$ -) and lateral ( $x$ -) dimensions of a typical BAS device, see Figure 1, a significant simplification can be achieved by averaging over the vertical direction and by describing certain effects phenomenologically. The resulting (2+1)-dimensional dynamical traveling wave (TW) model [1] can be resolved numerically orders of magnitudes faster, allowing for parameter studies in an acceptable time. The model is a degenerate system of second-order PDEs for the slowly varying complex amplitudes of the counter-propagating optical fields  $E(z, x, t) = (E^+, E^-)^T$ , nonlinearly coupled to a rate equation for the real carrier density distribution  $N(z, x, t)$ . It accounts for the diffraction of fields and for the diffusion of carriers in the lateral direction, whereas spatially non-homogeneous device parameters capture the geometrical design of the device. The normalized TW model reads as

$$\begin{aligned} \frac{\partial}{\partial t} E &= \left[ \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \frac{\partial}{\partial z} - \frac{i}{2} \frac{\partial^2}{\partial x^2} \right] E + [B(N, \|E\|^2, \omega) - \bar{\beta} I] E + F_{sp}, \\ \frac{1}{\mu} \frac{\partial}{\partial t} N &= D \frac{\partial^2}{\partial x^2} N + I(z, x) - R(N) - [E^{*T} B(N, \|E^\pm\|^2, \omega) E + c.c.], \end{aligned}$$

where  $\mu$  is small and the complex matrix  $B$  models the carrier- and frequency-dependent semiconductor material gain, thermal- and carrier-induced changes of the refractive index, as well as the distributed coupling of counter-propagating fields. The boundary conditions for the optical fields at the longitudinal edges of the device account for reflections of the counter-propagating fields, injection of external optical beams [2, 3], or optical feedback from an external cavity. At the lateral boundaries of the computational domain, the optical fields and carriers usually are well damped. Here, we assume either periodic boundary conditions [4] or mixed Dirichlet (for the carrier densities) and approximate transparent (for the field functions) boundary conditions [5]. This *basic* TW model can be extended for the modeling of various relevant properties of BAS devices. It can also be reduced to lower-dimensional systems, allowing for a more detailed analysis, understanding, and control of specific dynamical effects.

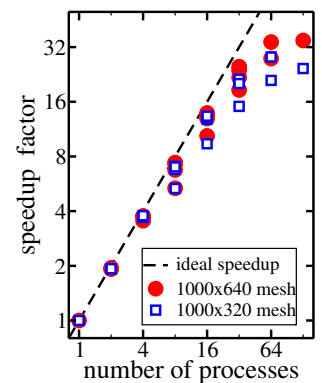
Precise dynamic simulations of long and broad devices and the tuning/optimization of the model parameters require huge process time and memory resources. A proper resolution of rapidly oscillating fields in typical BAS devices in a sufficiently large optical frequency range requires a fine space ( $10^6 - 10^7$  mesh points) and time (up to  $10^6$  points for typical 5 ns transients) discretization. Dynamic simulations of such devices can easily take several days or even weeks on a single processor. Some speedup of computations is achieved by using problem-dependent variable grid steps [5]. However, for extended parameter studies with the simulation times up to 1000 ns, parallel computers and parallel solvers have to be employed.

For the numerical integration of the TW model, we use either a split-step fast Fourier transform-based numerical method [4] or a full finite difference scheme [5]. The method of domain decomposition is used to parallelize the sequential algorithm. Exemplary simulations of two test problems on a parallel cluster of computers (see Figure 2) show a good scaling of the algorithm [4]. For example, the simulations performed on 32 processors give a speedup factor of 25. That is, the simulations requiring two weeks of process time on a single-processor computer can be efficiently performed over a single night. For a larger number of processes, the relative time needed for communications between them grows and implies a saturation of the speedup (see an increasing deviation of the test results from the ideal speedup in Figure 2).

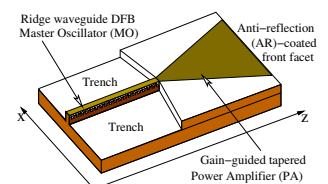
### Simulation of BAS devices

The TW model and our numerical algorithms were successfully used for simulations of different BAS lasers and amplifiers, also showing good agreement with experimental observations [1].

**Suppression of mode jumps in Master Oscillator Power Amplifier (MOPA) devices.** The master-oscillator (MO) tapered power-amplifier (PA) laser shown in Figure 3 was analyzed theoretically and experimentally in [1, 6]. The narrow waveguide of the distributed feedback (DFB) MO generates a stable stationary optical field determined by a single *transversal* mode, which later is amplified in the tapered PA part of the device. An ideal MOPA laser should be able to maintain a good quality of the emitted beam. The operation of realistic MOPA devices, however, is spoiled by the amplification of the spontaneous emission in the PA, by the small separation of the MO and PA electrical contacts, and by the residual field reflectivity at the PA facet of the device.

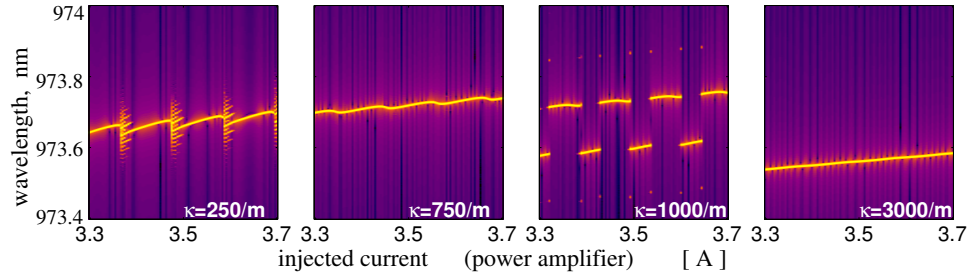


**Fig. 2:** Speedup of computations in multi-process simulations of two test problems

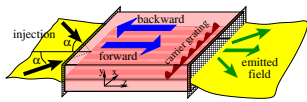


**Fig. 3:** Schematic of Master Oscillator Power Amplifier

**Fig. 4:** Simulated optical spectra of DFB MOPA devices with different DFB field coupling coefficients  $\kappa$  for increased injected current



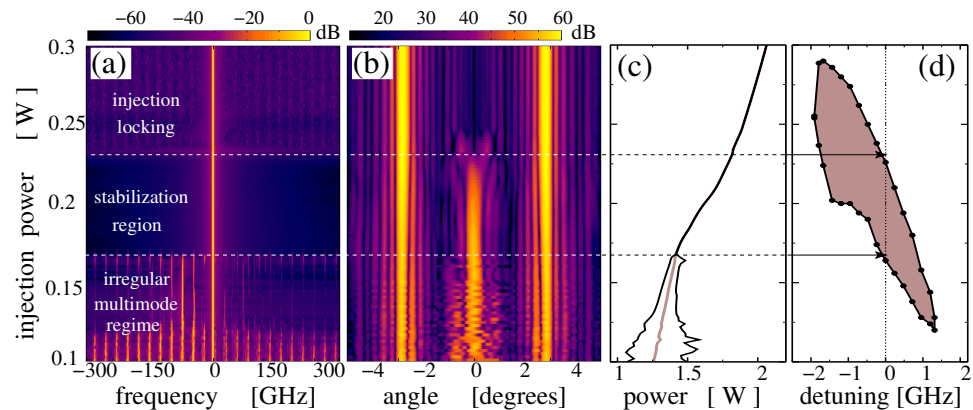
In [1], we analyzed how this residual reflectivity and thermally induced changes of the refractive index imply experimentally observable unwanted switchings between operating states determined by adjacent *longitudinal* optical modes. We found that these bifurcations are due to the changing phase relations of complex forward- and back-propagating fields at the interface of the MO and PA parts of the device. Simulations of a typical state-jumping behavior with increasing injected current is shown in the left panel of Figure 4. In the theoretical paper [6], we demonstrated that a proper choice of the field coupling parameter within the DFB MO part of the device makes it less sensitive to the optical feedback, leading to a stabilization of the laser emission; see second and fourth panels of Figure 4.



**Fig. 5:** Schematic of BAS laser with a dual optical injection

**Stabilization of BAS lasers by a dual off-axis optical injection.** In our theoretical paper [3], we proposed to stabilize the emission of a BAS laser by a pair of coherent optical plane waves injected into the laser along opposite angles to the optical axis; see Figure 5. Mathematically, this optical injection is given by the function  $\sqrt{P_0}e^{i\omega t} \sin(\alpha k_0 x)$  in the boundary conditions, where  $k_0$  is the central wavenumber,  $P_0$  is proportional to the injection intensity,  $\pm\alpha$  and  $\omega$  are the free space angles of the injected beams and the frequency detuning from the central frequency.

**Fig. 6:** Optical spectra (a) and far fields (b), as well as maximal, minimal, and mean emission power (c) for the increased injection power and fixed frequency detuning. (d): laser stabilization region in injection power / frequency detuning plane



We performed a series of simulations for fixed detuning  $\omega$  and increased intensity of the optical injection. Essential characteristics (optical spectra, far fields, field intensities) of typical observed dynamical states for  $\omega = 0$  and different injection intensities are shown in Figure 6. Here, one can distinguish three qualitatively different regimes, separated by thin horizontal lines. Once the injection intensity is too small, the spatial-temporal dynamics of the system is similar to that one



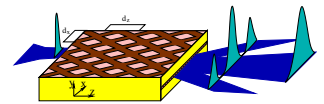
of the free-running BAS laser. Such dynamics can be recognized by multiple peaks of the optical spectrum (panel (a)), by scattered far-field instants (panel (b)), and by a non-stationary output field (panel (c)). For moderate and large injected field intensities the laser operates in a continuous wave regime (a single spectral line in panel (a) and coinciding minimal and maximal powers in panel (c)). An inspection of the far fields at these injections, however, allows us to distinguish two different regimes. Namely, for moderate injections, we have a stationary state, which has a well-pronounced central angular component (a stabilized mode of the laser). For larger injections, only the angular components corresponding to the injected beam angles  $\alpha$  are present. In this regime, our BAS laser is operating as an amplifier for the injected beams, but does not generate light by itself. Finally, panel (d) of the same figure, which shows a laser stabilization region in the injection power / frequency detuning plane, summarizes a series of simulations for different values of  $\omega$ .

It is noteworthy that the beam stabilization technique discussed above implies a coexistence of two or several stable continuous wave states, which have similar carrier and photon distributions and can be distinguished only by the phase of the complex field [3]. Thus, this beam stabilization technique can be especially attractive for applications in optical communications.

**Beam shaping in BAS amplifiers with periodically modulated electrical contacts.** An elegant way to improve the lateral beam profile in BAS amplifiers was analyzed in the recent theoretical work [3]. It was shown that a clever periodic modulation (PM) of the gain and refractive index in both longitudinal and lateral directions (see Figure 7) leads to a significant compression of the far fields, which is strongly desirable in real-world applications.

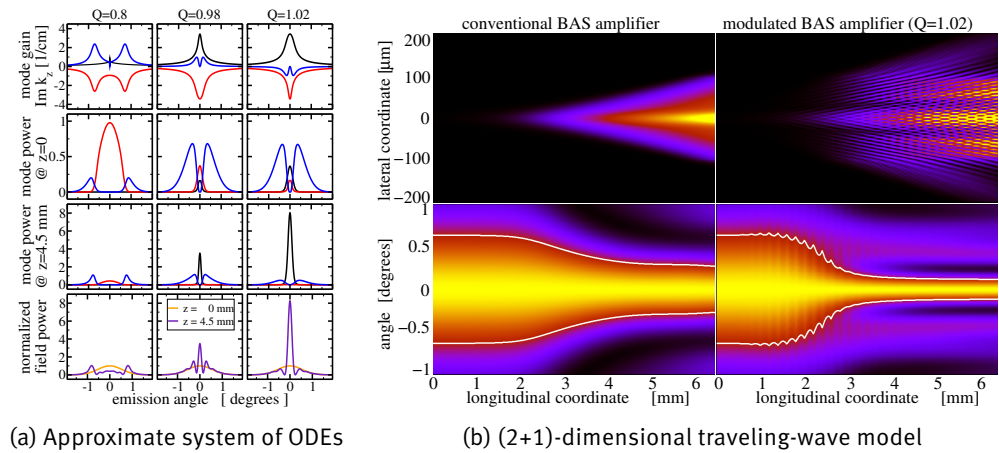
First of all, we analyzed a small field intensity regime in BAS amplifier. A harmonic expansion of the optical field allows us to approximate the original TW model by a linear system of three complex ordinary differential equations (ODEs). This simplified model describes the evolution of the optical fields for each emission angle that is close enough to the optical axis of the device. The propagating eigenmodes of this system grow or decay with the complex propagation wavenumber as  $\exp(-ik_z z)$ . Thus, the dependence of the mode gain functions  $\text{Im}k_z$  on the emission angle suggests a significant compression of the optical beam divergence around the zero angle, provided the modulation periods  $d_x$  and  $d_z$  satisfy the relation  $Q = k_0 d_x^2 \bar{n} / (\pi d_z) \approx 1$  ( $\bar{n}$ : background refractive index in semiconductor). Figure 8(a) illustrates the beam evolution and compression in a 4.5 mm-long BA amplifier for three different factors  $Q$ .

Next, to inspect the propagation and amplification of weak- and moderate-intensity beams in BAS amplifiers with  $Q \approx 1$ , we simulated our original *nonlinear* TW model. Even though the nonlinearities degrade the amplitudes of the spatial modulation in the BAS amplifier, the fundamental effect of beam divergence compression, which was observed in the linear ODEs, is preserved. The field compression is clearly seen in the right lower panel of Figure 8(b) (compare to left lower panel of the same figure, showing far fields of the conventional, non-modulated BAS amplifier).



**Fig. 7:** Schematic of BAS amplifier with periodically modulated electrical contact

**Fig. 8:** Angular shaping of the beam in BAS amplifiers. (a): mode gain, mode intensities at the beginning and the end of PM amplifiers with different  $Q$  as functions of the emission angle. (b): beam power distribution (top) and central part of the corresponding far field, with half maxima indicated by yellow lines (bottom) in conventional and PM amplifiers



Our first simulations of PM BAS *lasers* have also shown a promising beam divergence compression. We believe that the proposed periodic modulation of semiconductor media supplemented with additional beam-stabilizing techniques can become a standard method for beam quality improvement in edge-emitting BAS lasers.

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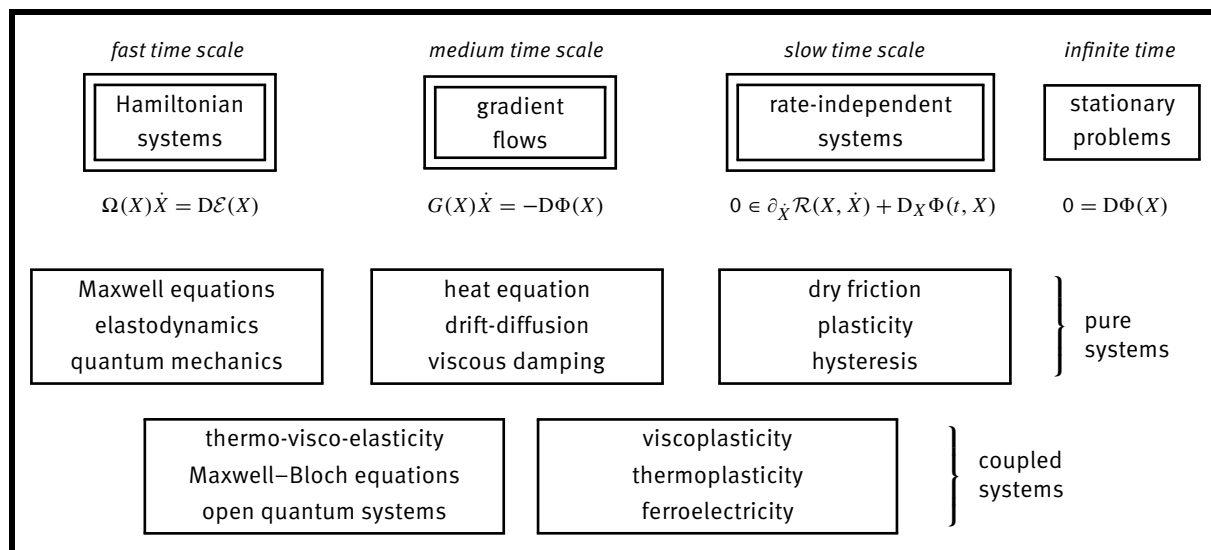


## 2.3 Multiscale Modeling and Evolutionary $\Gamma$ -Convergence

Karoline Disser and Alexander Mielke

Many processes and phenomena in the natural sciences take place on varying spatial and temporal scales, which strongly interact with each other. To describe their macroscopic evolution, the aim of multiscale mathematical modeling is to derive effective equations, which correctly take into account relevant micro- or mesoscopic quantities and structures.

The mathematical structure of fundamental equations in mechanics and physics is often given by driving functionals like energy or entropy. The differentials of these functionals provide the corresponding thermodynamic forces that drive the dynamics of the system. Moreover, the state space is equipped with geometric structures that turn the driving forces into rates of the state variables. A Hamiltonian or symplectic structure leads to classical systems without dissipation, while a Riemannian structure can act as a dissipation mechanism leading to gradient flows. Often these different mechanical phenomena give dynamics on different time scales; e.g., quantum mechanical oscillations or electromagnetic waves are typically much faster than dissipative effects in diffusion or heat transfer, which in turn are much faster than dry friction.



The diagram above gives a schematic overview of these types of evolutionary systems and their typical equations, where the fourth type is given by stationary problems. The boxes in the lower half give examples of mechanical systems and their couplings, which can be described in this way. One example is given by thermo-elasto-plasticity, where elastic oscillations are described by Hamiltonian dynamics, heat conduction is given by a gradient flow, and rate-independent effects come into play through the plastic flow rule. Similarly, for modeling quantum-well lasers, nanowires, and quantum-dot structures, one has to combine quantum mechanical effects given by a Hamiltonian system with a dissipative drift-diffusion system for classical semiconductor devices.

### ERC project “Analysis of multiscale systems driven by functionals”



This project is supported by the European Union within the Framework Programme 7 as an ERC Advanced Grant for the period from April 2011 to March 2016. The working group consists of six people and is integrated into the Research Group *Partial Differential Equations* (RG 1), but enjoys collaboration and synergies with many people at WIAS. The ERC funding supports two Ph.D. students and two postdocs for the whole time span.

The scientific topics of the project are focused on developing modeling and analysis tools for systems arising from couplings across multiple scales. The three main research areas are the following:

- (1) Analysis of systems driven by energy or entropy
- (2) Multiscale limits and evolutionary  $\Gamma$ -convergence
- (3) Applications in material modeling and optoelectronics

These areas are strongly interlinked, and the second area contains one of the main mathematical tasks, namely to develop a general theory of upscaling theory for evolutionary problems. For static problems given in terms of minimizing a single energy functional depending on a small parameter  $\varepsilon$ , there exists a well-developed theory of  $\Gamma$ -convergence, and the goal is to develop a corresponding theory for evolutionary problems defined in terms of two or more functionals. The general theory will provide a unified mathematical framework that hopefully applies to several classes of real-world multiscale systems.

### Evolutionary $\Gamma$ -convergence for gradient systems

As an important strategy in studying multiscale evolution, we highlight the concept of evolutionary convergence of gradient systems. Given a state space  $X$  and a family of energy functionals  $\mathcal{E}_\varepsilon : X \rightarrow \mathbb{R}$  as well as a family of dissipation potentials  $\mathcal{R}_\varepsilon$  parameterized by a small positive parameter  $\varepsilon$ , we call the triples  $(X, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$  *gradient systems*. They generate a gradient evolution via the differential equation

$$0 = \partial_{\dot{u}} \mathcal{R}_\varepsilon(u(t), \dot{u}(t)) + D\mathcal{E}_\varepsilon(u(t)), \quad u(0) = u_0^\varepsilon,$$

and we denote its solutions by  $u^\varepsilon : [0, T] \rightarrow X$ . Clearly, the evolution is driven by the two functionals  $\mathcal{E}_\varepsilon$  and  $\mathcal{R}_\varepsilon$ . We say that the family of gradient systems  $(X, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)_{\varepsilon \in (0,1)}$  *evolutionarily  $\Gamma$ -converges* to the limit system  $(X, \mathcal{E}, \mathcal{R})$  if the convergences of the initial conditions  $u_0^\varepsilon \rightarrow u_0$  and of the initial energies  $\mathcal{E}_\varepsilon(u_0^\varepsilon) \rightarrow \mathcal{E}(u_0)$  imply that for all  $t \in [0, T]$  we have  $u^\varepsilon(t) \rightarrow u(t)$  and  $\mathcal{E}_\varepsilon(u^\varepsilon(t)) \rightarrow \mathcal{E}(u(t))$ , where  $u : [0, T] \rightarrow X$  is the solution for the limit system with  $u(0) = u_0$ .

One of the major questions of evolutionary  $\Gamma$ -convergence is the derivation of sufficient conditions on the convergence of the pair  $(\mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$  to the limit  $(\mathcal{E}, \mathcal{R})$  that guarantee evolutionary  $\Gamma$ -convergence. This issue was first addressed on a general level by Sandier and Serfaty in 2004, and we refer to the survey articles [2, 6] for historic remarks and further details.

## Applications of evolutionary $\Gamma$ -convergence

We discuss some aspects of this theory and highlight three topics of recent research projects in some detail.

### 1. Discrete-to-continuum limit for gradient systems based on the Boltzmann entropy

In [1], we study the Fokker–Planck equation

$$\dot{u} = \operatorname{div}(\nabla u + u \nabla \Phi), \quad t > 0, \quad x \in \Omega, \quad (1)$$

describing general linear drift-diffusion processes in a physical domain  $\Omega \subset \mathbb{R}^d$ .

Jordan, Kinderlehrer, and Otto (1998) showed that this equation can be viewed as a gradient system of the Boltzmann entropy functional defined with respect to the steady state  $W = ce^{-\Phi}$ ,

$$\mathcal{E}(u) = \int_{\Omega} u \log(u/W) \, dx,$$

acting on the state space of probability measures endowed with the Wasserstein metric, which can be considered a Riemannian structure and which provides a dissipation potential  $\mathcal{R}$  for the system. Equation (1) can then be replaced by the condition that  $u$  obeys the *energy-dissipation principle*

$$(\text{EDP}) \quad \mathcal{E}(u(t)) + \int_0^t \mathcal{R}(u, \dot{u}) + \mathcal{R}^*(u, -D\mathcal{E}(u)) \, ds \leq \mathcal{E}(u(0)),$$

where  $\mathcal{R}^*(u, \cdot)$  denotes the Legendre dual of the potential  $\mathcal{R}(u, \cdot)$ . By the choice of  $\mathcal{E}$  and  $\mathcal{R}$  as driving functionals, this formulation assigns a particular physical structure to the problem, which is not determined by equation (1). The idea of the project is that, rather than the equation by itself, this additional structure might be helpful to determine accurate multiscale limits and couplings for the drift-diffusion process.

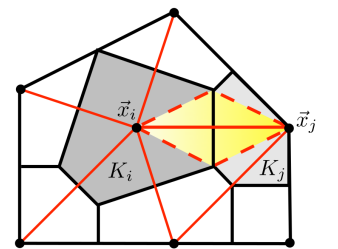
In numerical analysis, for  $n \rightarrow \infty$ , (1) can be approximated in space by a finite-volume scheme on Voronoi meshes generated by  $n$  points in  $\Omega$ . Traditionally, this approximation leads to an evolution governed by a discrete Laplace operator and a drift on a graph. Maas (2011) and Mielke (2011, 2013) independently showed that the spatially discrete evolution can again be viewed as a gradient system driven by the discrete relative entropy functional

$$\mathcal{E}_n(u) = \sum_{i=1}^n u_i \log(u_i/w_i)$$

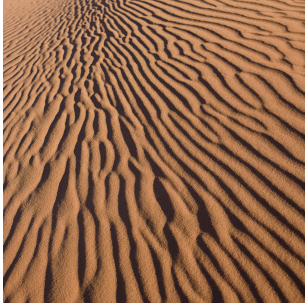
in the discrete state space of probability measures

$$X_n = \{u \in \mathbb{R}^n \mid u_i \geq 0, \sum_{i=1}^n u_i = 1\}$$

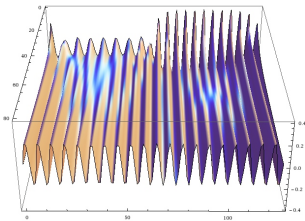
endowed with a discrete analogue of the Wasserstein metric, or a discrete-space dissipation func-



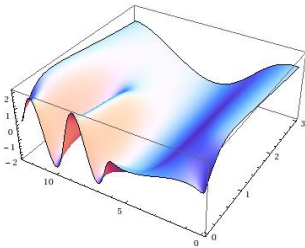
**Fig. 1:** On a Voronoi mesh with  $n$  positions  $\vec{x}_i$ , fluxes across cells  $K_i$  (grey) are approximated with respect to diamonds (yellow)



**Fig. 2:** Modulated period stripes on a sand beach (source: wikipedia)



**Fig. 3:** Solution of Swift-Hohenberg equation



**Fig. 4:**  $\text{Re}(A(t, x))$  of solution of Ginzburg-Landau equation corresponding to Figure 3

tional  $\mathcal{R}_n$ . The problem can be recast via the energy-dissipation principle (EDP) as

$$\mathcal{E}_n(u(t)) + \int_0^t \mathcal{R}_n(u, \dot{u}) + \mathcal{R}_n^*(u, -DE_n(u)) \, ds \leq \mathcal{E}_n(u(0)). \quad (2)$$

In [1], we consider general spatial discretizations in the one-dimensional case  $\Omega \subset \mathbb{R}^1$  and show the evolutionary  $\Gamma$ -convergence of the system  $(X_n, \mathcal{E}_n, \mathcal{R}_n)$  to  $(X, \mathcal{E}, \mathcal{R})$  for  $n \rightarrow \infty$ . Due to the structure of the problem, it is sufficient to show  $\Gamma$ -convergence of  $\mathcal{E}_n$  and a liminf estimate on the dissipation functional

$$J_n(u) = \int_0^t \mathcal{R}_n(u, \dot{u}) + \mathcal{R}_n^*(u, -DE_n(u)) \, ds.$$

It remains an open problem to establish the analogous result for general Voronoi meshes in higher space dimensions. The main difficulty is to construct a discrete gradient operator, which corresponds to the metric structure given by  $\mathcal{R}_n$  and which can be used to approximate the continuum gradient if the mesh size tends to 0.

## 2. Modulation equations

In specific situations, the loss of stability of a homogeneous solution in a partial differential equation can lead to spatially periodic patterns. In sufficiently large domains, these periodic patterns are modulated by a complex-valued amplitude function  $A(t, x)$ , which changes on a much larger spatial scale  $x$  and a long time scale  $t$ . As an example, we refer to the sand ripples on a beach depicted in Figure 2. A prototypical example exhibiting such a Turing instability is the so-called *Swift-Hohenberg equation*

$$(\text{SHe}) \quad \dot{u} = -\frac{1}{\varepsilon^2} (1 + \varepsilon^2 \partial_x^2)^2 u + Ru - u^3, \quad t > 0, x \in \mathbb{R}/L\mathbb{Z}.$$

Typical solutions, see Figure 3, have the form  $u(t, x) = \text{Re}(A(t, x)e^{ix/\varepsilon})$ , where  $e^{ix/\varepsilon}$  denotes the microscopic period pattern. The major question is how a given initial amplitude evolves with time. In [3], the  $L^2$  gradient structure of (SHe) involving the functional

$$\mathcal{E}_\varepsilon^{\text{SH}}(u) = \int_0^L \frac{1}{2\varepsilon^2} (u + \varepsilon^2 u'')^2 - \frac{R}{2} u^2 + \frac{1}{4} u^4 \, dx$$

is used to show the evolutionary  $\Gamma$ -convergence to the gradient system  $(L^2(\mathbb{R}/L\mathbb{Z}), \mathcal{E}^{\text{GL}}, 2\|\cdot\|_2)$  with the Ginzburg-Landau functional

$$\mathcal{E}^{\text{GL}}(A) = \int_0^L 2|A'|^2 - \frac{R}{2}|A|^2 + \frac{3}{8}|A|^4 \, dx.$$

The proof of the convergence of the solutions to the Swift-Hohenberg equation towards solutions to the Ginzburg-Landau equation can be done using *evolutionary variational inequalities*, which allows for a more advanced theory of evolutionary  $\Gamma$ -convergence than the energy-dissipation principle; cf. [3, Sec. 4]. This advanced theory uses the fact that the energy functionals  $\mathcal{E}_\varepsilon^{\text{SH}}$  are uniformly  $\lambda$ -convex, which allows us to prove the convergence under much weaker assumptions on the initial conditions. For instance, one does not need that the initial values have a finite energy.

### 3. Balanced-viscosity solutions in the vanishing-viscosity limit

Energy-driven systems can also be used efficiently for studying the limit of vanishing viscosity. Such problems occur if one considers a time-dependent generalized gradient system  $(X, \mathcal{E}, \mathcal{R}_\varepsilon)$ , where the dissipation potential has a part generating a rate-independent friction law as well as a very small viscous part, i.e.,  $\mathcal{R}_\varepsilon(v) = \mathcal{R}(v) + \frac{\varepsilon}{2} \langle \mathbb{G}v, v \rangle$ , where  $\mathcal{R}(\gamma v) = \gamma \mathcal{R}(v)$  for all  $v$  and all  $\gamma > 0$ . In particular, the friction forces contained in  $\partial \mathcal{R}(\dot{z})$  do not depend on the size  $\gamma$  of the rate  $\dot{z} = \gamma v$ , but only on the direction  $v = \frac{1}{|\dot{z}|} \dot{z}$ . The solutions for the generalized gradient system are given by the differential equation

$$0 \in \partial \mathcal{R}(\dot{z}) + \varepsilon \mathbb{G} \dot{z} + D\mathcal{E}(t, z).$$

If one is interested in the limit of vanishing viscosity, one may first consider the case  $\varepsilon = 0$ , which gives a rate-independent limit system. However, such rate-independent systems may develop jumps, and it is a major task to model the admissible jumps in a physically motivated way.

This can be done by the vanishing-viscosity method, i.e., we consider solutions  $z$  that are obtained as limits of solutions  $z^\varepsilon$  for  $\varepsilon \rightarrow 0$ . While the term  $\varepsilon \mathbb{G} \dot{z}$  will disappear for most parts of the solution, it will have some effect at jumps where  $\dot{z}$  may be of order  $1/\varepsilon$ . To characterize the limiting behavior correctly, the idea is to introduce a time rescaling  $t = \tau^\varepsilon(s)$  in such a way that  $\zeta^\varepsilon(s) = z^\varepsilon(\tau^\varepsilon(s))$  has a nicely bounded derivative with respect to  $s$ . Writing the energy-dissipation principle (EDP) in the rescaled variable, we obtain

$$\mathcal{E}(S, \zeta(S)) + \int_0^S M_\varepsilon(\tau'(s), \zeta'(s), -D\mathcal{E}(\tau(s), \zeta(s))) ds = \mathcal{E}(0, \zeta(0)) + \int_0^T \partial_t \mathcal{E}(\tau(s), \zeta(s)) \tau'(s) ds$$

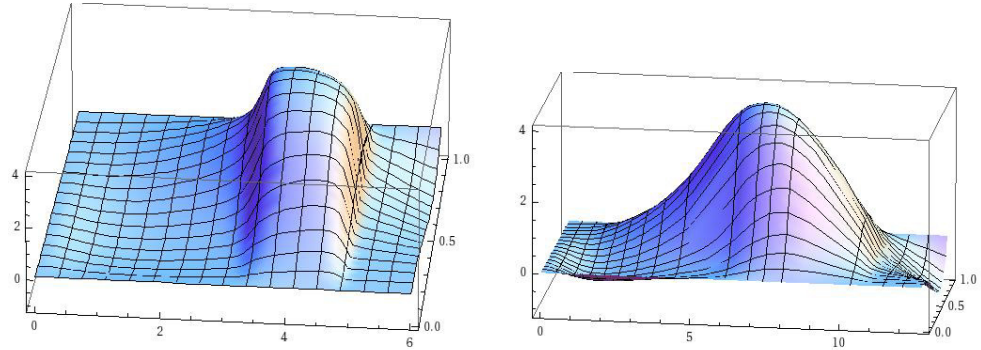
with the integrand  $M_\varepsilon(\alpha, v, \xi) = \mathcal{R}(v) + \frac{\varepsilon}{2\alpha} \langle \mathbb{G}v, v \rangle + \frac{\alpha}{2\varepsilon} \text{dist}_{\mathbb{G}}(\xi, \partial \mathcal{R}(0))^2$ . In this equation, the limit  $\varepsilon \rightarrow 0$  can be calculated in a suitable way, since the  $\Gamma$ -limit  $M_0$  of  $M_\varepsilon$  can be identified, namely

$$M_0(\alpha, v, \xi) = \mathcal{R}(v) + \chi_{\partial \mathcal{R}(0)}(\xi) \text{ for } \alpha > 0, \quad M_0(0, v, \xi) = \mathcal{R}(v) + \|v\|_{\mathbb{G}} \text{dist}_{\mathbb{G}}(\xi, \partial \mathcal{R}(0)).$$

The last expression for  $\alpha = \tau'(s) = 0$  corresponds to the behavior at jumps, where the macroscopic time  $t$  remains constant and shows clearly the balance of the different viscous terms arising from the viscosity operator  $\mathbb{G}$ . In [4], it is furthermore shown that balanced-viscosity solutions can be characterized independently of a parametrization  $t = \tau(s)$  and that they can be obtained by a time-incremental approach with a simultaneous limit of timestep  $\tau$  and viscosity tending to 0 as long as  $\varepsilon/\tau \rightarrow \infty$ . As an example, Figure 5 depicts the original solution  $z(t, x)$  having two jumps and a reparametrized solution  $\zeta(s, x)$ , which is Lipschitz continuous, for the small-viscosity equation

$$(**) \quad 0 \in \text{Sign}(\dot{z}) + \varepsilon \dot{z} - \Delta z - 6z(z-2)(z-4) - t(5-t)h(x), \quad t > 0, \quad x \in ]0, 1[.$$

**Fig. 5:** Solutions for (\*\*).  
Left:  $z(t, x)$ . Right:  
 $\zeta(s, x) = z(\tau(s), x)$



In some cases, the state space  $X$  splits into the form  $Y \times Z$  such that  $u = (y, z)$  splits into a purely viscous part  $y$  and a rate-independent part  $z$ . The generalized gradient systems  $(Y \times Z, \mathcal{E}, \mathcal{R}_\varepsilon)$  now lead to the evolutionary system

$$0 = \varepsilon^\beta \mathbb{G} \dot{y} + D_y \mathcal{E}(t, y, z), \quad 0 \in \partial \mathcal{R}(\dot{z}) + \varepsilon \nabla \dot{z} + D_z \mathcal{E}(t, y, z).$$

The analysis in [5] shows that the jump behavior of the limits  $(y, z)$  of the family  $(y^\varepsilon, z^\varepsilon)$  crucially depends on the parameter  $\beta$ . It is restricted to the case that  $\mathcal{E}(t, \cdot, z) : Y \rightarrow \mathbb{R}$  is strictly convex.

For  $\beta > 1$  the component  $y$  can relax into equilibrium much faster than the variable  $z$ . Denoting by  $y = Y(t, z)$  the unique minimizer of  $\mathcal{E}(t, \cdot, z)$ , one can describe the limiting behavior of  $(y^\varepsilon, z^\varepsilon)$  solely by constructing balanced-viscosity solutions for the reduced system  $(Z, \mathcal{I}, \mathcal{R}_\varepsilon)$ , where the reduced energy is given by  $\mathcal{I}(t, z) := \mathcal{E}(t, Y(t, z), z)$ . In contrast, in the case  $\beta \in (0, 1)$ , the jumps will occur such that, first, the variable  $z$  will jump for fixed  $y$  into a so-called *stable state* on the time scale  $\varepsilon$ , and, then, the variable  $y$  will converge into equilibrium together with  $z$  on the slower time scale  $\varepsilon^\beta$ . Again, the analysis relies on time reparametrization and follows from suitable  $\Gamma$ -limits of the energy-dissipation principle.

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## 2.4 Probabilistic Programming with Applications to Power Management

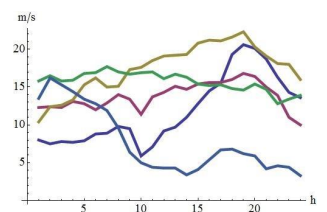
Ingo Bremer and René Henrion

### Introduction

Production and manufacturing processes are faced with the need for optimizing decisions in order to reduce costs or to increase profits, etc. The decisions to be taken are not free in general, but subject to technological, economic, or other constraints, typically expressed by means of equalities and/or inequalities. An example is given by the decision to produce an amount  $x$  of a certain good having to meet a given demand  $d$ , a relation that can be expressed as the inequality  $x \geq d$ . The task to minimize or maximize an objective function depending on constrained decisions is mathematically referred to as an *optimization problem*. Traditionally, all data of such problems, such as demand or physical coefficients, are supposed to be exactly known. In reality, however, one has to live with a significant level of uncertainty in the data.

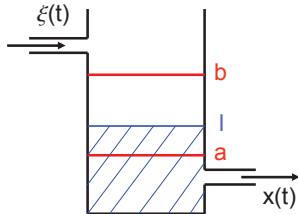
A prototypical example for production processes affected by uncertainty is power management, where optimal decisions to employ different power generation units (e.g., thermal, hydro, nuclear, wind, pumped storage) have to be taken in a cost-minimal way under various types of constraints (upper generation limits, demand satisfaction, level constraints for hydro reservoirs, or minimum down times for thermal units). Here, uncertainty appears in the guise of meteorological (e.g., precipitation, wind force, temperature), economical (e.g., demand of electricity or its price on the market), or technological (e.g., failure coefficients) parameters; see Figure 1. Most often, decisions have to be taken prior to observing the uncertain parameters. For instance, the switching on/off of thermal units is associated with a certain time delay and cannot be done as an immediate reaction to an increased or decreased demand. The latter is rather a task of more flexible units like pumped storage plants. Similarly, selling energy on a day-ahead market requires entering a contractual agreement on power delivery for each hour of the next day without knowing the exact conditions influencing the offer/demand relation and the profit (prices, demand, inflow to water reservoirs or wind force). Hence, one has to take so-called *here-and-now* decisions. In this environment of unknown future realizations of certain parameters, it is not clear how to solve or even to understand conceptually the arising optimization problem. A naive remedy would consist in replacing these parameters by their mean values observed in the past. As will be seen later, this approach suffers from a heavy lack of robustness.

Probabilistic programming is a discipline of stochastic optimization dealing with uncertain constraints by turning them into so-called *probabilistic constraints*. Here, it is assumed that uncertainty obeys a certain random law that can be identified or approximated on the basis of past observations. Then, inside some optimization problem whose constraints are given by a random inequality system, a decision is defined to be feasible if this inequality system is satisfied with a specified minimum probability, e.g., 95%.

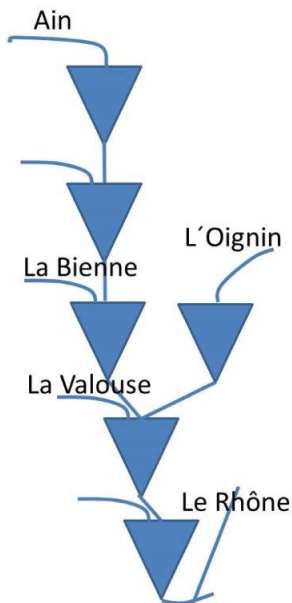


**Fig. 1:** Five wind speed scenarios

### Hydro reservoir management



**Fig. 2:** Level constraints in an abstract reservoir with random inflow and controlled release



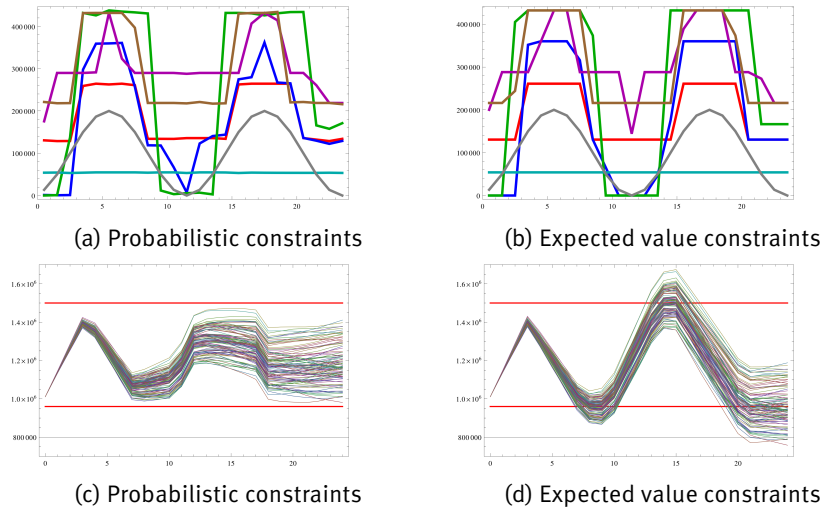
**Fig. 3:** Linked system of 6 hydro reservoirs

An important part of the total amount of electricity is generated by hydro plants (Germany: 5%, Brazil: 87%, Norway: 99.5%). Prior to turbinning, the water is collected in possibly large reservoirs with a random inflow process  $\xi$  governed by precipitation (rainfall, snow melt). From a perspective of production planning, the task consists in finding an optimal release policy  $x$  from the reservoir such that some objective is minimized or maximized while satisfying additional side constraints. An important constraint in this context is given by upper and lower limits  $a, b$  for the water level  $l$  in the reservoir; see Figure 2. There are ecological (e.g., flood reserve), technological, and economic reasons for imposing such constraints. As mentioned above, selling hydro energy on a day-ahead market requires a here-and-now decision on the release policy without knowing the random inflow to the reservoir on the next day. Thus, the water level in the reservoir is a random quantity and satisfying the given limits should be reasonably modeled via a probabilistic constraint.

In [2], we considered a linked system of six reservoirs of a hydro valley managed by *Electricité de France*; see Figure 3. Given an idealized price signal  $\pi$  (see gray curves in the top diagrams of Figure 4), the objective was to find an optimal release policy  $x$  for a horizon of two days ahead in order to maximize the profit  $\langle \pi, x \rangle$  by sale of energy subject to simple operational bound constraints of type  $0 \leq x \leq x^{max}$  and subject to the probabilistic level constraint described above. The time horizon was discretized into 24 intervals of two hours each in order to turn the problem into one of finite-dimensional nonlinear optimization. The probability for satisfying the level constraints in the reservoir was chosen as  $p = 0.98$ . We emphasize that the probabilistic constraint is a *joint* rather than an *individual* one. This means that, with the given probability, the filling levels in the reservoir stay between the imposed levels **throughout** the whole time horizon rather than for each of the 24 intervals individually.

Figure 4 shows in its diagrams on the top the optimal release policies for the six reservoirs for a model with joint probabilistic constraints (a) and with constraints replacing the random inflow by its expected value (b). One may see that these profiles tend to follow the given price signal as much as possible, but cannot do so perfectly due to the imposed constraints. Apart from a few peaks, the solution profiles look quite similar for both models. When assuming expected values, the resulting profit is slightly larger (2%) as compared to the probabilistic solution. In order to verify the effect of employing the respective release policies, a set of 100 inflow scenarios was simulated according a multivariate distribution identified from time series analysis. It has to be noted that these scenarios were not used for the mathematical solution of the problem, but just served the purpose of an a posteriori check. Given these scenarios (not plotted in the figure) and applying the obtained release policies, one arrives at 100 resulting scenarios for the filling levels in the reservoirs. They are plotted for only one reservoir in the bottom diagrams of Figure 4. As can be seen from Diagram (d), the expected value solution leads to a frequent violation of lower and upper limit constraints several times in the considered horizon. But the effect of neglecting distribution information is even worse: Among the 100 scenarios, there is not a single one satisfying the level constraints throughout the considered time horizon. This observation clearly rules out the use of expected values in random inequality constraints. In contrast, the probabilistic solution (Diagram (c)) does what it promises and yields a very robust solution by decreasing the amount of profit just a little bit. Given the chosen probability  $p = 0.98$ , one would expect that, on average, 98 out of

the repeatedly generated sets of 100 scenarios would satisfy the constraints uniformly over the whole time horizon.



**Fig. 4:** Reservoir management in hydro energy production: optimal release policies (top) and simulated level profiles (bottom)

For the specific simulation underlying Figure 4, even all scenarios are feasible.

## Probabilistic constraints

A probabilistic constraint as introduced above can be formalized as an inequality of the following type:

$$\mathbb{P}(g(x, \xi) \geq 0) \geq p. \quad (1)$$

Here,  $g(x, \xi) \geq 0$  represents an inequality system with several components defining the constraints on the decision vector  $x$  and being affected by some random vector  $\xi$ .  $\mathbb{P}$  denotes some probability measure, and  $p \in [0, 1]$  is a safety level (typically close to but not equal to 1). Introducing the probability function  $\varphi(x) := \mathbb{P}(g(x, \xi) \geq 0)$ , an optimization problem subject to probabilistic constraints can be written as

$$\min f(x) \quad \text{subject to} \quad \varphi(x) \geq p, \quad (2)$$

where  $f$  refers to some objective function. Formally, (2) represents a conventional nonlinear optimization problem. The main challenge in analyzing and solving it consists in the absence of an explicit formula for  $\varphi$  due to the joint distribution of  $\xi$  being multivariate. As a consequence, questions about analytical properties, algorithmic approaches, and the stability of (2)—well-understood in deterministic optimization theory—need to be answered again.

As (2) is at least formally a conventional optimization problem, one algorithmic approach to its solution relies on applying methods from nonlinear or, whenever possible, convex optimization. The main challenge here consists in evaluating  $\varphi$  and its gradients. This is the reason why major work has been devoted to the derivation of efficient gradient formulae for probability functions; see, e.g., [1, 4]). Equipped with these devices, a numerical solution of probabilistic programs using methods from convex optimization, such as a supporting hyperplane algorithm, or sequential quadratic programming methods in a potentially nonconvex setting, becomes possible.

### Application to a coupled hydro/wind system

In the following, an application of the above nonlinear optimization approach to a management problem of renewable energy will be described; see [3]. We consider a coupled hydro/wind system employed in order to meet a certain demand of electricity at hand and to sell the excess energy on a day-ahead market. We consider a time horizon of two days ahead, discretized into hours, half-hours, and quarters of hours. For simplicity, for this short-term problem, we assume all parameters with the exception of the wind energy to be deterministic. In particular, we assume the profiles of demand and day-ahead prices to be known and the inflow velocity to the hydro reservoir even to be constant. In contrast, the wind energy is modeled as a random parameter via the wind speed exploiting a long data series available from meteorological services.

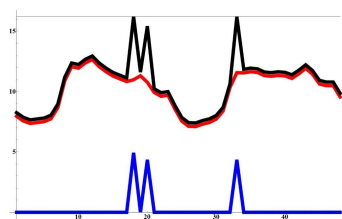
As the wind energy produced is out of our control, the only decision variable we consider is the release from the hydro reservoir. However, we do not only decide on the total release, but also on splitting it into two parts: one part supporting the wind energy production in order to meet the given demand, and the remaining part for sale at the day ahead market. Since the demand satisfaction is achieved partially by a random contribution (wind), it represents a stochastic inequality of “here-and-now” type and, therefore, is turned into a probabilistic constraint. In the rare event (according to the chosen safety level) of shortfall of energy, it is assumed that the balance is reestablished on the more flexible intraday market. The larger the safety level, the less likely that transactions on the more volatile intraday market are necessary. The resulting optimization problem looks as follows, with decision variables colored in blue, random parameters in red, and the remaining known data of the problem in black:

$$\begin{aligned}
 & \text{Maximize} \quad \sum_{t=1}^T p_t x_t \quad \text{subject to} \\
 & \mathbb{P}(y_t + \xi_t \geq d_t \quad \forall t = 1, \dots, T) \geq p \\
 & 0 \leq x_t, y_t \quad (t = 1, \dots, T) \\
 & x_t + y_t \leq h_{\max} \quad (t = 1, \dots, T) \\
 & l^{\min} \leq l^0 + tw - \sum_{\tau=1}^t \kappa(x_\tau + y_\tau) \leq l^{\max} \quad (t = 1, \dots, T) \\
 & l^0 + Tw - \sum_{\tau=1}^T \kappa(x_\tau + y_\tau) \geq l^*.
 \end{aligned}$$

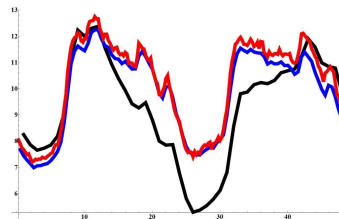
More precisely,  $d_t$ ,  $p_t$  refer to the demand and day-ahead price at time interval  $t$ , respectively,  $w$  is the constant inflow to the hydro reservoir,  $\xi_t$  is the generated wind energy, and  $x_t$ ,  $y_t$  represent the contributions of hydro energy used for the sale on the day-ahead market and for the support of wind in demand satisfaction, respectively. The objective is to maximize the profit on the day-ahead market subject to a set of constraints, the first of which is the probabilistic constraint on demand satisfaction throughout the whole time horizon with a safety level  $p$ . The following two simple constraints guarantee nonnegative releases from the reservoir such that the total amount of released water remains below some operational upper limit of the turbine. This is followed by level constraints for the hydro reservoir to be respected during the whole time horizon. The last inequality requires a minimum terminal water level in the reservoir in order to prevent degradation of initial conditions for later time horizons.

Figure 5 collects some numerical results of this problem. In (a), the optimal water releases (total:

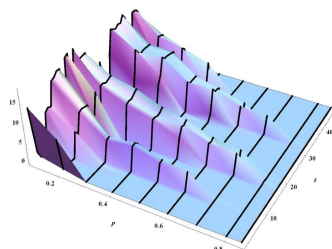
black; day-ahead sale: blue; contribution to demand satisfaction: red) are plotted for the safety level  $p = 0.7$ . The grey line represents the upper production limit. The diagram in (b) shows optimal solutions for the water release contribution to demand satisfaction with different discretization levels (black: 48 hours; blue: 96 half-hours; red: 192 quarters of hours). While there is a significant difference between the first two levels, the solutions to the finest levels almost coincide. The solutions demonstrate that the nonlinear programming approach is able to cope with probabilistic constraints where the random vector has a joint multivariate distribution of dimension up to a few hundred (here: number of time steps). In (c), the dependence of solutions (here: water release for day-ahead sale) on the safety level is illustrated: with increasing safety for demand satisfaction, a decreasing amount of hydro energy can be sold on the day-ahead market. Finally, Diagram (d) plots the demand satisfaction balance: The given demand profile (black) is opposed to 100 production scenarios resulting as the sum of the corresponding contributions by hydro energy and 100 wind energy scenarios calculated from 100 historical wind speed scenarios.



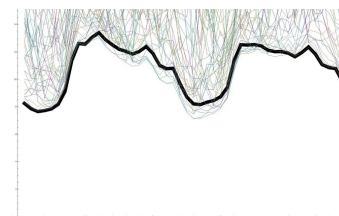
(a) Water releases (total and parts)



(b) Solutions for different discretization levels



(c) Day-ahead sale for different safety levels



(d) Demand satisfaction for 100 scenarios

**Fig. 5:** Numerical results for optimal water release in hydro/wind coupling

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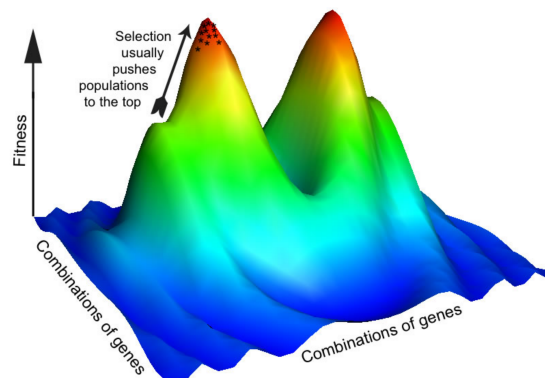
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## 2.5 Population Growth on Random Fitness Landscapes

Marion Hesse

In 1932, the American geneticist Sewall Wright [4] introduced the idea that evolution can be viewed as a hill-climbing process on a fitness landscape. Until today, this remains one of the most powerful images in evolutionary biology. Fitness landscapes are used to illustrate the relationship between genotypes and reproductive success. The reproductive success of a genotype is measured through its replication rate, which is then referred to as the fitness. The resulting fitness values are seen as the “height” of the fitness landscape; see Figure 1 for a schematic representation of a fitness landscape. The space over which the fitness landscape should be defined is the space of genetic sequences.

Even though Wright’s idea is now more than 80 years old, the study of fitness landscape has not been in the focus of the theory of evolutionary biology. This situation is currently changing. Long-term experiments on microbial populations which aim to determine fitness landscapes are bringing in first results. With this data in hand, it is now within reach to make the picture of the hill-climbing process precise and to ask questions about the timing and size of evolutionary events.



**Fig. 1:** Evolution as a hill-climbing process on a fitness landscape

In (most) fitness landscapes, there are peaks (areas of high fitness) and valleys (areas of low fitness). When an individual undergoes mutation, it changes its genotype and thus its location in the landscape. It thereby changes its fitness value to the one assigned to its new genotype. Since fitness is a measure of reproductive success, the higher the fitness value, the more likely it will create offspring into the next generation. By continuing this process over many generations, the population will eventually carry a genotype that sits at a peak of the landscape. A high mutation rate makes it easier for the population to cross valleys and/or find the genotype with the highest fitness value in the fitness landscape. The shape of the landscape and how frequently mutations occur will determine which paths the population can take and which peaks it can reach.

In this article, we present a probabilistic model for the evolution of a population on a fitness landscape. This model describes the behavior of a population of haploid, asexual individuals with high mutation rates and in which each individual is characterized by a genetic sequence. The population evolves on a random fitness landscape that assigns a random fitness value to each genotype.

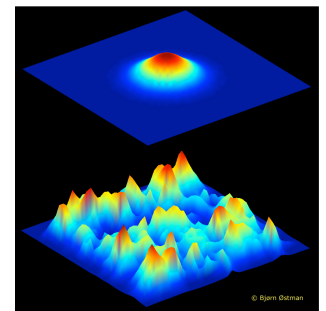


The population is thus exposed to mutations, which allow the population to move across the fitness landscape and thereby tend to increase the genetic variability, and selection, which is the comparative advantage of genotypes with high fitness and leads to concentration of the population in areas of higher fitness. Our model will help to understand when and on which time scales evolutionary events—that is, shifts of the population from one local peak to another (local) peak of the fitness landscape—can occur.

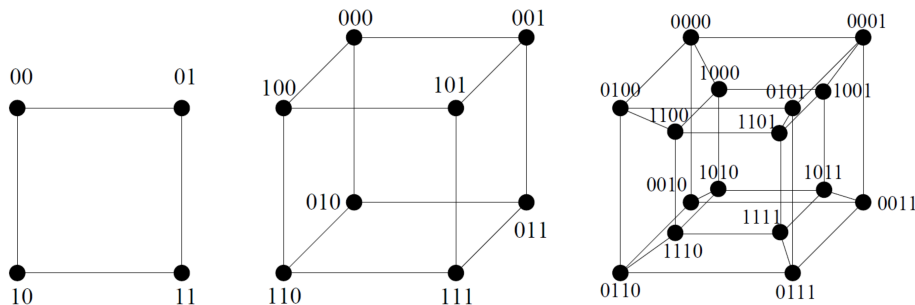
### Fitness as a rugged landscape

On a molecular level, each individual of the population is characterized by a sequence  $\sigma = \{\sigma_1, \dots, \sigma_N\}$  where each of the  $N$  entries  $\sigma$  is taken from a finite alphabet of size  $l \geq 2$ . We will often refer to  $\sigma$  as the type or genotype of an individual. For DNA- or RNA-based organisms, the alphabet is  $\{A, T(U), C, G\}$  corresponding to the nucleotide bases. For proteins the alphabet consists of the 20 amino acids. In classical population genetics,  $\sigma$  represents the configuration of alleles. In this case, the entry  $\sigma_i$  can take value 0 (wild type) or 1 (mutant) depending on which allele (wild type or mutant) is located at gene locus  $i$ .

For simplicity, we will assume henceforth that  $l = 2$  and  $\sigma_i \in \{0, 1\}$ . We can then view the space of all sequences as the  $N$ -dimensional hypercube  $\Sigma_N = \{0, 1\}^N$ .



**Fig. 2:** A smooth (top) and a more rugged (bottom) fitness landscape



**Fig. 3:** Hypercubes as a model for the space of genetic sequences

The idea of natural selection is that individuals with a relatively high fitness reproduce faster than individuals with a relatively low fitness. Thus the former and their corresponding genotypes become more abundant in the population while the latter get outnumbered.

Formally, a fitness landscape is the collection  $\{\zeta(\sigma), \sigma \in \Sigma_N\}$  where  $\zeta(\sigma)$  is the fitness value associated with type  $\sigma$ . Several different models of fitness landscapes have been proposed in the biology literature; see for example Figure 2. Recently, rugged fitness landscapes gained particular attention. In a rugged fitness landscape, also known as the *House of Cards model*, fitness values are random variables which are identical in distribution and independent of each other. For this reason, we also refer to this type of landscape as *random fitness landscapes*.

### A probabilistic model: A branching random walk in a random environment

The evolution of a population on a random fitness landscape can be modeled as a spatial branching process whose dynamics are given by the following steps:

- Each individual undergoes mutation by switching a uniformly chosen letter of its type sequence at rate 1 .
- An individual of type  $\sigma$  splits into two individuals at rate  $\xi(\sigma)$ .

The resulting process is called a *branching random walk in a random environment*. The term *random environment* refers to the random branching rates that form the fitness landscape. Our choice of landscape is the Random Energy Model (REM), which is borrowed from spin glass theory. As such we choose the fitness landscape  $\{\xi(\sigma), \sigma \in \Sigma_N\}$  to be an i.i.d. sequence of normal random variables with mean 0 and variance  $N$ .

We denote by  $v_N(t, \sigma; \sigma_0)$  the expected number of individuals alive at time  $t$  which are of type  $\sigma$  when the population is initiated from one individual of type  $\sigma_0$  at time 0. Our model can then be described through a system of differential equations with random potential

$$\frac{\partial}{\partial t} v_N(t, \sigma; \sigma_0) = \Delta_N v_N(t, \sigma; \sigma_0) + \xi(\sigma) v_N(t, \sigma; \sigma_0), \quad t \geq 0, \sigma \in \Sigma_N, \quad (1)$$

with initial condition  $v_N(0, \sigma; \sigma_0) = \delta_{\sigma_0}(\sigma)$ . Here,  $\Delta_N$  denotes the Laplace operator on  $\Sigma_N$ . The first term on the right-hand side of (1) describes the change in the number of individuals of a type through mutations, while the second term incorporates the change which is due to branching events.

### The mutation-selection model on a random fitness landscape

We can relate the differential equation (1) to a well-known mutation-selection equation by defining

$$u_N(t, \sigma; \sigma_0) := \frac{v_N(t, \sigma; \sigma_0)}{\sum_{\sigma' \in \Sigma_N} v_N(t, \sigma'; \sigma_0)}, \quad t \geq 0, \sigma \in \Sigma_N,$$

to denote the relative frequency of type  $\sigma_0$  at time  $t$  when the population is initially concentrated on the type  $x_0$ . The parallel mutation-selection model on the fitness landscape  $\{\xi(\sigma), \sigma \in \Sigma_N\}$  is then given by

$$\frac{\partial}{\partial t} u_N(t, \sigma; \sigma_0) = \Delta_N u_N(t, \sigma; \sigma_0) + (\xi(\sigma) - \bar{\xi}(t)) u_N(t, \sigma; \sigma_0), \quad t \geq 0, \sigma \in \Sigma_N, \quad (2)$$

with initial condition  $u_N(t, \sigma; \sigma_0) = \delta_{\sigma_0}(\sigma)$ . Here,  $\bar{\xi}(t)$  is the mean fitness of the population at time  $t$ :

$$\bar{\xi}(t) = \sum_{\sigma' \in \Sigma_N} \xi_N(\sigma') u_N(t, \sigma'; \sigma_0).$$

Similarly to (1), the first term on the right-hand side of (2) describes the change of type frequencies through mutation, while the second term is due to branching events. The latter can be interpreted

as selection mechanism since the frequency of types whose fitness lies above the mean fitness  $\bar{\zeta}(t)$  increases, while types of lower fitness than the mean fitness experience a decrease in type frequency.

## A phase transition in the fitness

In random fitness landscapes, the population is faced with the task of reaching ever higher fitness peaks by crossing through valleys of low fitness. The problem we have studied, and present here, is whether the population can move to a higher peak or stays at the initial location. In terms of the type frequencies, we are asking:

- Does the populations stay concentrated in the initial type or does it concentrate in a fitter type?
- What are the evolutionary time scales on which the population moves from one type to a fitter type?

Since fitness of a type is a measure of the type's reproductive success, we can approach this problem by studying the growth of the population. It is well known that the expected number of individuals grows exponentially fast and that the rate of growth depends on the fitness values. We can then rephrase the questions above as follows: Is the growth rate determined by the fitness of the initial type  $\sigma_0$  or can a higher growth rate be achieved via mutations to types with higher fitness? What are the evolutionary time scales on which the growth rate changes? A first step to answer these questions is our recent work [1], which we will now outline.

In the following, we parametrize time with the dimension on the hypercube  $\Sigma_N$ , that is, we set  $t = t(N)$ . For a fixed  $k \in \mathbb{N}$ , we assume that the initial individual is of the type that has the  $k$ th highest fitness value, and we denote this type by  $\sigma_k$ . We then analyze the asymptotics of the overall expected population size

$$v_N(t; \sigma_k) := \sum_{\sigma \in \Sigma_N} v_N(t, \sigma; \sigma_k), \quad \text{as } N \rightarrow \infty.$$

It turns out that the asymptotics exhibit the following phase transition: If  $t(N) \ll N \log N$ , then

$$\frac{1}{t} \log v_N(t; \sigma_k) = \zeta(\sigma_k) - \kappa + o(1), \quad \text{as } N \rightarrow \infty. \quad (3)$$

On the other hand, if  $t \gg N \log N$ , then

$$\frac{1}{t} \log v_N(t; \sigma_k) = \zeta(\sigma_1) - \kappa + O(N^{-2}), \quad \text{as } N \rightarrow \infty, \quad (4)$$

where  $\sigma_1$  is the fittest type.

The result can be interpreted as follows: If  $t(N) \ll N \log N$ , then the growth rate of the population depends mainly on the fitness  $\zeta(\sigma_k)$  of the initial type  $\sigma_k$ ; whereas, if  $t \gg N \log N$ , then the highest fitness value  $\zeta(\sigma_1)$  determines the growth rate. Coming back to our original question of concentration of types, the following interpretation is an easy consequence of the result above. In the case  $t(N) \ll N \log N$ , the population stays concentrated in the initial type  $\sigma_k$ , while in the case  $t(N) \gg N \log N$ , the population concentrates in type  $\sigma_1$ . This implies in particular that in the

latter case individuals are able to reach the fittest type through mutations which then outnumber all other types via the selection mechanism seen in (2).

As mentioned earlier, on a random fitness landscape, the population moves to higher fitness peaks by crossing fitness valleys, which typically gives rise to a sequence of time steps on which shifts of the population occur. So far, we have only explained a very small part of this picture, namely the case in which the population already starts from a high fitness value, the  $k$ th highest to be more precise. But how does the time scale change when we start from a lower fitness value or a randomly picked fitness value? We will address these questions in future work.

An even more important question: Is our assumption of an uncorrelated, random fitness landscape justifiable? There is more and more empirical evidence that indicates that real fitness landscapes, while possessing a considerable amount of randomness, are smoother than the random fitness landscape we consider here. A model combining both the smooth landscape (Figure 2 (top)) and the random fitness landscape (see again Figure 2 (bottom)) has recently been proposed in [3]. This model, the so-called *Rough Mount Fuji model*, seems to capture the features of real fitness landscapes better than completely smooth or completely random fitness landscapes. Our next goal should therefore be to understand the occurrence of evolutionary events on a Rough Mount Fuji landscape.

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## 2.6 Reduced-order Modeling for Blood Flows in the Pulmonary Artery

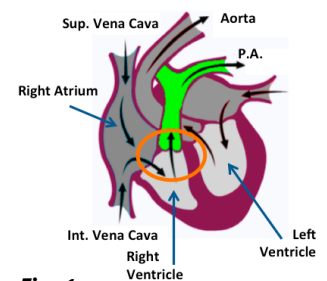
Alfonso Caiazzo

In recent years, computational simulations of blood flows have received increasing attention as a tool for gaining insight into the blood dynamics, for better understanding the relations between cardiovascular pathologies and changes in hemodynamics, as well as for exploring different scenarios of surgical intervention. This article focuses on computational models of pathological pulmonary circulation. The pulmonary artery (PA) is divided in main PA, connected to the heart (right ventricle), and in two branches (left and right PA), which end in the lungs (Figure 1). In healthy conditions, the blood coming from the venous system circulates from the right ventricle through the PA into the lungs, and the pulmonary valve is responsible of maintaining a one-way blood flow.

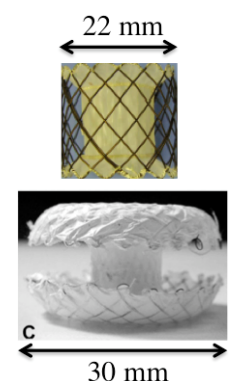
The Tetralogy of Fallot (ToF) is a severe heart defect characterized by an enlarged right ventricular outflow tract and, in some cases, by the absence of a functioning pulmonary valve. Without the valve, part of the blood flow regurgitates back into the right ventricle, which, besides having severe implications on the nutrients delivery throughout the circulatory system, might lead to progressive enlargement of the right ventricle and pulmonary arteries. For this pathology, clinicians are primarily interested in understanding how the artery is affected from the pathologic hemodynamics and, conversely, how blood regurgitation patterns are influenced by the shape of the deformed artery.

In particular, understanding the connections between artery shape and flow conditions is very important for surgery planning. In order to reestablish a normal (one-way) blood flow, treatment of ToF patients involves the design and the implantation of an artificial device able to act in the same way as the pulmonary valve. However, due to the enlarged shape of the ventricular outflow tract, the implantation of existing commercial devices (normally with diameter up to 22 mm) might result prohibitive. For these reasons, some authors have recently advocated the implantation, together with the artificial valve, of a torus-shaped stent (so-called *reducer*) [4] to reduce the diameter of the main PA (Figure 2). In this case, the main clinical questions concern the understanding of the flow patterns and the pressure gradients along the artery after implantation and of the forces acting on the reducer, in order to assess the long-term stability of the device.

Thanks to the advances in medical imaging, which allows extremely accurate three-dimensional reconstructions of vasculatures, *patient-specific* models are able to describe the blood flow in very complex shapes. However, increasing the resolution of the computational domain also increases the number of *degrees of freedom* of the solution, i.e., the dimension of the discrete problems to be solved, and thus the overall computational time for the simulation. This is still an important issue in medicine, where delivering results in a reasonable time is a critical aspect in the applications. This article describes two approaches for reducing the complexity of patient-specific simulations using *reduced-order modeling* (ROM), in which the dimension of the discrete problems is drastically reduced by seeking the solution as a combination of basis functions accounting for the main geometrical and physical characteristic of the flow field. In particular, the generation of ROM for the simulation of hemodynamics in ToF patients and for the design of artificial pulmonary valves will be discussed.



**Fig. 1:** Sketch of the pulmonary circulation showing the location of the pulmonary artery (green) and pulmonary valve (orange)



**Fig. 2:** Top: the artificial valve; bottom: the stent implanted to reduce the outflow tract diameter [4]

### Blood flow modeling in the pulmonary artery

For defining a mathematical model of pulmonary blood flow, the first step consists in describing the pulmonary arteries via a three-dimensional domain  $D$ , whose boundary is decomposed as

$$\partial D = B_{\text{in}} \cup B_{\text{wall}} \cup B_{\text{out}}, \quad (1)$$

denoting the *inlet*, connected to the heart via the right ventricle, the arterial *wall* and the two *outlet* boundaries, connecting to the lungs, respectively (Figure 3). The blood is modeled as an incompressible, Newtonian fluid, obeying the three-dimensional Navier–Stokes equations, formulated in terms of a velocity  $\mathbf{u}$  and a pressure  $p$ :

$$\begin{cases} \rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \mu \operatorname{div} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) = 0 & \text{in } D \times (0, T], \\ \operatorname{div} \mathbf{u} = 0 & \text{in } D \times (0, T]. \end{cases} \quad (2)$$

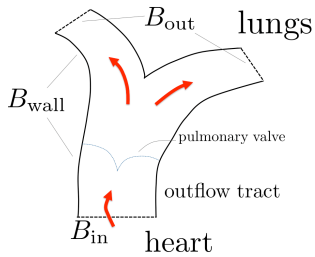
in a time interval  $(0, T]$  (e.g., the duration of a heart beat). In (2),  $\rho$  stands for the blood density ( $1 \text{ g/cm}^3$ ), while  $\mu$  denotes the blood dynamic viscosity ( $0.035 \text{ Poise}$ ). The system (2) is completed by the following boundary conditions on  $\partial D$ :

- On the inlet boundary  $B_{\text{in}}$ , a given velocity profile or a given pressure pulse is imposed. These data can be usually approximated from medical measurements of mean flows and mean pressures.
- *No-slip* boundary conditions (zero velocity) are imposed on the arterial wall  $B_{\text{wall}}$ .
- On the outlet boundary  $B_{\text{out}}$ , a pressure is imposed, which is computed dynamically as a function of the outgoing flux. With this approach, the effect of the neglected downstream vasculature can be taken into account through a simplified model.

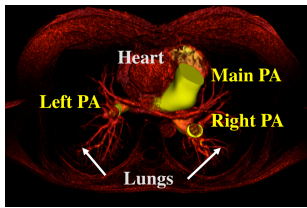
In practice, the domain  $D$  is obtained via a *segmentation*, i.e. reconstructing the patient-specific surface starting from a set of medical images (Figure 4). Then, the computational domain is generated discretizing the three-dimensional space in tetrahedral elements using the mesh generator TetGen. In order to solve problem (2) numerically, the two equations are first discretized uniformly in time. Next, at each time step the solution is computed using a finite element method, in which velocity and pressure are approximated by piecewise polynomials on each tetrahedron. In particular, using piecewise linear approximations, the dimension of the discrete space in which the solution is sought is proportional to the number of vertices of the tetrahedral mesh (one unknown for pressure and three unknowns for the velocity at each vertex).

### Proper orthogonal decomposition

Let  $\mathcal{U} = \{\mathbf{u}(t_1), \mathbf{u}(t_2), \dots, \mathbf{u}(t_M)\}$  denote a set of *snapshots* of the finite element solution to (2) for the blood velocity at times  $t_1, \dots, t_M$ . Each snapshot is a function belonging to the chosen finite element space, whose dimension depends on the discretization. For instance, if the solution is approximated by piecewise linear finite elements, the snapshots are defined by their values at the vertices of the tetrahedra. Hence, each function  $\mathbf{u}(t_i)$  belongs to a discrete space of dimension proportional to the number of vertices in the mesh, denoted by  $N$  in what follows.



**Fig. 3:** Sketch of the computational domain



**Fig. 4:** 3D rendering after segmentation of a patient's pulmonary artery surface (in yellow), taken from [3]



A proper orthogonal decomposition (POD) of the set  $\mathcal{U}$  (see, e.g., [5]) consists in finding a set of basis functions (orthogonal w.r.t. a given scalar product) that, even containing a small number of elements, typically much lower than the dimension of the finite element space, can represent the snapshots sufficiently well. In other words, the goal of POD consists in finding a set  $\{\phi_r(\mathbf{x}), \phi_r : D \rightarrow \mathbb{R}^3, r = 1, \dots, R\}$  (called a *POD basis*) and a set of coefficients  $\{a_{i,r}, i = 1, \dots, M, r = 1, \dots, R\}$ , that minimize the sum

$$\sum_{i=1}^M \left\| \mathbf{u}(t_i)(\mathbf{x}) - \sum_{r=1}^R a_{i,r} \phi_r(\mathbf{x}) \right\|^2 \quad (3)$$

according to a spatial norm that determines in which sense the best approximation is sought. Using the orthonormality of the basis  $\{\phi_r(\mathbf{x})\}_r$ , the minimization problem (3) can be rewritten as an eigenvalue problem in  $\mathbb{R}^N$  for a matrix  $U$  whose columns are defined by the snapshots:

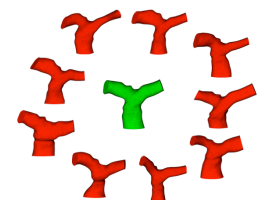
$$UU^T S \phi_r = \lambda_r \phi_r, \quad r = 1, \dots, R, \quad (4)$$

where the matrix  $S$  is defined by the inner products on the discrete space. A similar approach can be used to obtain a reduced-order model for the pressure [2]. Once having computed the POD bases for pressure and velocity, problem (2) can be discretized using only a subset of the POD bases, instead of the full finite element space of dimension  $N$ . In practice, the snapshot set can be very well approximated even by a small number of basis functions (often of the order of ten up to hundred) so that each time step only requires the solution of two small linear systems.

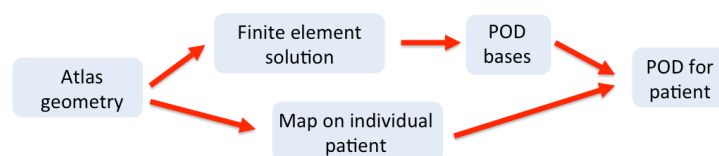
### Atlas-based reduced-order modeling

In the first application, let be given a set of pulmonary artery surfaces reconstructed from several ToF patients. Although the topologies of the blood vessels are similar, the individual shapes might differ considerably among each other. In this case, statistical image analysis allows to create a so-called *atlas* of the patient set, e.g., a sort of average patient (Figure 5). Hence, the key idea is to use the information about the fluid solution on the atlas geometry in order to precompute suitable reduced-order models for the individual patients (Figure 6).

First, the finite element solutions for velocity and pressure on the atlas geometry were computed, extracting the corresponding POD bases. Second, in order to generate a suitable POD basis for each individual patient geometry, the atlas POD bases were mapped onto the new meshes.



**Fig. 5:** Subset of the available patient surfaces (red) and the corresponding atlas (green)

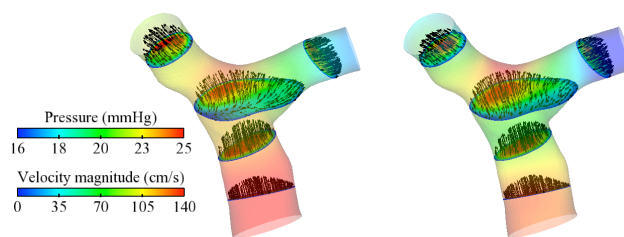


**Fig. 6:** The offline steps for computing a patient POD basis using the information on the atlas geometry

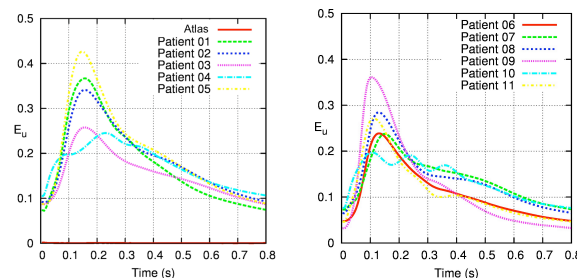
For this step, first a one-to-one mapping of each patient surface onto the atlas surface was computed. Then, this surface displacement was extended to the nodes of the three-dimensional domain via a nonlinear approximation computed solving a sequence of linear problems. This volume

mapping between these meshes was generated with the property that it preserves the topology of the mesh, i.e., mapping nodes on nodes and tetrahedra on tetrahedra. This procedure allows to define the individual POD bases for the pressure and the velocity on each individual patient via a *local* coordinate change (i.e., for each element of the mesh) to the atlas POD basis [3]. Using the individual POD bases, the fluid problem on the patient-specific domain can be formulated directly in terms of a reduced model.

Since all these steps can be performed *offline*, e.g., once for all before the simulation, the *online* computational effort, i.e., the operations needed at each simulation time step, reduces to the solution of two small linear systems for the velocity and the pressure. In preliminary numerical tests, reduced-order models with only 50 basis functions were able to decrease the simulation time by a factor of four. In order to validate the results also in terms of accuracy, the velocity and pressure fields obtained with the POD bases were compared with the numerical results of full finite element simulations on the individual patients.



**Fig. 7:** Velocity cut at two selected time steps comparing the results of a full finite element model (left) and of a POD formulation on a particular patient; cross sections are colored according to velocity magnitude, while the pressure profile is shown along the arterial boundary

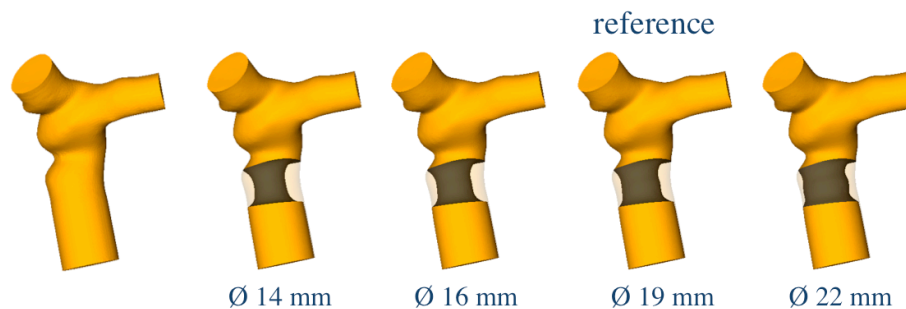


**Fig. 8:** Validation of the POD simulation on 11 patients

Figure 7 shows the comparison between the full finite element and the reduced solution for a selected patient. A more detailed validation is provided in Figure 8, which shows the relative differences (in  $L^2$ -norm) between the finite element solutions and the solution computed using, on each patient, the corresponding POD bases mapped from the atlas geometry.

### Efficient design study for artificial valves

The second application of the reduced-order modeling concerns surgery planning and implant optimization for ToF patients. In particular, the POD bases were used for performing a fast finite element analysis of devices composed of a reducer stent and an artificial valve (see Figure 2) with different geometrical parameters. To this aim, computational models of stents with different diameters were generated smoothly deforming the mesh of a *reference* device (Figure 9).



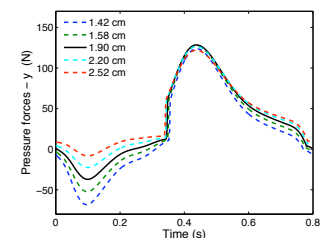
**Fig. 9:** Computational models of a ToF patient before the implantation of an artificial valve (leftmost picture) and of devices with different diameters (14 to 22 mm)

By construction, the resulting meshes for the different devices have exactly the same topology as the original one. A reduced-order model can hence be precomputed by solving only once the Navier–Stokes equations on the pulmonary artery with the reference device (diameter of 19 mm), then extracting the POD bases for velocity and pressure and mapping them on the new configurations through a proper coordinate change (as described in Figure 6). Then, the fluid solution on each configuration can be efficiently computed through a reduced-order model.

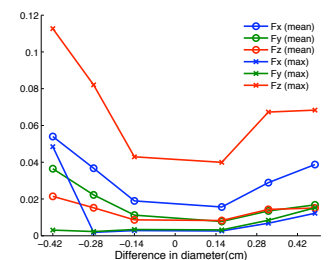
For this application, clinicians are particularly interested in quantifying the hydrodynamical forces acting on the artificial valve in the different cases, in order to estimate its long-term stability (Figure 10), and in the flow rates within the PA branches, after the implantation, in order to assure a correct post-operative pulmonary circulation. Hence, in order to assess the properties of the reduced-order model, both full finite element simulations and POD simulations were run on the geometries with different device diameters, comparing then the resulting pressure forces on the implant. Figure 11 shows that, although in all cases the POD basis is computed *offline* using only the results on the reference domain, the discrepancies in pressure forces are below 5%, reaching 10% only in the case of the configuration with the largest deformation. However, POD simulations reduced the computational time by up to a factor of four.

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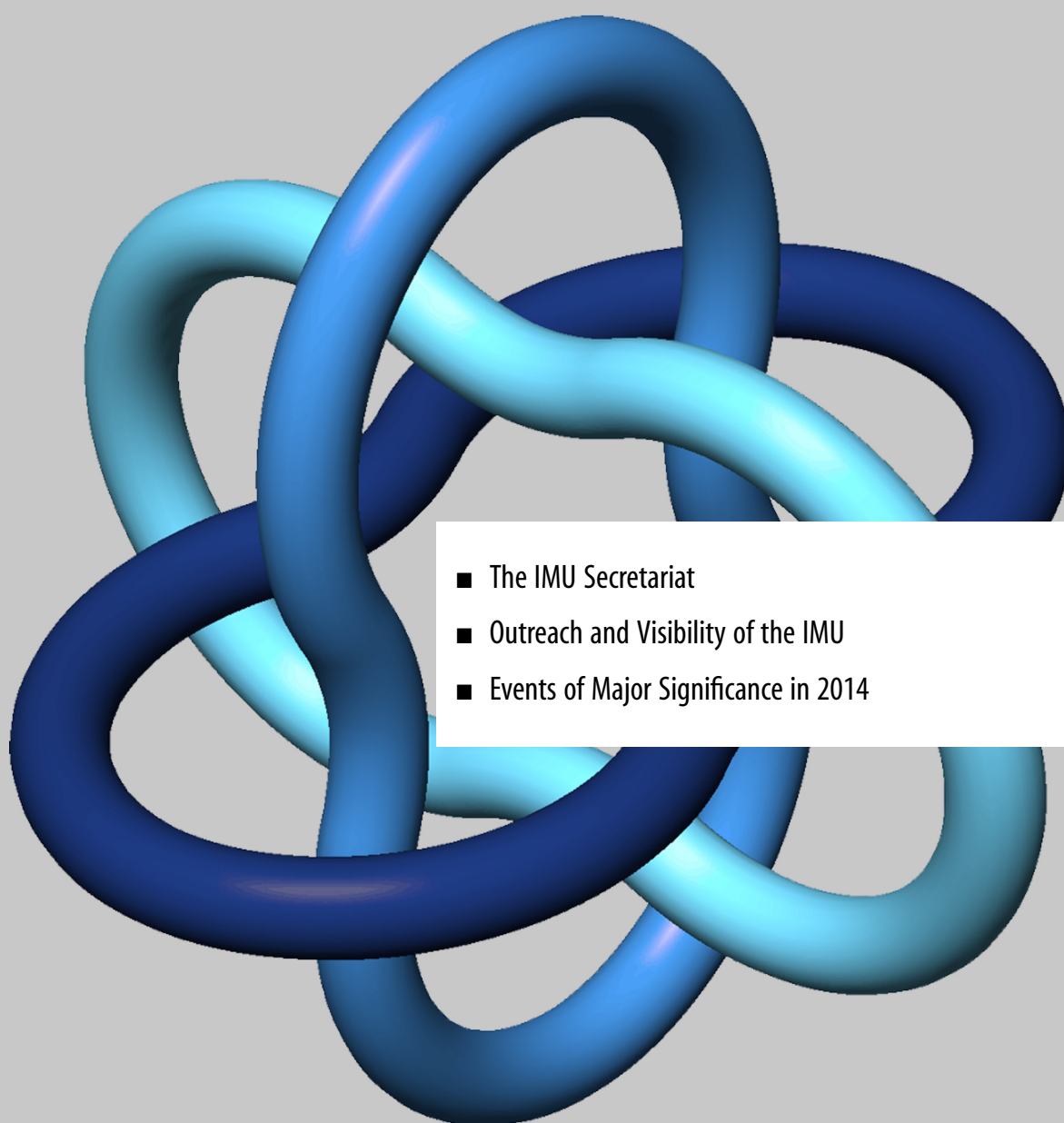
**Fig. 10:** Pressure forces during a cardiac cycle for devices of different diameters



**Fig. 11:** Difference between finite element and POD simulations in pressure forces for devices of different diameters



# 3 IMU@WIAS



- The IMU Secretariat
- Outreach and Visibility of the IMU
- Events of Major Significance in 2014

### 3.1 The IMU Secretariat

*Sylvia Markwardt*

Since January 2011, the Secretariat of the International Mathematical Union has been permanently based in Berlin, Germany, at the Weierstrass Institute. Under the supervision of the IMU Executive Committee, the Secretariat runs IMU's day-to-day business and provides support for many IMU operations, including administrative assistance for the International Commission on Mathematical Instruction (ICMI) and the Commission for Developing Countries (CDC). The IMU Secretariat also hosts the IMU archive.

For the first time in its almost 100-year history, IMU has a permanent secretariat. In the past, IMU conducted its business at the institution of the IMU Secretary which usually also served as the legal domicile of IMU. At the General Assembly 2010 in Bangalore, India, the Weierstrass Institute in Berlin was elected as the host institution of the permanent secretariat. The operation of the secretariat is supported by grants from the German Federal Ministry of Education and Research (BMBF) and the State of Berlin.



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

Staff members (Figure 1):

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

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

Lena Koch, *ICMI/CDC Administrator*. L. Koch is responsible for supporting administratively the activities of the Commission for Developing Countries and the International Commission on



Mathematical Instruction. She is, in particular, in charge of promoting the work of both commissions, managing their Web presence including public relations and communication, handling grant applications and support programs.

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

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

Gerhard Telschow, *IT and Technical Support*. G. Telschow is responsible for running the IT operations of the IMU Secretariat. This includes taking care of running the hardware and software infrastructure, in particular, the IMU server and mailing lists and planning the extension of IMU's IT services for its members, commissions and committees.

Helge Holden (not in the picture) is the new IMU Secretary (see page 61).

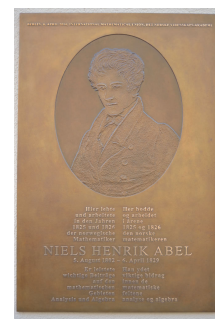
The Secretary is responsible for conducting the ordinary business of the Union and for keeping its records.

## 3.2 Outreach and Visibility of the IMU

Important events took place in “IMU's life” in 2014. After four years of preparation, the International Congress of Mathematicians (ICM) 2014 was held. Preceding the ICM, the IMU organized its 17th meeting of the General Assembly where account was given on the previous four-year term and IMU's leadership and development for the next four-year term were decided. The “Mathematics in Emerging Nations: Achievements and Opportunities” (MENA0) Symposium was organized. And IMU commemorated Niels Henrik Abel in Berlin. The events are described in more detail below in chronological order.

### Abel commemorative plaque

The Norwegian mathematician Niels Henrik Abel (1802–1829), famous for his results in the fields of analysis and algebra (the abelian groups, abelian manifolds, or abelian integrals are named after him), has been living and working in Berlin in the years 1825 and 1826. During this period, Abel was supported by August Leopold Crelle who published mathematical articles of Abel in his “Journal für die reine und angewandte Mathematik” (Journal for the Pure and Applied Mathematics). It was in Berlin and especially thanks to the support of Crelle that Abel had his scientific breakthrough internationally. Norway pays tribute to this fact, among other things, by inviting the winning team of each “Tag der Mathematik” (mathematics competition for pupils annually taking



**Fig. 1:** Abel commemorative plaque

place in Berlin) to the Abel Prize award ceremony in Oslo. Since 2003, the Norwegian Academy of Science and Letters (DNVA) has been awarding the Abel Prize which is besides the Fields Medal the most prestigious award in mathematics.

The International Mathematical Union, in cooperation with the Norwegian Academy of Science and Letters, commemorated Abel's stay in Berlin and created a bronze plaque (Figure 1) that was mounted on the facade of the house at *Am Kupfergraben 4A, 10117 Berlin*, where Abel used to live. The inauguration (Figure 2) of the plaque was on April 6, 2014, the 185th anniversary of Abel's death; present were Sven Erik Svedman, Ambassador of the Royal Norwegian Embassy in Berlin, Øivind Andersen, Secretary General of the DNVA, Helge Holden, President of the Niels Henrik Abel Board, Tom Lyche, University of Oslo, Martin Grötschel, Secretary of the IMU, Jürg Kramer, President of the German Mathematical Society (DMV), Jürgen Sprekels, Director of WIAS, representatives of the Berlin mathematical community, and Erika Klagge who designed the plaque.



**Fig. 2:** Inauguration of the plaque on April 6, 2014

## IMU General Assembly 2014

**About the IMU General Assembly.** The General Assembly (GA) is the main body of the International Mathematical Union. It admits IMU members, elects the IMU officers and the members of the IMU Executive Committee, establishes commissions and the budget, and decides about the IMU statutes, the rules of conduct, and many other issues. The GA consists of Delegates appointed by the IMU Adhering Organizations, together with the members of the Executive Committee, and of the Representatives of Associate and Affiliate Members. Guests and observers may be invited additionally. Only Delegates have voting rights. The IMU Statutes contain a detailed description of the rights and duties of the GA. The GA normally meets once in four years, usually at a place and date close to an International Congress of Mathematicians.

**IMU GA 2014.** In 2014, the 17th meeting of the IMU General Assembly took place from August 10 to 11 in Gyeongju, Korea. The agenda of this GA meeting covered, among other things, the following items: appointment of the Credentials Committee, the Finance and Dues Committee, the Election Committee, the Resolutions Committee, and the Tellers Committee. These committees are very important for the proper functioning of the GA meeting. Other items were: review of the activities of the Union, Finances and Dues, Resolutions; presentation of the slates and election of the officers for the IMU Executive Committee (EC), the Commission for Developing Countries (CDC), and the International Commission on the History of Mathematics (ICHM) for the term 2015–2018; report of the ICM 2014 Program Committee; reports of Affiliate IMU members and IMU-related organizations; report of the Office Committee; the decision on the location of the International Congress of Mathematicians 2018; IMU membership issues.



**Fig. 3:** Impressions from the IMU General Assembly 2014

#### Elected IMU Executive Committee for the term 2015–2018.

- *IMU President:* Shigefumi Mori (Japan)
- *IMU Secretary:* Helge Holden (Norway)
- *IMU Vice Presidents:* Alicia Dickenstein (Argentina), Vaughan Jones (New Zealand/USA)
- *IMU Members at Large:* Benedict H. Gross (USA), Hyungju Park (Korea), Christiane Rousseau (Canada), Vasudevan Srinivas (India), John Toland (UK), Wendelin Werner (Switzerland)
- *Ex Officio:* Ingrid Daubechies (USA)

#### Elected Commission for Developing Countries for the term 2015–2018.

- *CDC President:* Wandera Ogana (Kenya)
- *CDC Secretaries:* C. Herbert Clemens (USA) (Policy), Srinivasan Kesavan (India) (Grant Selection)
- *CDC Members:* Alf Onshuus (Colombia), Mama Foupouagnigni (Cameroon), Polly Sy (Philippines), Budi Nurani Ruchjana (Indonesia), Angel Pineda (USA/Honduras), Angel Ruiz (Costa Rica)
- *Ex Officio:* Shigefumi Mori (Japan)

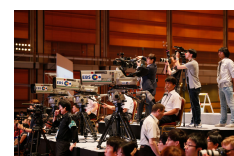
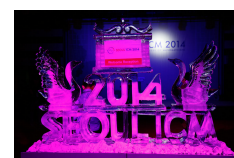
#### Elected International Commission on the History of Mathematics for the term 2015–2018.

- Ciro Ciliberto (Italy)
- Shrikrishna G. Dani (India)

**ICM 2018.** The GA decided that the International Congress of Mathematicians 2018 will be held in Rio de Janeiro, Brazil, August 2018.

#### International Congress of Mathematicians 2014 – ICM 2014

**About the International Congress of Mathematicians (ICM).** The scientific prizes awarded by IMU are the highest distinctions in the mathematical world, and they are presented in the opening ceremony of an ICM: Fields Medals (two to four medals have been given since 1936), the Rolf Nevanlinna Prize (since 1986), the Carl Friedrich Gauss Prize (since 2006), and the Chern Medal Award (since 2010). At the closing ceremony of the ICM, the Leelavati Prize, sponsored by Infosys, for excellence in mathematical outreach is awarded (since 2010).



**ICM 2014.** ICM 2014 took place in Seoul, Republic of Korea, from August 13–21, 2014. The IMU prizes of 2014 were presented on August 13, 2014, during the Opening Ceremony of ICM 2014 by Park Geun-hye, the Honorable President of Korea.

**Fields Medal 2014.** To recognize outstanding mathematical achievement for existing work and for the promise of future achievement.

- Artur Avila (France/Brazil)
- Manjul Bhargava (USA)
- Martin Hairer (UK)
- Maryam Mirzakhani (USA)

**Rolf Nevanlinna Prize 2014.** For outstanding contributions in Mathematical Aspects of Information Sciences.

- Subhash Khot (USA)



**Carl Friedrich Gauss Prize 2014.** For outstanding mathematical contributions with significant impact outside of mathematics.

- Stanley Osher (USA)



**Chern Medal Award 2014.** Is awarded to an individual whose accomplishments warrant the highest level of recognition for outstanding achievements in the field of mathematics.

- Phillip Griffiths (USA)

**Leelavati Prize, sponsored by Infosys 2014.** For outstanding contributions for increasing public awareness of mathematics as an intellectual discipline and the crucial role it plays in diverse human endeavors.

- Adrián Paenza (Argentina)

### MENAO Symposium at ICM 2014

*Alan Anderson and Lena Koch*



The status of mathematics development efforts has been described in three “regional reports” covering Mathematics in Africa, Southeast Asia, and Latin America and the Caribbean and its challenges and opportunities. These reports were presented at the MENAO symposium. In August 2014, the IMU held a day-long symposium prior to the opening of ICM 2014, entitled Mathematics in Emerging Nations: Achievements and Opportunities (MENAO). More than 250 participants from around the world, including representatives of embassies, scientific institutions, private business, and foundations attended the symposium.

Attendees heard inspiring stories from individual mathematicians and from several developing nations that have progressed substantially in mathematics over the last half-century. A parallel poster session featured the work of sixteen international centers, projects, commissions, foundations, and initiatives supporting mathematicians and mathematics educators. During MENAO, IMU President Ingrid Daubechies officially announced that the five inaugural laureates of the *Breakthrough Prize in Mathematics* would each give \$100,000 for a new IMU fellowship and mentorship program for talented young mathematicians from some of the least developed countries.

**A vision of mathematics' power.** The symposium showed that a mathematically educated population is a powerful force to spur economic development in all nations. Major challenges, such as disease, hunger, climate change, environmental degradation, and energy development, require strong mathematical, computational, statistical, and other quantitative skills.

Given such challenges, more support is needed for those who wish to become educators and researchers in mathematics. Raising international mathematical literacy has been a goal of the IMU since its founding, but the resources to achieve such a goal have been—for the majority of the history of the IMU—insufficient. IMU has recently initiated a drive for public and private sector funding to allow it to take a more active role in supporting mathematics in developing countries. In that context, the goals of the MENAO symposium were not only to hear the stories from the developing world but also to build partnerships and networks between mathematical communities, their governments, international agencies, private business, and foundations.

The symposium demonstrated the importance of mathematics to economic and social development in several countries and concluded that supporting mathematics and mathematics education in the developing world requires concerted efforts of mathematicians and the public and private sectors.

### 3.3 Events of Major Significance in 2014

#### Grants

**IMU won ICSU grant 2014.** IMU's application to ICSU (International Council for Science) for a €30,000 grant was successful. The grant project was entitled "East African Capacity and Network Project", supporting applicants were ICMI, UNESCO, the ICSU Regional Office for Africa (ICSU ROA), the Tanzania Commission for Science and Technology (COSTECH), the Aga Khan University Institute for Educational Development East Africa, Dar es Salaam, Tanzania (AKU), and the African Academy of Sciences (AAS).

## Meetings

**ICMI Study 23 IPC meeting.** The International Program Committee for ICMI Study 23 “Primary Mathematics Study on Whole Numbers” held its meeting at the IMU Secretariat in Berlin from January 19–24, 2014 (Figure 1). The ICMI Study Series is a major program of the International Commission on Mathematical Instruction (ICMI). Each study initiated by ICMI addresses an issue or topic of significance in contemporary mathematical education, and is conducted by an international team of leading scholars and practitioners; see <http://www.mathunion.org/icmi/conferences/icmi-studies/introduction/>.



**Fig. 1:** ICMI Study 23 IPC meeting

**CEIC meeting.** The Committee on Electronic Information and Communication (CEIC) held its annual meeting at the IMU Secretariat in Berlin from July 12–13, 2014. The CEIC is a standing committee of the IMU Executive Committee (EC). CEIC’s mandate is to advise the EC on matters concerning information and communication; see <http://www.mathunion.org/ceic/>.

## Events

**Inauguration of the Abel Commemorative Plaque.** A bronze plaque commemorating the Norwegian mathematician Niels Henrik Abel was inaugurated on April 6, 2014, the 185th anniversary of Abel’s death. The plaque is a joint project of the International Mathematical Union and the Norwegian Academy of Science and Letters. See also 3.2.

**Heidelberg Laureate Forum.** The second Heidelberg Laureate Forum (HLF) took place from September 21–26, 2014, 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. Manjul Bhargava and Martin Hairer, recipients of the 2014 Fields Medal at the ICM in August 2014 were among the laureates attending this year’s HLF.



**Guests of the IMU Secretariat.** The table below gives an overview of guests who visited the IMU Secretariat in 2014.

Date	Guests	Event
Jan. 19 – 24	Abraham Arcavi, Israel; Ferdinando Arzarello, Italy; Sybilla Beckmann, USA; Mariolina Bartolini Bussi, Italy; Sarah Gonzales, Dominican Republic; Roger Howe, USA; Maitree Imprasitha, Thailand; Berinderjeet Kaur, Singapore; Joanne Mulligan, Australia; Jarmila Novotna, Czech Republic; Xuhua Sun, China; Hamsa Venkatakrishnan, South Africa; Lieven Verschaffel, Belgium	ICMI Study IPC
Jan. 21 – 23	Guillermo Curbera, Spain	IMU Archive
Feb. 13	Petra de Bont, Netherlands; Lex Zandee, Netherlands	Individual visit
April 1	Martin Burger, Germany	Individual visit
April 6	Helge Holden, Norway	Individual visit
April 10	Stefano Angioletti-Uberti, Italy; L. S. Anusha, India; Zhenning Cai, China; Jordi Casanellas, Portugal; Holger Dell, Germany; Chang-Song Deng, China; Azat Gainutdinov, Russia; Matthias Gritschneider, Germany; Guoying Gu, China; Thiem Hoang, USA; Mario Kieburg, Germany; Semyon Klevtsov, Belarus; Maxim Komarov, Russia; Ercan E. Kuruoglu, Italy; Guanjun Liu, China; Alex Markowitz, USA; Rainer Moll, Germany; Vijay Natarajan, India; Carlo Nitsch, Italy; Niurka Quintero, Spain; Sam Sanders, Belarus; David Torres-Teigell, Spain; Erick Trevino, Mexico; Nikki Vercauteren, Switzerland; Qi Wu, China; Ming Xu, China	Alexandervon Humboldt network Meeting
April 25 – 27	Leif Abrahamson, Sweden; Bernd Bank, Germany; Claude Cibils, France; Giulia Di Nunno, Norway; Alice Fialowski, Hungary; Herbert Fleischner, Austria; Gert-Martin Greuel, Germany; Andreas Griewank, Germany; Marie-Françoise Roy-Coste, France; Marta Sanz-Solé, Spain; Barbara Strazabosco, Germany; Joana Teles, Portugal; Olaf Teschke, Germany; Sheung-Tsun Tsou, UK; Bengt-Ove Turesson, Sweden; Paul Vaderlind, Sweden; Begona Vitoriano Villanueva, Spain; Michel Waldschmidt, France; Anders Wandahl, Sweden	EMS Council of Developing Countries
May 7	Ragni Piene, Norway	Individual visit
May 12 – 20	Bernard Hodgson, Canada	ICMI Archive
May 27	Mihyun Kang, Austria	Individual visit
July 12 – 13	Thierry Bouche, France; Olga Caprotti, Finland; Tim Cole, USA; James Davenport, UK; Carol Hutchins, USA; László Lovász, Hungary; Peter Olver, USA; Ravi Vakil, USA	CEIC meeting
Sep. 30	Livia Giacardi, Italy	ICMI Archive
Dec. 15 – 16	Helge Holden, Norway	Individual visit

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

- IMU Executive Committee meeting, Princeton, USA (M. Grötschel, S. Markwardt, A. Mielke)
- ICMI Klein workshop, Rio de Janeiro, Brazil (L. Koch)
- ICMI Executive Committee meeting, Rio de Janeiro, Brazil (L. Koch)
- Abel Prize events, Oslo, Norway (M. Grötschel, A. Mielke)
- IMU General Assembly, Gyeongju, Korea (M. Grötschel, S. Markwardt, A. Mielke)
- International Congress of Mathematicians ICM 2014, Seoul, Korea (M. Grötschel, L. Koch, S. Markwardt, A. Mielke, A. Orłowsky, B. Seeliger, G. Telschow)
- MENAO Symposium, Seoul, Korea (M. Grötschel, L. Koch, S. Markwardt, A. Orłowsky)
- Heidelberg Laureate Forum, Heidelberg, Germany (M. Grötschel, L. Koch)



#### The IMU Secretariat from the perspective of the IMU.

John Toland who presented the report of the IMU Office Committee to the IMU General Assembly 2014 made the following résumé:

*“The benefits of these modern efficient office facilities and highly motivated professional staff at no cost to IMU cannot be exaggerated. They have already transformed the work of the IMU Executive Committee, Commissions and Committees.”*

(According to the Memorandum of Understanding between the IMU and WIAS, it is the purpose of the IMU Office Committee, which is not part of the Secretariat, “to monitor the performance of the IMU Secretariat on behalf of the IMU Executive Committee and Adhering Organisations.”)

The IMU General Assembly showed its appreciation of the IMU Secretariat by passing Resolution 3 that reads as follows:

#### Resolution 3

*“The General Assembly of the IMU thanks Alexander Mielke, Sylwia Markwardt, Lena Koch, and all the other staff at the IMU Secretariat in Berlin for their dedicated work and for all their multiple contributions to the IMU.”*

# 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 & Analysis of Phase Transitions*
- YSG *Modeling of Damage Processes*
- LG 3 *Mathematical Models for Lithium-ion Batteries*
- LG 4 *Probabilistic Methods for Mobile Ad-hoc Networks*
- ERC 1 *EPSILON*
- ERC 2 *EntroPhase*

## 4.1 Research Group 1 “Partial Differential Equations”

The objective of this research group is the analytical understanding of partial differential equations and 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 semiconductors; in particular, organic semiconductors and optoelectronic devices
- 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:

- 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
- Existence, uniqueness, and regularity theory for initial and boundary value problems in non-smooth domains and with nonsmooth coefficients, thereby also including nonlocal effects
- Coupling of different models; in particular, coupling of surface and volume effects
- Iterative and variational methods using physically motivated energetic formulations

The qualitative study of partial differential equations provides a deeper understanding of the underlying processes and has a considerable impact on 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.

### Analysis of multiscale systems driven by functionals



European Research Council  
Established by the European Commission

The ERC project “Analysis of multiscale systems driven by functionals” is devoted to the study of evolution problems driven by energy or entropy functionals, which act on a state space with a Hamiltonian, Riemannian, or Finslerian structure and to systems arising from the coupling of these dynamics. In particular, such coupled problems may include several spatial or temporal scales.

Some recent results are presented in the Scientific Highlights article on page 35, for example, a limit passage from the Swift–Hohenberg to the Ginzburg–Landau equations and the definition and analysis of balanced-viscosity solutions for rate-independent systems. In particular, these results use the notion of *evolutionary  $\Gamma$ -convergence* or *E-convergence*, which helps to transfer the theory of  $\Gamma$ -convergence known from the calculus of variations to evolution problems.

A focus of the project lies on the analysis of applications from material modeling and optoelectronics. One part of it is concerned with the mathematical study of Maxwell–Bloch-type systems. Using their GENERIC structure, reduced models were derived coupling the evolution of the amplitude of an electromagnetic wave with the evolution of the inversion density. For these systems, results on the existence of solutions and their long-time behavior can be proved.

In another part of the project, heterogeneous thin films are studied, combining homogenization and dimension reduction of functionals with differential constraints. It is shown that the lower-dimensional effective limit models depend critically on the relative magnitude between the two scales of film thickness and material heterogeneities. In particular, an explicit example indicates that if the heterogeneities are larger than the film thickness, the limit behavior is nonlocal, so that the energy of the limit cannot be expressed in terms of an integral functional.

Yet another part is devoted to the study of the time evolution of elastoplastic materials in the context of rate-independent processes, with a focus on the interplay between dynamics and relaxation effects. If the dissipation functional for this system includes discontinuities, which is normally the case in relevant applications, relaxation is expected to result in a nontrivial interaction between energy and dissipation, as well as in a critical dependence on the full deformation history. To support this thesis, an antiplane model in linearized elastoplasticity is investigated, with two active slip systems, infinite cross-hardening, and a dissipation with a monotonicity constraint using the two different concepts of Young measure relaxation and  $\Gamma$ -limit expansion of weighted energy-dissipation (WED) functionals.

In [1], the asymptotic behavior of rigid bodies is studied, which contain a cavity filled by a viscous Navier–Stokes liquid. The system has a mixed dissipative and Hamiltonian structure because the kinetic energy is dissipated due to viscosity and fluid motion, and the modulus of angular momentum is conserved. For a general class of geometries, a rigorous proof of Zhukovskiy’s theorem is given, which states that in the limit of time going to infinity the body will rotate around one of the principal axes of inertia.

### Regularity theory for differential operators and geometric measure theory

In last years, it became apparent that geometric measure theory is an adequate instrument to improve regularity results for elliptic and parabolic operators. With the focus on applied problems, which include mixed boundary conditions, one succeeded in the meanwhile to pass from previously more topological conditions for the Dirichlet part of the boundary to measure-theoretic conditions. As before, bi-Lipschitzian charts are needed for the points of the (closure of the) Neumann boundary, but a much weaker condition suffices for the Dirichlet part, namely the Ahlfors–David condition, i.e., if  $d$  is the space dimension, then  $D$  is  $(d - 1)$ -set in the spirit of Jonsson/Wallin. Under these conditions, the following results could be proved in the last years:

- I) Interpolation on the scale of spaces  $\{W_D^{1,q}(\Omega)\}_q$  performs as in the case where  $\Omega$  is the unit ball in  $\mathbb{R}^d$  and  $D$  is the whole boundary of  $\Omega$ .
- II) Gröger’s isomorphism theorem  $-\nabla \cdot \mu \nabla + 1 : W_D^{1,q}(\Omega) \rightarrow W_D^{-1,q}(\Omega)$  can be reproduced for  $q$  close to 2 in this geometrically wider context.
- III) Under the above conditions on the boundary, Hardy’s inequality was proved for  $W^{1,q}$  functions  $u$  with partially vanishing trace on the Dirichlet boundary part  $D$ .
- IV) Having III) at hand, one succeeds by following an idea of Pascal Auscher to develop a Calderon–Zygmund decomposition for functions on  $\Omega$  with trace-zero condition on  $D$ , *respecting this trace condition*. This idea is one of the essential ingredients for the proof that  $(-\nabla \cdot \mu \nabla + 1)^{1/2} :$

$L^q(\Omega) \rightarrow W_D^{-1,q}(\Omega)$ ,  $q \in [2, \infty]$ , is a topological isomorphism. This isomorphism property allows to carry over relevant properties of the operators  $-\nabla \cdot \mu \nabla$ , known when they act on  $L^p$  spaces, to the spaces of the  $W_D^{-1,q}(\Omega)$  scale. The most important consequences are here the *existence of a bounded holomorphic calculus* and *maximal parabolic regularity*. The latter is also to be seen, in the light of the results of Clement, Li, and Prüss, as an extremely general and most effective tool for the treatment of *nonlinear parabolic equations*.

V) Lastly, a condition, similar, but slightly more restrictive than the (lower) Ahlfors–David condition, together with the *outer volume condition* for the whole domain  $\Omega$ , leads to a reproduction of the classical Hölder regularity results for elliptic second-order divergence operators—as could be shown jointly with Tom terElst (Auckland). Here, even suitable Hölder properties could be proved for the heat kernels of the corresponding semigroup—which has been, in this generality, an outstanding problem for many years.

### Material modeling

The research in this field deals with the mathematical modeling and the analysis of the elastic behavior of solids undergoing dissipative processes. This research 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*.

**Shape memory alloys, elastoplasticity, and damage.** The MATHEON project C18 “Analysis and numerics of multidimensional models for elastic phase transformations in shape memory alloys” ended in May 2014. In its last period, rate-independent models for dimension-reduced shape memory alloys were studied. Moreover, by means of  $\Gamma$ -convergence, non-interpenetration conditions in linearized hyperelasticity for materials with cracks were derived in general space dimensions.

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”, which expired in December 2014. In its last phase, the evolution of a rate-independent system within a non-convex energy landscape modeling phase separation was studied. Using an evolutionary version of  $\Gamma$ -convergence, an effective macroscopic model was identified. It was shown that this macroscopic model incorporates the essential information of the microstructure evolution and, at the same time, allows for a numerical approximation in a finite element framework. But non-convexity in the energy landscape plays a role in “pure” elasticity as well. Here, the effective macroscopic energy is the essential object, yet hard to determine in general. In [2], a new characterization is given for the structure of the quasiconvex hull in the regime of planar elasticity. This result helps to characterize macroscopic strain tensors, which are states of minimal energy and, hence, give information about the effective macroscopic energy.

October 2014 was the start of the project “Finite element approximation of functions of bounded

**MICROPLAST**



variation and application to models of damage, fracture, and plasticity” within the DFG Priority Program 1748 “Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis”, funded by the German Research Foundation. This is a joint project with Sören Bartels (U Freiburg) funding one full position for the period 10/2014–09/2017. The aim of this project is to establish reliable and efficient numerical methods for models of solids with spatial discontinuities caused by the evolution of dissipative processes, such as plasticification, damage or fracture. In particular, the project focuses on such prototypical models that use the class of functions of bounded variations (BV) to describe mathematically the discontinuities. This class guarantees the convergence to a solution of the infinite-dimensional model and for which iterative solution methods can be constructed. Emphasis is on unregularized numerical approaches that lead to sharp approximations of discontinuities on coarse grids and rigorous convergence proofs. The main objectives are the development, analysis, and implementation of finite element methods for model problems describing discontinuities in BV. This approach includes the derivation of a priori and a posteriori error estimates as well as the construction of adaptive and extended approximation methods for BV-prototype models such as the Rudin–Osher–Fatemi and the Mumford–Shah model. The techniques will be transferred to analytically justified and closely related models for the description of rate-independent inelastic processes, in particular, perfect plasticity, damage and fracture.

Such a model for rate-independent, brittle delamination with spatial BV-regularization, where the internal variable is the characteristic function of a set of finite perimeter, has been studied in [3]. In this setup, it was possible to obtain the existence of so-called *local solutions*. While the defining properties of the well-studied energetic solutions consist of a global energy balance and a stability inequality that has to hold jointly for the displacements and the internal variable, local solutions are defined via an upper energy dissipation estimate, and the joint stability splits into a weak formulation of the quasistatic mechanical force balance for the displacements and a semistability inequality for the internal variable. Via an adhesive contact approximation incorporated in an alternate minimization scheme, the existence of solutions to the time-discrete model is shown. The limit passage to the time-continuous model heavily relies on an additional regularity property of quasiminimizers of the perimeter, which is called a *lower density estimate* and which coincides with the definition of  $(d-1)$ -dimensional sets. Thanks to the fact that this regularity property could be verified for semistable internal variables, it was possible to apply the results on Hardy’s inequality mentioned in the regularity paragraph in order to construct a suitable recovery sequence for the test functions of the quasistatic mechanical force balance and, thus, to pass from time-discrete adhesive contact to time-continuous brittle delamination.

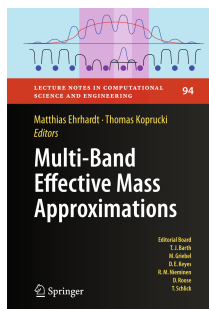
**A coupled reaction-diffusion system on two scales.** The Collaborative Research Center 910 “Control of Self-organizing Nonlinear Systems” was under review in June 2014, and all projects received a very positive recommendation. In particular, the project A5 “Pattern formation in systems with multiple scales” at WIAS will continue another four years starting from January 1, 2015. Within the scope of this project lies the analytical study of nonlinearly coupled reaction-diffusion systems involving different diffusion lengths on the macroscopic and on the microscopic length scales. In 2014, based on a general two-scale homogenization result obtained for reaction-diffusion systems with degenerating diffusion coefficients, convergence rates of the solutions of the approximating



systems towards a solution of the homogenized system were studied by exploiting arguments on the well-preparedness of the initial data and their regularity properties.

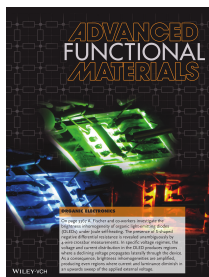
## Semiconductors

Semiconductor nanostructures, such as quantum wells or quantum dots, form the active region of modern optoelectronic devices. Their operation principle relies on quantum mechanical effects. A volume in the Springer series “Lecture Notes in Computational Science and Engineering” [4] has been edited by WIAS in cooperation with BGU Wuppertal addressing mathematical models for the electronic states in semiconductor nanostructures from the most relevant class of  $k$ p-Schrödinger systems. The book covers many interdisciplinary aspects ranging from mathematical modeling to accurate and stable numerical simulation methods.



**Modeling of germanium-on-silicon lasers.** June 2014 was the start of the Einstein Center for Mathematics Berlin (ECMATH)-funded MATHEON project OT1 “Mathematical modeling, analysis, and optimization of strained germanium microbridges”, which is a joint project with the Humboldt-Universität zu Berlin (M. Hintermüller, T. Surowiec), that also involves the close collaboration with the Department for Materials Research at the Leibniz Institute for Innovative High Performance Microelectronics, Frankfurt Oder (IHP). The goal of this project is to make germanium microbridges, integrated on silicon wafers, capable of light emission. The strategy is to suitably increase the optical gain in the germanium by both mechanical strain and high doping. To this aim, mathematical models were established at WIAS, which are based on the van Roosbroeck system for semiconductors coupled with equations for optical fields.

So far, for the description of the optoelectronic properties of strained germanium, a microscopic quantum mechanical model based on tight-binding Hamiltonians has been developed at IHP in collaboration with partners at Pisa University. It allows for the computation of the optical gain in dependence on mechanical strain, doping, and wavelength. To utilize these microscopic gain calculations for device simulation, a special macroscopic gain model adapted to strained germanium is developed, which was implemented into the device simulation package WIAS-TeSCA. First numerical simulations with WIAS-TeSCA affirm that the band structure engineering in germanium via strain and doping optimization is indeed a promising way to go to obtain a germanium laser.



**Electrothermal modeling of organic devices.** In the field of organic semiconductors, the successful cooperation with the Institut für Angewandte Photophysik (TU Dresden) [5] was continued. Additionally, the ECMATH-MATHEON project SE2 “Electrothermal modeling of large-area OLEDs” started in June 2014.

The self-heating of homogeneous organic materials is based on Arrhenius-like conductivity laws and their non-Ohmic current voltage relation. To describe the spatially inhomogeneous current flow in larger inhomogeneous structures with organic layers, the idea is to involve a spatially resolved PDE-based  $p(x)$ -Laplace thermistor model, where  $p = 2$  represents the Ohmic case. In two spatial dimensions and spatially constant  $p > 2$  a priori estimates for the temperature and the

electrostatic potential were verified, and the existence of weak solutions is proved by Schauder's fixed point theorem. For the treatment of the Joule heat term, higher regularity results for problems with  $p$ -structure were exploited.

Moreover, a finite volume approximation of the full PDE model was derived, where the code contains an accurate implementation of the non-standard electrical conductivity law and the Joule heat expression in the case of non-Ohmic materials. Under certain assumptions concerning the device geometry, the resulting scheme coincides with coupled electrical and thermal network models for the description of large area OLEDs used in [5]. Furthermore, a prototype simulation program for  $p$ -Laplace thermistor models based on the in-house software `pdelib2` was established.

Members of the group coorganized the Kick-Off Meeting of the ECMI Special Interest Group "Sustainable energy" at the Technische Universität Berlin and initiated a session on electrical and electrothermal modeling and simulation of organic materials and devices.

**Numerical analysis for reaction-diffusion equations.** In cooperation with the Research Group RG 3 *Numerical Mathematics and Scientific Computing*, Voronoi finite volume discretizations were studied that preserve qualitative properties of the continuous problems at the discrete level. Especially, for reaction-diffusion problems in heterostructures with mass-action-type reversible reactions, uniform energy estimates and global upper and lower bounds for the discrete solutions for classes of Voronoi meshes could be derived; see [6]. As in the continuous case, the uniform bounds were obtained by Moser iteration. In a further paper, these uniform energy estimates were generalized to admissible finite volume meshes by proving a uniform Poincaré-like estimate of the relative free energy by the dissipation rate for implicit Euler, finite volume discretized reaction-diffusion systems. This result was proven indirectly and ensures the exponential decay of the relative free energy with a unified decay rate.

Annegret Glitzky was involved as one of the co-organizers in the preparation and operation of the FVCA7 – The International Symposium of Finite Volumes for Complex Applications VII in Berlin, June 15–20, 2014, whose main organizer was Jürgen Fuhrmann (RG 3).

## Further highlights of 2014

**Second Conference of Women in Leadership Positions.** On October 15, 2014, Marita Thomas participated in the Second Conference of Women in Leadership Positions, which was hosted by Angela Merkel in the chancellery. About 70 women in leadership positions in industry, media, public services, and research, together with about 20 women at the start of their careers in MINT fields (mathematics, information sciences, natural sciences, and technology), were invited to this one-day workshop. This year, it consisted of four parallel morning sessions on the topics "The glass ceiling – What prevents women from taking leadership positions" and "Strategies of companies to attract women for leadership positions". After a joint lunch, the results of the discussions in the morning sessions were presented in a plenary session to the Chancellor Angela Merkel.

**The ISIMM Junior Award.** This award was given to Stefan Neukamm in 2014. The prize is awarded to scientists below 35 years of age for their exceptional contributions towards building a link between Mathematics and Mechanics.

**Mentoring for women scientists in Leibniz institutions.** As in 2011/2012 Marita Thomas, this year, Karoline Disser participated in the “Mentoring for women scientists in Leibniz institutions”

**Einstein Foundation Berlin.** Within the Einstein Foundation program, Dr. Tulkin Rasulov (Bukhara State University, Uzbekistan) and Dr. Chi Vinh Pham (Hanoi University of Science, Vietnam) did an extended research stay in RG 1.

**Young European Probabilists XI: Mass transport in analysis and probability.** Michiel Renger was a co-organizer of this conference that took place in Eindhoven from March 10–14, 2014. The field of optimal transport has recently seen a major boost of activity with many different focal points, including: geometry in discrete/continuous and general metric spaces, Sobolev inequalities and gradient flows, random measures, hydrodynamic limits and large deviations of particle systems, and applications to financial mathematics, kinetic theory, and quantum mechanics. This year's YEP workshop aimed at bringing together promising young European researchers from both analysis and probability.

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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*.

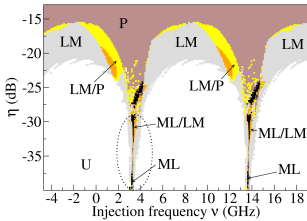
The research group contributes to the application-oriented research topics *dynamics of semiconductor lasers* and *pulses in nonlinear optical media*. External funding was received in 2014 within the DFG Research Center MATHEON (projects D8 and D14), the Collaborative Research Center (SFB) 787 (projects B4 and B5), the Marie Curie Initial Training Network (ITN) PROPHET, the DFG Individual Grant “Ab-initio description of optical nonlinearities in femtosecond filaments”, the BMBF-supported project MANUMIEL between the Technical University of Moldova, the Ferdinand Braun Institute for High Frequency Technology (FBH), Berlin, and WIAS, as well as the new MATHEON Project OT2 “Turbulence and extreme events in nonlinear optics”.

### Dynamics of semiconductor lasers

The research in this field is characterized by its close relations to various experimental partners, and it presently covers a particularly wide range of different types of devices. An important event was the Workshop “Nonlinear Dynamics in Semiconductor Lasers” (NDSL14), organized with the support of MATHEON, SFB 787, and PROPHET, which aimed at bringing together applied mathematicians, theoreticians, and experimentalists working in the field of semiconductor physics and nonlinear dynamics to exchange experience and discuss new trends in the field of nonlinear phenomena in semiconductor lasers. For the activities on broad-area (BA) lasers and amplifiers—an important class of high power devices—we refer to the Scientific Highlights article by M. Radziunas on page 30.



**Fig. 1:** Participants of the Workshop NDSL14



**Fig. 2:** Parameter scan (injection rate and frequency detuning) of the dynamical regimes of an optically injected MLL, cf. Pimenov et al., *Phys. Rev. E*, **89**(5) (2014), 052903

**Mode-locking.** A new technique of coherent passive mode-locking (CML) due to coherent light-matter interaction was studied theoretically, resulting in a practical realization in semiconductor lasers. In particular, the CML was shown to be self-starting, such that no external seeding pulse is required. In the Marie Curie Initial Training Network (ITN) PROPHET, hybrid mode-locking in two-section edge-emitting semiconductor lasers was studied theoretically, based on a set of delay-differential equations (DDE). Recent experiments by the group's partners in PROPHET showed that in optically injected ML lasers the locking behavior is strongly affected by bistability and hysteresis between different dynamical regimes. Numerical simulations, see Figure 2, showed in fact bistability and hysteresis between different locked and unlocked regimes similar to the experimental results, and could clarify the relevance of the phase-amplitude coupling in the gain and absorber sections for the experimentally observed phenomena.

For the estimation of the pulse timing jitter from the DDE model, a semi-analytical method was developed, which allows a very efficient estimation of this jitter and which was applied to study noise characteristics of other multimode laser devices. In contrast to previous theoretical results, it could be demonstrated that the dependence of the timing jitter on the injection current can be highly non-monotonous. Specifically, a peak in the dependence of the timing jitter on the gain can be observed, which is related to a transition between two fundamental ML regimes. Moreover, the timing jitter suddenly drops when the laser switches to a certain ML branch. These theoretically predicted properties were later observed in experiments with quantum dot lasers in Cork [1].

**Ring lasers, coupled lasers.** An algorithm allowing to calculate instantaneous longitudinal optical modes of the (1+1)-dimensional traveling wave model in nearly arbitrary coupled laser configurations was developed. Analysis on this basis can explain the origin of different operational regimes, including their dependence on important parameters for a variety of edge-emitting semiconductor lasers, such as multi-section lasers, ring lasers, or coupled laser devices. Such an analysis was performed in collaboration with partners in the frame of the EU-ITN PROPHET and with TU Moldova and FBH Berlin in the frame of the project MANUMIEL.

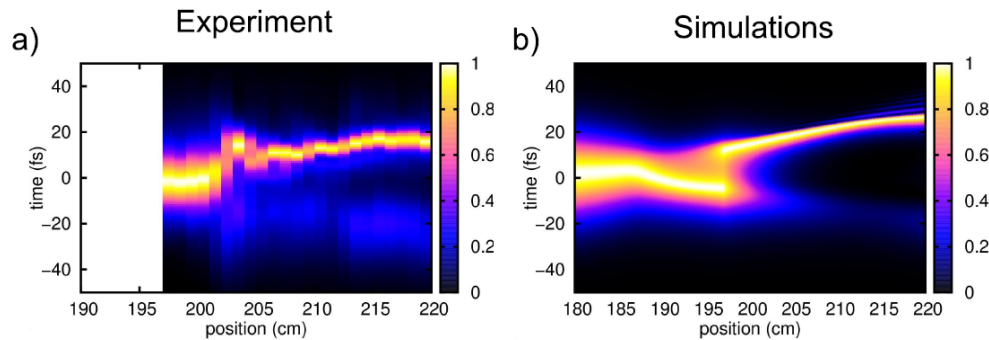
**Dynamics of frequency-swept laser sources.** Frequency-swept lasers with a tunable intra-cavity spectral filter are novel compact sources for optical coherence tomography (OCT), which is an imaging technique for the acquisition of high-resolution real-time images of biological tissues. In particular, OCT is used as a clinical diagnostic tool, in particular, for monitoring the eye, but the field of its application has expanded greatly in recent years. The group analyzed such lasers theoretically, based on a set of delay-differential equations that describes well the experimental results by the group's partners in the frame of the EU-ITN PROPHET. The model was also used to determine important quantities of such devices, together with a physical interpretation of important characteristics. The potential impacts on optical coherence tomography applications were analyzed [2].

### Pulses in nonlinear optical media

The dynamics of temporal self-compression of optical pulses in femtosecond filaments was investigated in [3]. The evolution of the temporal pulse envelope along the filament axis was determined



experimentally and found to be in excellent agreement with numerical simulations of a unidirectional approximation of Maxwell's equations; see Figure 3.



**Fig. 3:** Evolution of a temporal pulse envelope a) on axis of a filament in experiment and b) in numerical simulations

In a News&Views article in Nature Photonics, an experimental scheme for extending the propagation range of femtosecond filaments figured out by Scheller et al. was discussed; cf. Figure 4.

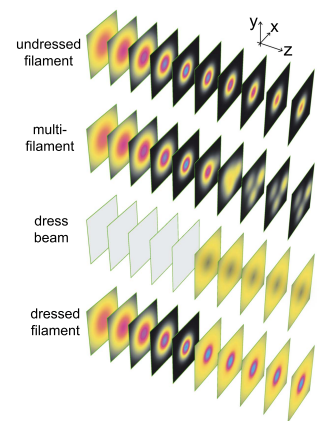
Investigations of optical pulses in nonlinear media with a special accent on complex/turbulent states and on extreme solitons/rogue waves were concentrated on typical settings in fiber optics. The results obtained are based on a systematic use of the Hamiltonian approach for nonlinear waves. The most important achievements include a new method of supercontinuum generation and extreme pulse compression by multiple collisions of a seed pulse with resonant dispersive waves. A mathematical structure that strictly limits the largest possible “extremeness” of optical pulses was found [4]. A review book chapter on Hamiltonian methods for optical systems was finished (to be published in 2015). Together with Raimondas Čiegis from TU Vilnius, higher-order numerical schemes for generalized nonlinear Schrödinger equations were studied.

### Dynamical systems

A major highlight in this field was the positive evaluation of the DFG Collaborative Research Center (SFB) 910 “Control of Self-organizing Nonlinear Systems” with the new project A3 “Activity patterns in delay-coupled systems”. Another outstanding event was the Workshop “Collective Dynamics in Coupled Oscillator Systems” from November 24–26 at WIAS with 75 participants from 10 countries.

**Synchronization of coupled oscillators.** A new approach to the stabilization and control of chimera states was published [5]. The paper presents a general control scheme that is able to find and stabilize an unstable chaotic regime in a system with a large number of interacting particles. The control allows to track a high-dimensional chaotic attractor, for example, a chimera state, through a bifurcation where it loses its attractivity.

Motivated by the fundamental question how the classical Kuramoto-type synchronization scenario extends to various types of spatially extended systems, a one-dimensional model of phase oscillators with nonlocal coupling was considered, showing that the transition from incoherent to synchronized behavior is mediated by the emergence of partially coherent twisted states. The bifurcation scenario resembles the classical Eckhaus instability, which describes the emergence of stable wave patterns in partial differential equations [6].



**Fig. 4:** Extending the propagation range of a filament by dressing it with a Bessel beam; cf. G. Steinmeyer, C. Brée, Extending Filamentation, *Nature Photonics*, **8** (2014), pp. 271–273

**Complex Ginzburg–Landau equation (CGLE) with delayed feedback.** Multistability and snaking behavior of plane wave solutions of the cubic and the cubic-quintic CGLE with delayed feedback were investigated analytically and numerically. Numerical bifurcation analysis for various delay times and asymptotic stability analysis in the limit of large delay revealed the borders of strong and weak instabilities of the plane waves. Direct numerical integration of the model equation confirmed the results of the analytical analysis.



**Fig. 5:**  
Participants of the Workshop  
“Collective Dynamics in  
Coupled Oscillator Systems”  
(DON14) at WIAS

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## 4.3 Research Group 3 “Numerical Mathematics and Scientific Computing”

RG 3 studies the development of numerical methods, their numerical analysis, and it works at implementing software for the numerical solution of partial differential equations and differential-algebraic systems. Many of the research topics have been inspired by problems from applications; see the Scientific Highlights article by Alfonso Caiazzo on page 51. Below, a selection of research topics of the group will be sketched. Further topics include stabilized and physical property-preserving discretizations for problems coming from computational fluid dynamics (CFD), the simulation of semiconductor devices (in collaboration with Research Group RG 1 *Partial Differential Equations*) and population balance systems, uncertainty quantification (in collaboration with Research Group RG 4 *Nonlinear Optimization and Inverse Problems*), and reduced-order modeling.

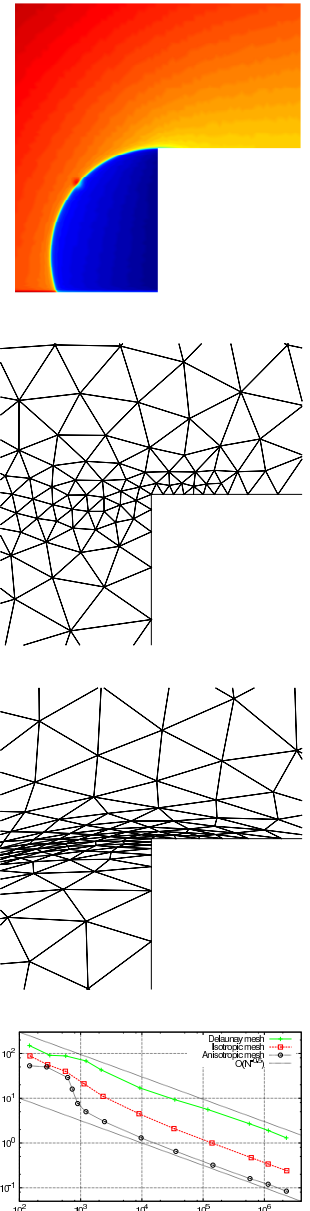
### Anisotropic mesh generation and adaptation

The objective of this project is a better understanding of adaptivity and its impact on all stages of a numerical simulation: from the discretization to the solution of the resulting linear systems. In particular, the group is interested in anisotropic mesh adaptation and its application to problems with distinct anisotropic features and/or strongly anisotropic and heterogeneous full tensor coefficients.

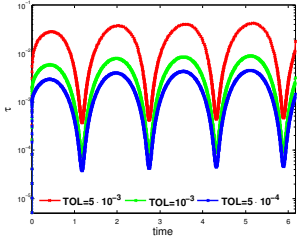
Anisotropic mesh adaptation is a more general approach than the classical (isotropic) adaptation and can significantly improve the accuracy of the solution and enhance the computational efficiency (Figure 1). Further, it can be of significant advantage for designing numerical schemes with particular properties. A better understanding of anisotropic mesh adaptation is inevitable for the development of new, more efficient and effective numerical algorithms.

One area of current emphasis is an important question connected with the generation of adaptive meshes. It consists in obtaining the directional information of the solution, which is required for the optimal anisotropic mesh adjustment. Two major approaches are considered: based on post-processing of the numerical approximation (recovery of solution derivatives) [5] and on a posteriori error estimates. Also the possibilities of mesh improvement algorithms (e.g., mesh smoothing) are explored, and mesh quality measures are developed in order to make a qualified judgment of the quality of the generated grids.

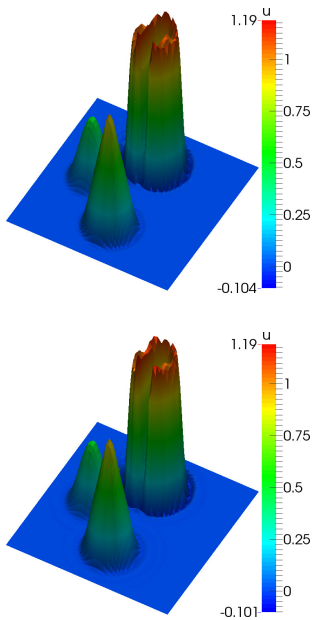
Another research topic is the investigation of the impact of adaptive grids on the last stage of a numerical simulation: the solution of linear systems arising from the discretization of PDEs. Since an anisotropic mesh is expected to contain elements of large aspect ratio, there exists a concern that the discretization based on adaptive and, particularly, anisotropic meshes can lead to extremely ill-conditioned linear systems, which may outperform the accuracy improvements gained by adaptation. Most of the results available on conditioning are for the special case of isotropic adaptation and, typically, too pessimistic to be of any use for the general case. A new analysis was necessary. For elliptic second-order problems, the group was able to show that the conditioning of finite element equations with anisotropic adaptive meshes is much better than generally assumed [6],



**Fig. 1:** Example of an adaptive finite element solution, close-ins at the re-entrant corner of the corresponding isotropic and anisotropic adaptive meshes, and the energy error norm for uniform (green), isotropic (red), and anisotropic (black) mesh adaptation



**Fig. 2:** Temporal evolution of the length of the time step,  $cGP(2)$  with different tolerances for the PC11 controller



**Fig. 3:** Solution at final time. Top:  $cGP(2)$  with adaptive time step and  $TOL=10^{-3}$  (1533 steps), bottom:  $cGP(2)$  with equidistant time step  $\tau = 10^{-4}$  (61646 steps).

especially in one and two space dimensions. To the best of the group's knowledge, this result is the first that has been proven for the general case (that is, without any assumptions on the mesh regularity or topology).

### Higher-order variational time stepping schemes

The numerical solution of convection-dominated flow problems needs stable discretizations both in space and in time. The instabilities caused by the convection-dominated phenomena are often treated by stabilized finite element methods, like the streamline-upwind/Petrov–Galerkin (SUPG), continuous interior penalty (CIP), or local projection stabilization (LPS) methods. For the stiffness caused by the small mesh sizes in time, A-stable or strongly A-stable time-stepping schemes are used. In [2], a stabilized finite element method was analyzed for convection-dominated convection-diffusion-reaction equations. Here, the LPS method in space is combined with the higher-order continuous Galerkin–Petrov (cGP) and discontinuous Galerkin (dG) methods in time. The cGP methods are a class of finite element methods using discrete solution spaces in time consisting of continuous piecewise polynomials of degree less than or equal to  $k$  and test spaces built by discontinuous polynomials of degree up to order  $k - 1$ . In dG methods, both solution and test spaces are constructed by discontinuous polynomials of degree less than or equal to  $k$ . Since the test functions in time are allowed to be discontinuous at the discrete time points, for both considered temporal discretizations the solution of cGP and dG schemes can be calculated by a time-marching process.

The use of higher-order time stepping schemes results in higher computational costs. However, the computational costs per time step can be compensated if only the necessary number of time steps is applied. The advantage of variational time-stepping schemes is that by means of simple post-processing, one obtains a solution of one order higher than the solutions computed with  $cGP(k)$  or  $dG(k)$ . Thus, well-understood techniques from the numerical analysis of ordinary differential equations can be used for performing an adaptive time-step control. In [1], adaptive higher-order variational time-stepping schemes applied to time-dependent convection-diffusion-reaction equations are described in detail. They are compared with respect to the performance (efficiency, accuracy) with an adaptive Crank–Nicolson scheme. For a rotating body problem with variable speed of rotation, the evolution of the length of the time step is illustrated in Figure 2. Small time steps correspond to fast rotations. It can be seen in Figure 3 that there are no visible differences in the solutions obtained with the adaptive time-step algorithm and the application of a small equidistant time step.

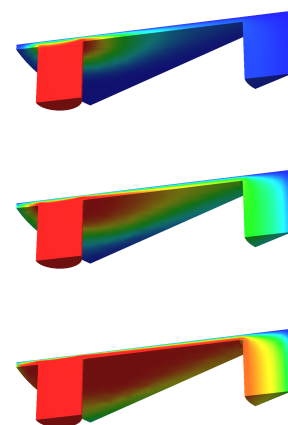
### Macroscopic modeling of transport and reaction processes in magnesium-air batteries

WIAS participates in an ongoing project in an interdisciplinary research network on “Perspectives for Rechargeable Magnesium-Air Batteries” in the Research Initiative “Energiespeicher” funded by the German Ministry of Education and Research. Together with project partners from the Universities of Bonn and Ulm and the Center for Solar Energy and Hydrogen Research Baden-Württemberg, fundamental research is performed to study possible setups, in particular, electrode and electrolyte materials, and the processes inside the batteries. The advantages of magnesium-air batter-

ies compared with lithium-ion batteries are the higher availability of magnesium and their higher energy density due to the lighter air cathode and the two-electron charge.

The WIAS subproject concentrates on macroscopic models for components of the magnesium-air batteries. Major efforts were invested in the improvement of a simulation tool that allows to simulate species transport in a moving fluidic electrolyte. A Voronoi box-based finite volume method for the transport equation simulates the species transport and involves a discrete velocity of the Navier–Stokes equations that should be divergence free to ensure mass conservation. A novel approach of a modified nonconforming Crouzeix–Raviart finite element method based on [7] led to a very inexpensive mass-conservative method [4]. However, it is of lowest order and exhibits a slow convergence of the velocity error at high flow rates. Thus, for the present application a higher-order discretization by Taylor–Hood or Scott–Vogelius finite element methods appears more suitable. The latter is divergence free but expensive. To achieve the mass conservation also for the less costly Taylor–Hood finite element method, an appropriate reconstruction of the discrete velocity into a divergence-free subspace of Brezzi–Douglas–Marini finite elements is under investigation.

The simulation tool is used to determine diffusion coefficients and to verify data from thin-layer flow cell experiments by project partners in Bonn; see Figure 4. Future intended applications include the calculation of other parameters like reaction coefficients. Another focus are pore models for the gas cathode to understand the coupling between species transport and oxidation. The magnesium peroxide precipitates and clogs the cathode and so reduces the available transport cross section. For this purpose, discretizations for the Nernst–Planck models developed in the Leibniz Group LG 3 *Mathematical Models for Lithium-Ion Batteries*, which take into account volume constraints and ion solvation effects, were investigated. A finite volume discretization strategy from semiconductor analysis together with a reformulation of the original problem in species activities results in a numerical model focusing on the proper reflection of qualitative properties of the physical model at the discrete level [3].



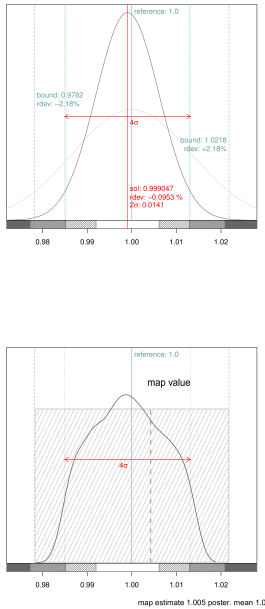
**Fig. 4:** Concentration of dissolved ions in a simulated thin-layer flow cell with inflow (left) and outflow (right) and an anode on the top of the cell for different flow rates (top: slow, middle: medium, bottom: fast)

### BOP: Deterministic and stochastic numerical methods in gas turbine performance modeling

The development of the process simulator BOP is a long-term project with successful applications in different industrial areas as exhaust sensor simulation, chemical engineering, and gas turbine performance modeling. The numerical kernel of BOP provides different modes for steady-state, transient, Monte Carlo, correction-curve, homotopy, and script simulations to treat large-scale systems of differential-algebraic equations arising in process simulation problems. During the last years, a number of add-ons were developed for the simulator. Two recently developed add-ons of BOP, the deterministic *Modified Least-Squares* approach and the stochastic *Bayesian* approach may be used for the parameter calibration in gas turbine models.

In gas turbine performance modeling, calibration techniques are used to adjust the gas turbine model to corresponding measurement data. Since both the calibration parameters and the measurement data are uncertain, the calibration process is intrinsically stochastic. If the deterministic *Modified Least-Squares* approach, which uses an algorithm of Levenberg–Marquardt type, is used for parameter calibration, the quantification of the uncertainty of the calibrated gas turbine model





**Fig. 5:** Posterior of a gas turbine inlet mass flow calibration parameter from BOP's Least-Squares method (top) and BOP's Bayes method (bottom)

is not clearly derived. But this uncertainty quantification is essentially needed for the prediction of the gas turbine performance, which has to be guaranteed to the customer. Moreover, such performance prediction might also be required for new gas turbine models when no measurement data for this model are available. In this case, the quantification of the uncertainty of the model is required, e.g., for risk-assessment reasons. For these reasons, a fully *Bayesian* approach is used for the nonlinear model, and the posterior of the calibration problem is computed based on a Markov chain Monte Carlo simulation using a Metropolis–Hastings sampling scheme; see Figure 5. To consider the dependence of the calibration parameters on the operating conditions, a *Gaussian process regression* approach is used. The latter approach was implemented, in collaboration with the Research Group RG 6 *Stochastic Algorithms and Nonparametric Statistics*, as an R package add-on of BOP. It now enables a higher dimensionality of the regression and a variable prior signal variance. Additionally, the script mode of BOP was extended to efficiently perform the complex simulation scenarios in case of the *Bayes* approach as well as the computation of the Jacobian in the *Modified Least-Squares* approach. In case of the Jacobian computation, e.g., speedup factors of about three were achieved.

Besides the new numerical features, the process description interpreter of BOP was extended, e.g., with respect to the treatment of analytic derivatives of process models, the repeated use of user-defined equation blocks, and the usage of process parameters.

The new version of the simulator, BOP3.1, including the new features and improvements, will be released to a leading manufacturer of heavy-duty gas turbines in March 2015. Additionally, a cooperation in the field of aerospace gas turbine simulation is in preparation.

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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.

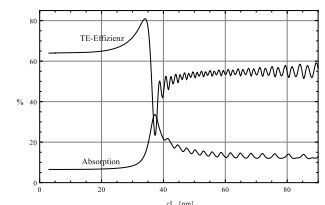
2014 was a year of endings and new beginnings for the research group. With the end of the third MATHEON funding period, four projects could be successfully completed. Five Ph.D. students successfully defended their theses, four former Ph.D. students and a postdoc left the group to take up new positions in industry or research. At the same time, the new ECMath/MATHEON project SE13 “Topology optimization of wind turbines under uncertainties” started. Moreover, the group acquired a project in the new Collaborative Research Center/Transregio (TRR) 154 “Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks”.

A special highlight of last year’s work was the organization of the Committee for Mathematical Modeling, Simulation and Optimization (KoMSO) Challenge Workshop “Math for the Digital Factory”, May 7–9, 2014. This event was also the kick-off meeting of the new Special Interest group (SIG) on Digital Manufacturing of the European Consortium for Mathematics in Industry (ECMI). ECMI SIGs serve as a platform of scientific exchange between researchers from academia and industry and form the central part of ECMI’s research activities in industrial mathematics. Participants from 10 European countries and Japan, 41 from academia and 10 from industry discussed scientific challenges related to digital manufacturing. In 22 talks, participants discussed topics like multibody and PDE systems of production processes, discrete and continuous models of production planning, as well as aspects of energy efficiency related to machine tools and more complex production systems. In an extra session, funding opportunities in “Horizon 2020” connected to nano-sciences, nano-technologies, materials and new production technologies (NMP) were discussed. A member of the European technology platform Manufuture provided insight in the preparation of new framework calls related to production.

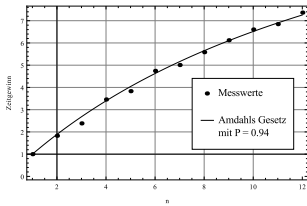
In the following, selected scientific achievements of the research group in 2014 are detailed.

### Inverse problems

In 2014, the design and analysis of algorithms for the simulation of time-harmonic wave scattering was continued. The ZIM (Central Innovation Program for SMEs) project “Grating simulation in field tracing” with LightTrans GmbH Jena was successfully completed. In particular, a new version of an integral equation solver for conical diffraction was developed. This solver is an enhanced and robust simulation tool for optical devices with many interesting features, not available in other software packages; see [4]. As an example, results for a coated echelle grating in Littrow mounting are explained, coping with challenging numerical problems (high wavenumber, thin coating layers, singularity of solutions). A grating with a period of about  $12\ \mu\text{m}$  is illuminated by a laser



**Fig. 1:** Efficiency of mode -122 and absorption as function of  $c_L$



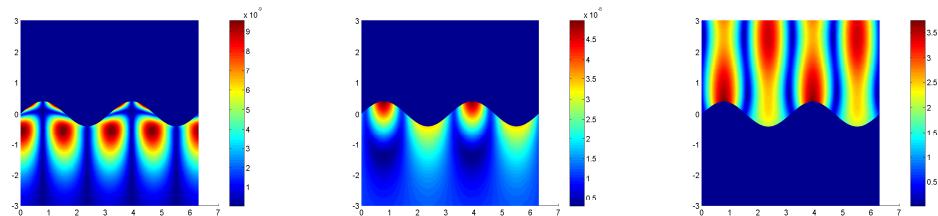
**Fig. 2:** Amdahl's law

of wavelength 193.35 nm under an incidence angle of  $78.7^\circ$ . In Figure 1, the efficiency of mode -122 and the absorbed energy are given depending on the coating thickness  $c_L$ , varying from 3 to 90 nm. The numerical solution of the integral equations uses spline functions with about 2000 graded mesh points. The computations were performed for 425 different values of  $c_L$  to see the oscillations of the graphs.

In order to reduce the computing time for such problems, the main work in 2014 was devoted to the development of new parallel discretization algorithms for the integral operators. The resulting code is highly optimized and very efficient, and can be adapted to the field tracing approach and software of the project partner. The computational results shown above need a computing time of about 12 hours on a PC with 16 cores. The parallel performance of the code can be estimated by Amdahl's law, i.e., the speedup  $Z$  is given by  $Z = 1 / [(1 - P) + P/N]$ , where  $P$  denotes the parallel fraction of the programs and  $N$  the numbers of processors. In Figure 2, the computational speedup versus the number of processors is shown, which fits to the high value of  $P = 0.94$ .

In connection with the diffraction of general time-harmonic fields by gratings, Floquet–Fourier transform techniques were developed, which lead to a sequence of solutions of usual diffraction problems with plane wave incidence for adaptively chosen incidence parameters. Their choice can be determined from the values of cubature nodes for the approximation of two-dimensional integrals. A theoretical and experimental investigation of optimal and efficient cubature methods for higher-dimensional integrals was initiated to find algorithms with a minimal number of incidence parameters. In particular, known adaptive algorithms were extended with higher-order formulas and applied to the approximation of nonsmooth diffracted fields. Exploiting the oscillatory structure of the integrands together with appropriate splittings of the integration domain is expected to result in a further performance improvement of these algorithms.

**Fig. 3:** Left: first component of displacement, middle: second component, right: pressure



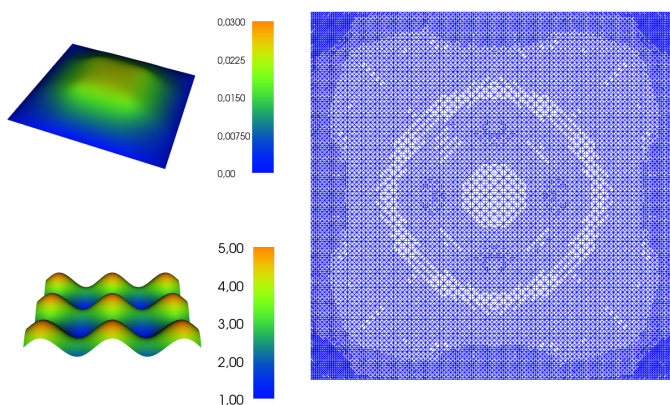
Besides light scattering, numerical algorithms for the fluid-solid interaction on biperiodic surface structures were developed and analyzed [6]. Here, acoustic waves are reflected by and transmitted into elastic bodies. A variational approach in the domain around the surface coupled with Dirichlet-to-Neumann mappings over the domain boundary leads to existence and uniqueness results. This technique with further modifications extends even to the case of Rayleigh frequencies (i.e., if modes propagate along the surface plane) and implies a unique acoustic far-field wave for, e.g., Jones frequencies (i.e., if the elastic body admits eigenmodes).

### Optimization and optimal control

The research group continued its efforts in the field of stochastic optimization with a focus on the analysis and numerics of probabilistic constraints. This engagement experienced a new im-

pulse by starting a participation in the above-mentioned TRR 154 with a project entitled “Nonlinear probabilistic constraints in gas transportation problems”. Here, earlier results obtained from models with linear probabilistic constraints are supposed to be extended to the nonlinear case and applied to gas networks with uncertainties (demand etc.). A theoretical prerequisite for this objective is the gradient formula derived in [1]. A major step forward could be achieved by integrating the algorithmic solution of probabilistic optimization problems into a sequential quadratic programming (SQP) environment. Applications to renewable energies (hydro/wind) illustrate the benefits of this approach (see the Scientific Highlights article on page 41). At the same time, in the area of hydro reservoir management under uncertainty, an existing cooperation with Electricité de France (EDF) was intensified (joint publications, plenary talk at an EDF-organized conference on optimization, mutual research visits) and a new cooperation with the Brazilian Energy Research Institute CEPEL (Rio de Janeiro) was started. An estimate for the condition number of linear-quadratic two-stage stochastic optimization problems could be proven by using tools from second-order non-smooth variational analysis. The paper appeared as a contribution to a special volume of “Mathematical Programming” dedicated to the 50th anniversary of Convex Analysis.

Previous results on adaptive numerical methods for PDEs with stochastic data were extended in two directions. First, a fully adaptive stochastic Galerkin finite element method with guaranteed error bounds was developed for a model problem with affine dependence on an infinite set of random parameters (see Figure 4). The estimator is based on recent equilibration techniques for the deterministic problems. Second, a goal-oriented adaptive Multilevel Monte Carlo (MLMC), which employs a problem-adapted mesh hierarchy, was derived (together with RG 3 *Numerical Mathematics and Scientific Computing*). Since a posteriori error estimators for deterministic problems play an important role for discretizations of stochastic problems, a functional error estimator for the convection-diffusion problem was analyzed. Moreover, in an interdisciplinary project with biology, the geometry dependence of cell polarization was investigated with a numerical simulation of a coupled bulk-surface problem.



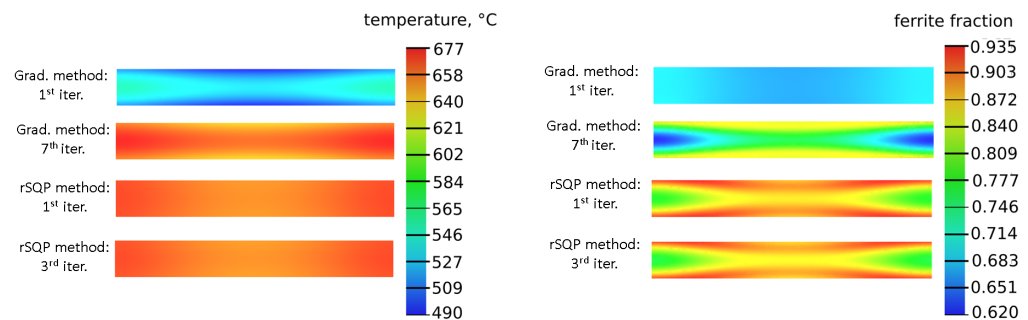
**Fig. 4:** Solution of a model problem with an inhomogeneous diffusion coefficient on a square and adaptively refined mesh. This kind of PDE data is relevant for stochastic problems, since random fields can be expanded in functions exhibiting similar properties.

In collaboration with Pierluigi Colli, Gianni Gilardi (both Pavia), and Jürgen Sprekels (RG 7), an optimal control problem for a viscous Cahn–Hilliard equation with a dynamic boundary condition and obstacle potentials was analyzed, and an optimality system was constructed by a thermodynamically justified approximation procedure [2]. Moreover, a second-order analysis of the op-

timal control problem for a viscous Cahn–Hilliard equation with a dynamic boundary condition was established. This second-order analysis paves the road for future research directions, i.e., to derive Newton methods (second-order methods) to solve numerically the optimal control problem for viscous Cahn–Hilliard equations with dynamic boundary conditions. In collaboration with Noriaki Yamazaki from the Kyoto University of Education, who visited WIAS for four weeks in August/September, the singular limit of an Allen–Cahn equation with double obstacle potential was analyzed.

In [5], sufficient optimality conditions and an SQP-solver for the optimal control to produce dual-phase steels were developed. The control problem was solved numerically, using `pdelib` (see page 197). In Figure 5, some iterations of the optimization procedure are shown, both the simulated final temperature and phase distribution in the cross section of the steel slab. In connection with the work on multi-phase steels, nucleation and growth models were revisited, including the identification of temperature-dependent growth coefficients and evolution laws for the grain size evolution of ferrite grains allowing an efficient estimate of mesoscopic microstructure-avoiding phase field models.

**Fig. 5:** The simulated final temperature (left) and phase distribution (right) in the cross section of the steel slab in a certain number of iterations of the optimization procedure. In both pictures, the 1<sup>st</sup> and 7<sup>th</sup> (final) iteration of the gradient projection method and the 1<sup>st</sup> and 3<sup>rd</sup> (final) iterations of the reduced SQP method are depicted in order from top to bottom.



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## 4.5 Research Group 5 “Interacting Random Systems”

The group continued their research activities on a number of topics like stochastic models for genetics (see the Scientific Highlights article on page 46), connectivity in large mobile ad-hoc systems, spectra of random operators, particle systems with coagulation and other interactions, and more. Further topics entered the group’s research spectrum by the addition of new members, due to the success in recent applications for third-party funded projects: the Leibniz Group *Probabilistic Methods for Mobile Ad-hoc Networks* (see also page 106), a DFG project on “Random mass flow through random potential”, and a project in a new DFG-funded Collaborative Research Center “Scaling Cascades in Complex Systems” at the Freie Universität Berlin. In this way, a number of current applications of large interacting random systems are under study in various areas, like kinetic theory, biological evolution, statistical mechanics, and telecommunication networks.

RG 5 maintains a number of collaborations with other Leibniz institutes and other research groups of WIAS. The group is a partner in a successful Leibniz application for 2015 of the Leibniz Institute for Zoo and Wildlife Research (IZW) about a project on the spread of viruses in water. In collaboration with the Research Group RG 3 *Numerical Mathematics and Scientific Computing*, a Ph.D. project was initiated on coagulating particle systems in turbulent flows.

In fall 2014, the head of RG 5, Wolfgang König, organized a Summer School of the Berlin Mathematical School on “Applied Analysis for Materials” at the Technische Universität Berlin with several speakers of WIAS; about 70 young people from all over the world attended. Two further workshops were organized by members of RG 5: one of the three days of the “Berlin – Padova Young Researchers Meeting on Stochastic Analysis and Applications in Biology, Finance and Physics”, which was attended by some 50 young people from Padua, Berlin, and other parts of Germany, and one day of a workshop on “Extrema of Branching Processes and Gaussian Free Fields” (supported by the Einstein Foundation and Technische Universität Berlin), which presented world-class speakers and attracted some 30 interested people.

RG 5 was also active in the education of young people in 2014. Its head supervised 20 bachelor and four master theses at the Technische Universität Berlin on various subjects in the research spectrum of the RG 5. At the same university, he acted as the main organizer of the 19th Day of Mathematics, a one-day mathematical contest for about 1000 pupils from Berlin and Brandenburg, which is one of the most popular public events in mathematics in Berlin. And also the INSPIRATA, the Leipzig Center for Education in Mathematics and the Sciences (headed by the head of the group) proceeded successfully in the sixth year of its existence: The *Aktion Mensch* awarded the center a position for two and a half years.

A closer description of some of the group’s achievements in 2014 follows.

### Extreme values of random fields with long-reaching correlations

Log-correlated Gaussian fields are random fields  $X(x)$  in  $\mathbb{R}^d$  in which the variance diverges logarithmically as  $|x| \rightarrow 0$ . Hence, they are distribution-valued stochastic processes arising from

physics, where they are used to define quantum gravity in conformal field theory. One of the main challenges is to show the universal behavior of extrema in any dimension  $d \geq 2$ .

In [3], the group approximated a wide class of log-correlated Gaussian fields by suitable cut-off random variables  $X_\epsilon(x)$ , which converge to  $X(x)$  as  $\epsilon \downarrow 0$ . The group's choice covers several models including the massive and the massless Gaussian free field. Given a parameter  $a > 0$ , one studies the invariance under cut-offs of the Hausdorff dimension of the “ $a$ -thick points”, i.e., points  $x \in \mathbb{R}^d$  where  $X_\epsilon(x) \approx a \text{Var}(X_\epsilon(x))$ . The group showed that the dimension equals  $d - a^2/2$ , as predicted by the theory of Gaussian multiplicative chaos. The group showed also that, under very general conditions, any two arbitrary cut-offs possess almost surely the same set of  $a$ -thick points.

This result allows the group to “wrap up” the question of the universality of extrema of log-correlated Gaussian fields: Independently of the choice of the approximating cut-off, the behavior of the extremal set is the same at any dimension.

### Concentration phenomena of mass transport through random media

The parabolic Anderson model concerns the solution to the Cauchy problem for the differential equation

$$\frac{\partial u(x, t)}{\partial t} = \Delta u(x, t) + \zeta(x)u(x, t), \quad x \in \mathbb{Z}^d, t \in [0, \infty), \quad (1)$$

where  $\Delta$  is the discrete Laplace operator acting on real functions of  $\mathbb{Z}^d$  and  $\zeta = (\zeta(x))_{x \in \mathbb{Z}^d}$  is an i.i.d. random field. The operator  $\Delta + \zeta$  is known as the Anderson tight-binding operator and is important in solid-state physics, e.g., in the modeling of electronic properties of disordered materials. The solution to (1) is relevant in a variety of applications related to mass transport in random media including chemical kinetics and population dynamics.

An important feature of the solution of (1) with localized initial datum  $u(\cdot, 0) = \mathbf{1}_0(\cdot)$  is the occurrence of *intermittent islands*, i.e., relatively few and small regions in space outside of which the mass of  $u$  is negligible in comparison to the mass inside. These islands are random, time-dependent and typically far away from the origin. Indeed, for certain choices of the distribution of  $\zeta(0)$  it is known that the mass is asymptotically carried by a single point of  $\mathbb{Z}^d$ , a phenomenon known as *complete localization*.

In contrast, a case is considered where the relevant islands have a non-trivial structure and cannot be reduced to points. The relevant (i.e., extreme) spectral properties of the Anderson operator in this case were studied by the group in [1], as reported in the Annual Research Report 2013 on page 39ff. Relying on their results, the group was able to show that the solution strongly concentrates in a single non-trivial island whose size stays bounded as time increases. The scaling limit of the center of this island can also be described, as well as aging properties of the solution. A manuscript is in preparation. The distributional properties of the leading eigenvalues of the Anderson operator were studied by the group in [2] in terms of a central limit theorem.



### Pair formation in biological populations

Pair formation in zoological populations comprised of females and males is an important aspect of sexual selection, one of the main deriving forces of evolution. A crucial concept in the mating of animals is assortativeness: In a positively (resp. negatively) assortative population, similar (resp. different) types prefer to mate together, while in a non-assortative population, individuals mate completely randomly, independent of their types. However, deriving the assortativeness properties of a species is an important challenge that receives attention in both biology and game theory communities (the latter being due to the related matching problems in economy such as secretary and college-student problems). For most species the mating process has two main ingredients: the preferences of individuals depending on their types and the mechanism with which the animals encounter each other for mating. In [4], the group introduced a very general class of *stochastic* permanent pair formation models that incorporates these two aspects. Using probabilistic techniques (in particular of Markov chains), it gave a complete characterization of assortativeness of a species, depending on the parameters of the model. Moreover in [5], the group investigated in detail the special case where the times individuals search for mates are given by Poisson processes. For large populations it explicitly calculated the limiting mating patterns which paves the way for hypothesis testing for the preferences in the population.

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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 *Stochastic modeling, optimization, and algorithms*. 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 a leading position with important mathematical contributions and the development of statistical software. Members of the research group participate in the DFG Research Unit FOR 1735 “Structural Inference in Statistics: Adaptation and Efficiency”.

Members of the group were also involved in several industrial contracts and cooperations, such as a project with Alstom (Switzerland) Ltd. on “Gas turbine process simulation”, the HSH Nordbank, and Deloitte.

Scientific highlights achieved by the research group in 2014 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 2014:

- Outstanding publications:
  - THORSTEN DICKHAUS, *Simultaneous Statistical Inference*, Springer, Berlin et al., 2014.
  - VLADIMIR SPOKOINY, THORSTEN DICKHAUS, *Basics of Modern Mathematical Statistics*, Springer Texts in Statistics, Springer, Berlin et al., 2015.
  - W.K. HÄRDLE, V. SPOKOINY, V. PANOV, W. WANG, *Basics of Modern Mathematical Statistics: Exercises and Solutions*, Springer Texts in Statistics, Springer, Berlin et al., 2014.
- FOR 1735 with WIAS participation (subprojects 1 und 4) was prolonged until 3/2018
- Cooperations with the Leibniz Institute for Neurobiology, Magdeburg, and the Wellcome Trust Centre for Neuroimaging, London, were established
- Two offers to Thorsten Dickhaus: professorship (W3) Universität Bremen, professorship (W2) Technische Hochschule Wildau

In cooperation with the Wellcome Trust Center for Neuroimaging, new methods for the analysis of high-resolution multi-shell diffusion magnetic resonance (MR) experiments were developed. Data from such experiments are characterized by an extremely low signal-noise ratio leading to severe bias and variability of estimated characteristics. Two essential tools to address these problems

were proposed. The multishell position-orientation adaptive smoothing (msPOAS) approach [5] enables a variance reduction employing the data-inherent spatial homogeneity structure in orientation space  $\mathbb{R}^3 \times \mathbb{S}^2$ . Adequate modeling as well as variance reduction by msPOAS require a correct assessment of distributional characteristics of the observed data that is achieved by a new locally adaptive procedure for estimating the scale parameter of the signal distribution [4].

Together with partners from the Leibniz Institute for Neurobiology, the investigation of the dynamics of functional connectivity networks in learning experiments was started. First results were presented at the Human Brain Mapping Conference 2014 in Hamburg. Preliminary investigations concern the alignment of individual learning curves.

The cooperation with the Department of Neurology, Universität Münster, focuses on the investigation of multi-modal imaging problems.

Copula-based multiple test procedures controlling the family-wise error rate (J. Stange et al., *ASTA Adv. Stat. Anal.*, doi: 10.1007/s10182-014-0241-5) and the false discovery rate (T. Bodnar, Th. Dickhaus, *Electron. J. Stat.*, **8**:2 (2014), pp. 2207–2241), respectively, under general dependencies were developed.

A mathematical analysis regarding least favorable parameter configurations for step-up-down multiple tests was performed (G. Blanchard et al., *Statist. Sinica*, **24**:1 (2014), pp. 1–23).

New results in structure adaptive estimation and convergence of expectation-maximization-type alternating algorithms were obtained in [1].

M. Panov and V. Spokoiny showed that the Bayesian posterior follows the Bernstein–von Mises phenomenon under rather broad and mild conditions including noise misspecification and finite samples [2].

The validity of the classical multiplier bootstrap procedure under non-classical assumptions and the so-called *modeling bias* effect were investigated in [3]. The bootstrap validity is shown under the *small modeling bias* condition and extended in a slightly different form to the case of large modeling bias.

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### Stochastic modeling, optimization, and algorithms

The project focuses on the solution of challenging mathematical problems in the field of optimization, stochastic optimal control, and in the field of stochastic and rough differential equations. These problems are particularly motivated by applications in the finance and energy 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 appearing in energy and storage markets, for instance. Also, there is a strong expertise in financial (interest rate and equity) modeling, volatility modeling, effective calibration, and the modeling of financial derivatives, such as complex structured interest rate, energy, and volatility derivatives.

Further, the group has expertise in the highly active field of rough path analysis and regularity structures, which led, in particular, to a recent joint text book by Peter Friz and the Fields medallist Martin Hairer.

#### Highlights 2014:

- Granting of ECMath-MATHEON project SE7 “Optimal strategies in energy and storage market” (John Schoenmakers, Vladimir Spokoiny) for 2014–2017
- Granting of ECMath-MATHEON project SE8 “Stochastic methods for the analysis of lithium-ion batteries” (Wolfgang Dreyer, Peter Friz) for 2014–2017
- Book publication: PETER FRIZ, MARTIN HAIRER, *A Course on Rough Paths: With an Introduction to Regularity Structures*, Universitext, Springer, Berlin et al., 2014
- Best Paper Award in Optimisation Letters for Roland Hildebrand
- Offer to Christian Bayer: senior lecturer (equivalent to W2) at Linköping University (Sweden)

The innovative forward-reverse approach in the context of the simulation of conditional diffusions developed in [2] was continued in the reporting year and applied to statistical inference under incomplete observation. Indeed, one of the most prominent algorithms for maximum likelihood estimation is the celebrated expectation-maximization (EM) algorithm, which naturally leads to computations of conditional expectations amenable to calculation with the forward-reverse algorithm. The theoretical properties of the coupled forward-reverse-EM algorithm are explored, including a detailed convergence proof, in the context of a discrete-time Markov chain (with general state space). Furthermore, also the forward-reverse-EM algorithm is studied in practice for examples in the context of Stochastic Reaction Networks, a class of pure-jump Markov processes with state-dependent intensities heavily used in computational chemistry and other engineering fields.

A hot topic in the simulation of asset prices or interest rate models equipped with stochastic volatility processes (e.g., Heston-type models) is the effective simulation of the square root process involved, also called the *Cox–Ingersoll–Ross (CIR) diffusion process*,

$$dV = k(\lambda - V)dt + \sigma\sqrt{V}dW,$$

with  $W$  being a standard Brownian motion. Simulation of the CIR process is particularly difficult when the Feller condition  $\sigma^2 \leq 2k\lambda$  is violated. In this case, the behavior of  $V$  at the boundary zero becomes critical. For the case where  $4k\lambda > \sigma^2 > 2k\lambda$ , that is to say, when the Feller condition

is weakly violated, the development of a new simulation algorithm was started in 2013 (WIAS Preprint no. 1763). This approach, based on a Doss–Sussmann formalism in connection with a novel concept of uniform stochastic differential equation simulation, was developed further, and a substantially extended version of the former preprint is meanwhile to appear (in Adv. Appl. Prob.). Treatment of the case of strong valuation of the Feller condition, i.e.  $\sigma^2 \geq 4k\lambda$  will involve the study of the local time at zero and will be one of our next challenges.

The ideas on surely optimal dual martingales for American options developed in the project in the preceding years (J. Schoenmakers, J. Huang, J. Zhang 2013) were worked out further in the context of penalized convex optimization. As a result, a new efficient path-wise dual maximization approach for the optimal stopping problem was proposed with an analysis of its convergence properties (WIAS Preprint no. 2043).

In the area of modeling and interference of economic processes, nowadays time changed Lévy processes are quite popular. In this respect, a new estimation method for estimating the time change of a rather general time-changed Lévy process is developed and studied in all its statistical aspects in WIAS Preprint no. 1960.

Before the financial crisis, LIBOR rates were regarded more or less as risk free. However, after the crisis, it became necessary to take credit risk into account in LIBOR rates and, as a result, multi-curve LIBOR models are needed. To this topic, the project contributed with a multi-curve affine LIBOR model that incorporates multi-curve LIBORs with nonnegative stochastic spreads and overnight index swap basis rates in a mathematically consistent way (WIAS Preprint no. 1951). It is demonstrated that the model is capable to fit a huge system of liquid market data simultaneously.

Monte Carlo simulations critically depend on a proper choice of the stopping criterion, i.e., of the number of simulated samples (potentially adaptively chosen depending on preliminary results of the simulations such as sample variances of the quantity of interest). Usual stopping criteria are based on asymptotic properties of the sampler, such as asymptotic normality of the sample mean. Hence, they may fail in actual Monte Carlo simulations, which are always based on a finite number of samples, especially in heavy-tailed situations. In [3], a particular stopping criterion is presented, for which empirical studies suggest very good performance even for heavy-tailed models.

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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

**Analysis of sweeping processes.** Sweeping processes are an important topic of elastoplasticity. Mathematically, they are represented by a class of evolution differential inclusions. Sweeping processes were introduced by the French scientist J.J. Moreau in the early seventies. Currently, that model system is also used to describe the dynamics of machines and masonry and to generate animated computer graphics.

Olaf Klein, jointly with Vincenzo Recupero from Dipartimento di Scienze Matematiche, Politecnico di Torino, gave a counterexample to show that the transfer of the model to new applications is accompanied by some subtleties. In [1], they proved: *“There is no continuous extension of sweeping processes to functions of bounded variation.”*

**Analysis of processes in the context of electrochemistry.** Pierre-Étienne Druet developed a setting that allows succinct answers to a series of still open problems of generalized potential theory. To this end, he introduced weak notions of *div* and *curl* operators as functionals on Sobolov spaces. The electrotechnical limit of Maxwell’s equations serves as an example to illustrate the mathematical rigor of the formalism: Higher regularity and compactness of the solution operator are proved under extremely weak requirements on the data [2].

A further topic concerns the analysis of the electrolyte model that was developed in the research group jointly with the Leibniz Group 3 *Mathematical Models for Lithium-ion Batteries*. The newly



introduced coupling of the transport equations with the momentum balance exhibits a challenge from the analytical point of view. Many of the well-known theorems for elliptic-parabolic systems are no longer applicable. Within an ongoing thesis project, Paul Gajewski proved existence and uniqueness of equilibrium for the generalized Nernst–Planck–Poisson system [3].

**Analysis and optimal control of phase field systems.** Jürgen Sprekels, jointly with colleagues from the University of Pavia and with Elisabetta Rocca from the ERC Group *Entropy Formulation of Evolutionary Phase Transitions*, achieved new important results in the systematic analysis of optimal control problems for phase field systems modeling phase separation phenomena occurring in a container  $\Omega \subset \mathbb{R}^n$ ,  $n \leq 3$ . In such problems, strong and singular nonlinearities occur that render the analysis difficult. The main focus of research was directed toward (i) dynamic boundary conditions modeling effects of surface diffusion on the boundary  $\Gamma$  of  $\Omega$ , and (ii) situations in which the phase separation takes place in a fluid flow. Both local and nonlocal evolution systems were studied.

Among the local models, the optimal boundary control problems involving dynamic boundary conditions for viscous and non-viscous Cahn–Hilliard systems were solved. For example, [4] treated the case of differentiable nonlinearities. First-order necessary optimality conditions were derived for the viscous case.

However, the main direction focused on *nonlocal* models, in which the free energy comprises a nonlocal term. Most challenging was the analysis of the optimal distributed control of the nonlocal Cahn–Hilliard/Navier–Stokes system

$$\partial_t y - \Delta w = -\mathbf{u} \cdot \nabla y \quad \text{and} \quad w = a y + f'(y) - K * y \quad \text{in } Q, \quad (1)$$

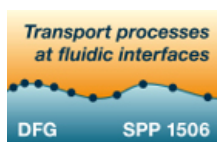
$$\partial_t \mathbf{u} - 2 \nabla \cdot (m(y) D\mathbf{u}) + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \pi = \mu \nabla y + \mathbf{v} \quad \text{and} \quad \nabla \cdot \mathbf{u} = 0 \quad \text{in } Q. \quad (2)$$

Here,  $D\mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u})$  is the symmetric gradient,  $\mathbf{v}$  plays the role of the control parameter, and the two-dimensional situation was discussed. Fréchet differentiability of the control-to-state mapping  $\mathbf{v} \mapsto (y, \mathbf{u})$  could be shown, and the first-order necessary optimality conditions were established in terms of a variational inequality and the adjoint system.

**Modeling of electrolytes.** In 2014, the outstanding Ph.D. thesis “*Theorie der elektrochemischen Grenzfläche*” appeared. Clemens Gohlke passed the examination at the Technische Universität Berlin with the grade *summa cum laude*. The subject of his thesis is one of the two cornerstones of the research on lithium-ion batteries within the Leibniz Group 3 *Mathematical Models for Lithium-Ion Batteries*. Its starting point is the observation that the classical Nernst–Planck–Poisson model (NPP), which is even today still applied by most scientists in this area, has serious deficiencies: The NPP model (i) is not capable of correctly predicting the distribution of species in the adjacent layers at the interface between an electronic and an ionic conductor, (ii) is not thermodynamically consistent, (iii) ignores the role of the local pressure and does not take into account the ion-solvent interaction. A detailed description of these shortcomings is found in the Scientific Highlights article “*Crucial Revisions of Electro-Chemical Modelling*” of the Annual Research Report 2013 of WIAS on page 29.

The “*Theorie der elektrochemischen Grenzfläche*” not only removes these deficiencies, in fact, it represents a rational approach to the full coupling of continuum thermodynamics and electrodynamics. Particularly, the new derivation of the electrodynamic surface balance equations of the interface between different materials is among the highlights of this thesis. There is no other author who has found the key for unique surface equations, viz. the identification of interfacial electromagnetic energy and force. Even the subject of magnetization, which is a distant subject for battery research, is included. Moreover, the thesis contains numerous subtle details of greatest importance that have been overlooked in the past.

### 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”.

Within this project, Sebastian Jachalski successfully finished his Ph.D. thesis “*Derivation and Analysis of Lubrication Models for Two-Layer Thin-Films*” at Technische Universität Berlin. The thesis deals with the mathematical modeling and analysis of dewetting phenomena and equilibrium states of a thin liquid bilayer.

The modeling of the interface equations takes into account intermolecular forces in the setting of Navier-slip boundary conditions. The analysis of the model concerns (i) existence of solutions of the equilibrium, (ii) derivation of the corresponding sharp interface model by means of matched asymptotic analysis, (iii) calculation of contact angles, (iv) rigorous derivation of the sharp limit energy, (v) determination of minimizer and proof of equivalence to the matched asymptotic solution. The results are compared with experimental data.

Finally, the analysis of non-equilibria without and with intermolecular forces is studied in detail. The former case implies non-negative, globally weak solutions, while in the case with molecular forces the existence of positive smooth solutions could be proved.

### Funded by the Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin (PVcomB)



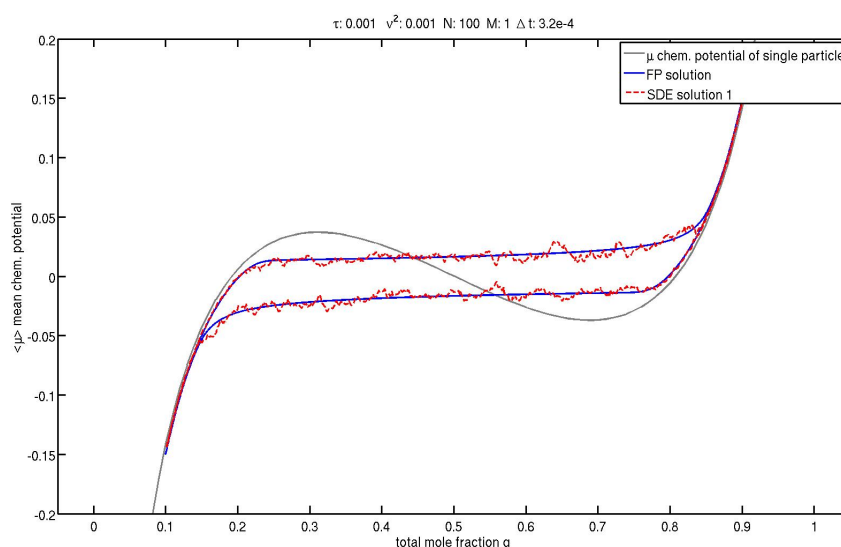
Modeling and analysis for epitaxial growth of anisotropic quantum dots is important to understand and control dewetting processes of crystalline silicon layers that are used to develop nanostructured thin-film photovoltaic cells. In this area, Barbara Wagner, jointly with colleagues from PVcomB, Humboldt-Universität zu Berlin, Martin-Luther-Universität Halle-Wittenberg, Helmholtz-Zentrum Berlin, and the Institute for Silicon Photovoltaics, established within a fundamental study a direct quantitative comparison between measured equilibrium structures and the equilibrium solutions of the model equations [6]. The model is represented by convective Cahn–Hilliard equations of the 6th order, which are not treatable by standard methods of analysis.

### MATHEON projects

The research group contributed with the following two projects to the application area *Mathematics for Sustainable Energies* of the DFG Research Center MATHEON funded by the Einstein Center for Mathematics Berlin (ECMath):

The project SE4 “Mathematical modeling, analysis and novel numerical concepts for anisotropic nanostructured materials” is headed by Barbara Wagner, jointly with Christiane Kraus (Young Scientists’ Group *Modeling of Damage Processes*), and Gitta Kutyniok (Technische Universität Berlin). Its topic is the prediction of damage and life time of modern materials as they are found, e.g., in lithium-ion batteries. The intercalation electrode of the battery suffers large volume variation up to 7% during the charging and discharging processes. These large deformations induce unwanted inhomogeneous stresses, and even cracks may appear, decreasing the life time of the battery. The project studies mathematical models describing coupled processes of diffusion, phase separation, and the evolution of stresses.

The project SE8 “Stochastic methods for the analysis of lithium-ion batteries” is headed by Wolfgang Dreyer and Peter Karl Friz from the Research Group RG 6 *Stochastic Algorithms and Nonparametric Statistics*. The challenging project needs mathematical techniques from both analysis and stochastics. The aim is to achieve the understanding if the speed of battery charging is limited due to the application of many-particle electrodes in lithium-ion batteries. The strange behavior of many-particle electrodes was explained a few years ago by Wolfgang Dreyer and Clemens Gohlke jointly with Michael Herrmann from Westfälische Wilhelms-Universität Münster. The mathematical core of their model is a nonlocal and nonlinear partial differential equation of Fokker–Planck type. It predicts the evolution of the probability density  $w(t, y)$  to find a single storage particle of the many-particle electrode in a certain filling state  $y$ . The evolution is controlled by two small parameters inducing a variety of analytical as well as numerical problems.



**Fig. 1:** Voltage versus charge according to the Fokker–Planck equation and its stochastic correspondence, respectively

The strategy of the project relies on the conjecture that there is a system of stochastic ordinary differential equations with “nicer” properties than the Fokker–Planck equation, but describing the same physics. In 2014, that conjecture has already been confirmed. Figure 1 shows the hysteretic behavior of the charging/discharging process of the many-particle electrode in the two settings. The smooth hysteresis represents the prediction of the Fokker–Planck equation describing the many-particle ensemble in the limit  $N \rightarrow \infty$ , while the rough hysteresis is generated by the corresponding system of  $N$  stochastic ordinary differential equations for  $N = 100$  storage particles.

## MURPHYS-HSFS-2014

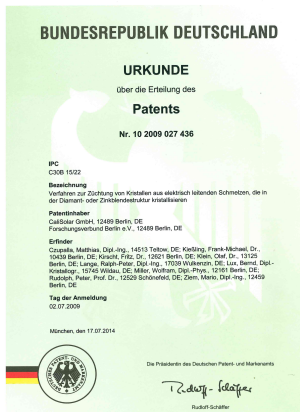
The “7th International Workshop on Multi-Rate Processes & Hysteresis”, associated with the “2nd International Workshop on Hysteresis and Slow-Fast Systems”, was organized by Olaf Klein (RG 7) jointly with M. Dimian (Suceava), P. Gurevich (Berlin), D. Knees (WIAS/Kassel), D. Rachinskii (Dallas), and S. Tikhomirov (Leipzig). It took place at WIAS from April 7–11, 2014 (see also page 126).

## Miscellaneous

The industry-funded research on crystal growth techniques for photovoltaic applications was stopped in 2013. However, there are still some activities. For example, in 2014 a patent was awarded in the context of crystal growth from electrically conducting melts.

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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.

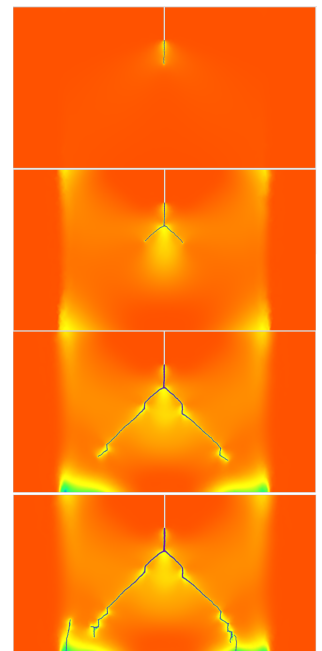
### Modeling, analysis, and numerics of damage processes

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 the calculus of variations for nonlinear and nonsmooth evolution systems and from geometric measure theory.

Based on previous works in the group, a unifying model describing coarsening, phase separation (Cahn–Hilliard/Allen–Cahn equations), damage processes, and elasticity was investigated; cf. [3]. More precisely, inertial effects were considered in the coupled system to account for elastic waves that may also affect the propagation of damage. For the resulting hyperbolic-parabolic system, a suitable notion of solutions was adapted, which utilizes energetic principles to describe the damage evolution. The inertia term in the balance equations of forces requires a careful analysis of the time-incremental system to establish existence results. These results were achieved by some higher-order regularization, approximation techniques for a certain class of functions, and by passing to the limit system via energy estimates.

For a realistic material model, temperature effects should also be taken into account, since they significantly influence the elastic properties via thermal expansions. To this end, strongly coupled systems of partial differential equations describing heat conduction, elasticity, and damage processes were studied; cf. [4]. A novelty of the analyzed model was a damage-dependent heat expansion coefficient, which, in turn, leads to several new coupling terms in the system. To handle the resulting equations analytically, a weak formulation was established, which is based on previous works in the YSG regarding coupled systems of phase separation and damage phenomena. Existence of weak solutions was proven by adapting two different approximation schemes: time-discretization and truncations of the heat conductivity coefficient and of the temperature function. A main challenge was the passage between these approximations to the corresponding limit system. Due to the new coupling terms, arising from the damage-dependent heat expansion coefficient,

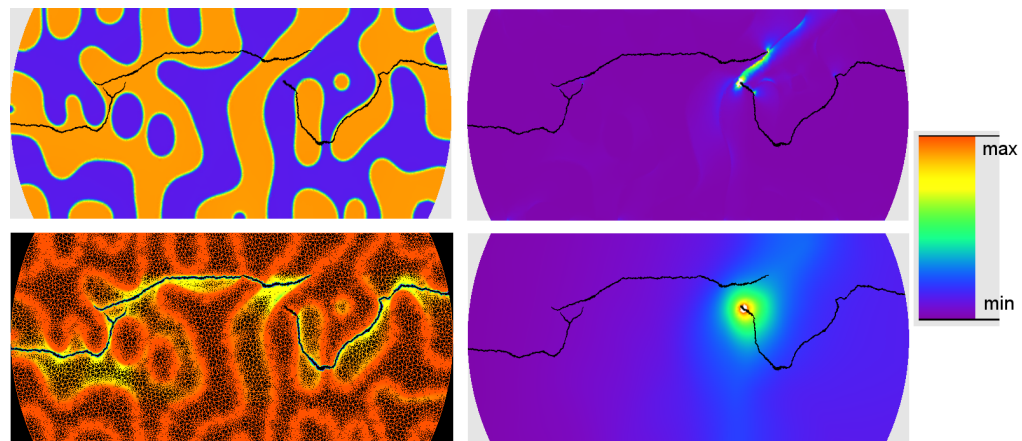


**Fig. 1:** Snapshots from a numerical simulation of damage with time-dependent loading

cient, well-established a priori estimation techniques developed from Boccardo–Gallouet could not be applied here. Thus, new tailored a priori estimates had to be devised in order to deal with the nonlinear terms.

Complementary to the analytical work done in the group, numerical methods were developed to examine solutions for a class of models that, in particular, are suitable to describe the interplay of phase separation and damage in alloys. The numerical schemes, dealing with the resulting non-convex problem, are not trivial and involve the approximation of inclusion equations to account for the irreversibility of damage evolution. At each discrete time step, an implicit constraint system of nonlinear equations had to be solved. A combined alternate minimization and trust-region scheme appeared to have sufficient robustness to accomplish this task. An additional challenge is the presence of multiple spatial and temporal scales during crack propagation. In order to resolve fine structures at the crack tip, without dealing with a very large number of computational nodes, spatially adaptive mesh generation for the finite element discretization was implemented. In addition, a time step control was introduced in the rate-dependent case. In the rate-independent case, the software allows for backtracking to ensure compliance with the energy inequality.

**Fig. 2:** Snapshots from a numerical simulation of phase separation and damage with material-dependent elasticity tensor and time-varying loading. From top left to bottom right: Phase field, elastic energy, damage field (with grid), and temperature field (Markus Radszuweit)



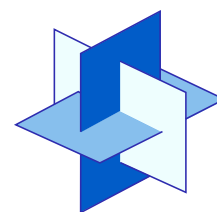
Typically, damage models claim phenomenological constitutive relations between the damage variable (used to model damage progression mathematically) and the material constants (modeling the elastic behavior of the considered material). Starting with a damage process of a body showing a very fine microstructure with respect to the material distribution, the group succeeded in justifying rigorously an effective description of this relation. Taking into account the underlying microstructure, these effective models describe damage progression from a macroscopic point of view. Such effective models are advantageous, since not all of the material's microscopic details have to be considered. This approach reduces the number of degrees of freedom inherent in the models, which simplifies and hence speeds up numerical simulations. Depending on the type of microscopic defects occurring in the considered material (e.g., inclusions of damaged material, voids, or microscopic cracks), different effective models were derived. In addition, it turned out that the existence of solutions is an immediate consequence of the rigorous limit process, which is performed in the framework of evolutionary  $\Gamma$ -convergence and uses multiscale convergence techniques. Hauke Hanke successfully defended his Ph.D. thesis on this topic in 2014; cf. [2].



As a further topic, jointly with the Research Group RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, a novel thermodynamically consistent diffuse interface model was derived for compressible electrolytes with phase transitions; cf. [1]. The fluid mixtures may consist of  $N$  constituents with the phases liquid and vapor, where both phases may coexist. In addition, all constituents may consist of polarizable and magnetizable matter. The introduced thermodynamically consistent diffuse interface model may be regarded as a generalized model of Allen–Cahn/Navier–Stokes/Poisson type for multi-component flows with phase transitions and electrochemical reactions. For the introduced diffuse interface model, physically admissible sharp interface limits were investigated by matched asymptotic techniques. Two scaling regimes were considered, i.e., a non-coupled and a coupled regime, where the coupling takes place between the smallness parameter in the Poisson equation and the width of the interface. In the sharp interface limit, a generalized Allen–Cahn/Euler/Poisson system was recovered for mixtures with electrochemical reactions in the bulk phases equipped with admissible interfacial conditions. The interfacial conditions satisfy, for instance, a generalized Gibbs–Thomson law and a dynamic Young–Laplace law.

### Projects

The research group participates in the Research Center MATHEON with the project SE 4 “Mathematical modeling, analysis and novel numerical concepts for anisotropic nanostructured materials”. The MATHEON project C32 “Modeling of phase separation and damage processes in solder alloys” was successfully finished at the end of May 2014. In addition, third-party funding was secured within the SFB 1114 “Scaling Cascades in Complex Systems” for the project “Effective models for interfaces with many scales”.



### Further activities

The International Workshops “Multi-Rate Processes and Hysteresis” (MURPHYS) and “Hysteresis and Slow-Fast Systems” (HSFS) with the local organizers Dorothee Knees (YSG) and Olaf Klein (RG 7), took place at WIAS, February 6–8, 2014. The lectures focused on multiple scales, singular perturbation, phase transition, and hysteresis phenomena in economic, engineering, and information systems.

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## 4.9 Leibniz Group 3 “Mathematical Models for Lithium-ion Batteries”

The Leibniz group has been 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 is working on the modeling based on continuum thermodynamics and electrodynamics, 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 electrochemical processes and transport phenomena involved are modeled by partial differential equations in the bulk regions and by jump conditions across the interfaces.

The group started in July 2012 and according to the Pact for Research and Innovation the external funding will end in June 2015. Due to the important achievements of the Leibniz group, its issues hereafter will again be among the topics of Research Group RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*.

The research in 2014 was based on revisions of the classical electrochemical models that were established in the last years by members of the Leibniz group jointly with RG 7. Particularly in the neighborhood of the interface between an electrolyte and a solid electrode, those revisions are unconditionally necessary. The resulting mathematical model includes a system of partial differential equations in the boundary layers on both sides of the interface, which is coupled to an algebraic system relating the corresponding fields across the interface. The motivations for the need of a new model are given in the Scientific Highlights article “Crucial Revisions of Electro-Chemical Modelling” of the Annual Research Report 2013 of WIAS on page 29. The continuum physical foundations are to be found in the 2014 Ph.D. thesis “*Theorie der elektrochemischen Grenzfläche*” written by the group member Clemens Gohlke [1].

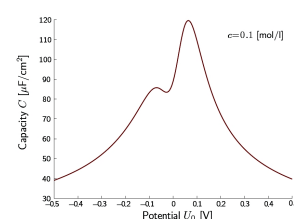
### Highlights

**Metal-electrolyte interface I: Interfacial solvation effects and electron transfer reactions.** Crucial processes controlling the performance of a rechargeable battery happen at the interface between an electrode and an electrolyte. From an experimental point of view, the so-called *differential capacity* is best suited to characterize those processes. However, a rational predicting theory that relates the differential capacity to the interfacial processes has been missing for almost 80 years. The differential capacity  $C$  [ $\mu\text{F}/\text{cm}^2$ ] relates the total charge of interface and electrolytic boundary layer to the voltage  $U$  between the metal electrode and the electrolyte. The de-

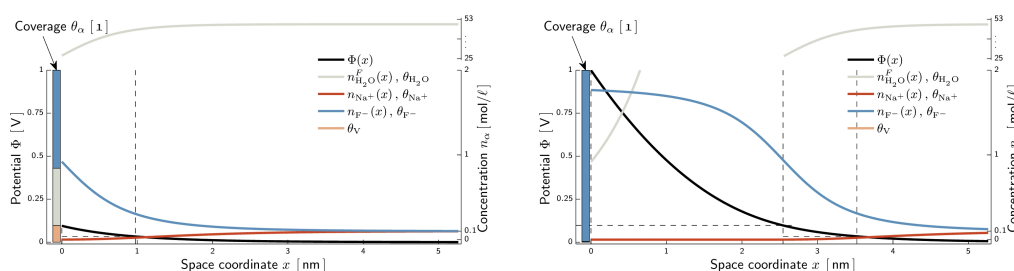
termination of the highly nonlinear function  $C(U)$  relies on an intricate boundary value problem for the interface and the adjacent boundary layers. The group's model incorporates three essential electrochemical phenomena, which are mandatory for a realistic prediction of capacity functions.

1. The solvation phenomenon whereupon the ions of the electrolyte form solvation shells around each other has not been modeled within a continuum setting in the chemical literature. The new model represents solvation by finite and different volumes of the involved ions. The evolution of solvated ions is governed by an intimate coupling of the diffusion process and the local pressure generated by thermal motion and by the local electric field.
2. Due to the two-dimensionality of the interface, and, moreover, due to interfacial electron transfer reactions, the solvated ions lose a part of their solvation shells when they appear as adsorbates.
3. The determination of the interfacial electron density needs a model of the metal. The Leibniz group complemented the old Sommerfeld model of free conduction electrons in the bulk region by a simple surface model allowing to calculate the density of available interfacial electrons involved in the electron transfer reactions with the adsorbates.

By now, there is quite a fundamental knowledge of each parameter in the theory. Consequently, it is not astonishing that a quantitative and qualitative agreement to experimental capacity data can be stated. Note that the interface capacity is a highly nonlinear curve with various maxima and minima throughout the potential range. Nevertheless, the model covers the whole nonlinearity and achieves also experimental agreement in variations of the salt concentration. Such an accuracy of predicting electrochemical interface properties is outstanding. It is a milestone in the continuum description of the electrolytic double layer and allows for an in-depth investigation of many electrochemical phenomena [1], [3].



**Fig. 1:** Capacity as a function of the applied voltage. Each point relies on the complete distribution of the constituents on the interface and within the electrolytic layer



**Fig. 2:** Distribution of electrolytic constituents and interfacial coverages. Left: Applied voltage 0.1 Volt. Right: Applied voltage 1.0 Volt.

**Metal-electrolyte interface II: Rational derivation of Butler–Volmer equations.** The prediction of the capacity function requires the full resolution of the boundary layers. There are other problems in the context of electrochemical interfaces where a reduced model is sufficient that does not resolve the interfacial neighborhood. This fact relies on the observation that the complete model contains a small parameter  $\lambda$  representing the ratio of the width of the boundary layer to the length of the bulk domain. By application of the method of asymptotic analysis to the complete model, a reduced model and corresponding new boundary conditions across the interface can be attained in the limiting case  $\lambda \rightarrow 0$ . The method is developed and extensively described in [1]. Among the new boundary conditions, one finds a relation of Butler–Volmer type that relates the rate of interfacial chemical reactions to the particle densities of the bulk phases at the interface and to

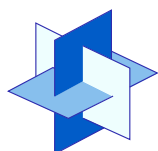
a certain difference of the electric potential. The chemical literature provides a variety of Butler–Volmer equations; however, a generally accepted representation is missing. Even if Butler–Volmer equations look similar to each other, they crucially differ in the way functions for the interfacial reaction rates, or the potentials are defined.

It is thus an important achievement that the Leibniz group could establish a rational derivation of the Butler–Volmer function [1], [4]. Its design relies on paying careful attention to two facts:

1. The reaction rate is the difference of the corresponding rates for the forward and backward reaction. These latter rates can not be modeled independently of each other. Their ratio is restricted by the second law of thermodynamics. Thus, only one of the two rates can be modeled in a thermodynamically consistent way.
2. The definition of the relevant potential difference is a priori not given in the complete model. It requires some connection between variables of the bulk regions and the interface.

A further subtlety in the derivation of the Butler–Volmer function has brought confusion in the classical literature. It concerns the dependence of the interfacial reaction rate on the electric potential, which, however, is continuous across the interface. Thus there arises the question: Which potential difference drives the chemical reaction on the interface? The answer within the group's model is simple: The complete model, i.e.  $\lambda > 0$ , does not imply the Butler–Volmer function at all. Rather it can only be deduced in the limiting case  $\lambda \rightarrow 0$ . Here appears exclusively a dependence of the interfacial reaction rate on the electric potential difference between the bulk domains [4].

### Projects



The Leibniz group, jointly with Research Groups RG 6 and RG 7 *Stochastic Algorithms and Nonparametric Statistics* and *Thermodynamic Modeling and Analysis of Phase Transitions*, participates in the Einstein Center Berlin-funded MATHEON project SE8 “Stochastic methods for the analysis of lithium-ion batteries”.

### Further activities

The international and interdisciplinary workshop ECI 2014 “Electrochemical Interfaces: Recent Topics and Open Questions” organized by the Leibniz group jointly with Jürgen Fuhrmann from Research Group RG 3 “Numerical Mathematics and Scientific Computing” took place at WIAS from September 30 to October 2, 2014; see also page 128.

In 2014, the group started a collaboration with Martin Burger's group at Westfälische Wilhelms-Universität Münster on the transport of ions through nano-channels. The objective is the application of the improved model of the Leibniz group for electrolytes in the context of biological and synthetic pores.



**Fig. 3:** ECI 2014 workshop at WIAS in Berlin

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**Fig. 4:** Dr. Clemens Guhlke at the “Energy Science Slam” of the Berlin-Brandenburg Cluster Conference Energy Technology on December 5, 2014, at the Berlin-Brandenburg Airport



## 4.10 Leibniz Group 4 “Probabilistic Methods for Mobile Ad-hoc Networks”

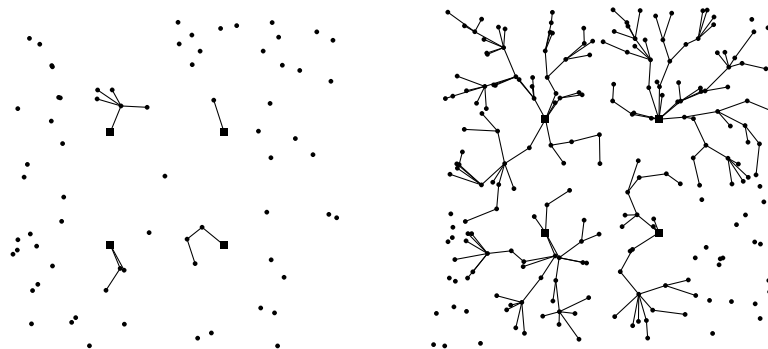
The Leibniz group resulted from a successful proposal by Wolfgang König and Robert Patterson within the competition procedure of the Leibniz Association in the Pact for Research and Innovation. The group started in July 2014. Its external funding will end in June 2017.

In cooperation with the Leibniz Institute for Innovative High Performance Microelectronics (IHP) in Frankfurt (Oder), connectivity in large mobile ad-hoc systems is studied.

### Bounded-hop percolation

The following is an account of the first research results obtained.

The first three generations of wireless telecommunication networks were based on simple cellular networks. That is, the operator installed base stations at certain fixed locations. Then, each base station was responsible for providing service at a sufficiently high level of quality to all users within a certain region of the Euclidean plane. One of the major new aspects in fourth-generation technology consists in an extension of this cellular topology through the concept of relaying. In other words, instead of sending directly to the base station, a message can be transmitted via multiple hops, where other users act as relays.



**Fig. 1:** Bounded-hop model with  $k = 5$  in the sub- (left) and supercritical (right) regime

In order to describe the behavior of this novel network type, the group developed and investigated the model of *bounded-hop percolation*. The users form a homogeneous Poisson point process in  $\mathbb{R}^d$  with some intensity  $\lambda > 0$ , whereas the base stations are installed at the sites of the hypercubic lattice  $r\mathbb{Z}^d$  for some scaling factor  $r > 0$ . In order to communicate with the base station, other users that are within a certain communication radius of a given user can serve as relay. For assessing the quality of the multi-hop network, one considers the average proportion of users in large boxes that connect to a base station in at most  $k \geq 1$  hops. Then, the group showed that, as  $r \rightarrow \infty$ , the asymptotic behavior of this quantity is closely related to continuum percolation properties of the underlying Poisson point process of users. In the subcritical regime,



the proportion of connected users tends to 0, regardless of the choice of  $k$ . In contrast, in the supercritical regime, if  $k$  grows linearly in  $r$ , then this quantity converges to a deterministic non-zero value that can be expressed in terms of certain basic characteristics of continuum percolation. The two regimes are illustrated in Figure 1, where users and base stations are represented by dots and squares, respectively.

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### 4.11 ERC Group 1 “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. The postdoc Stefania Patrizi is a member of his group, and more collaborators visited the institute to establish scientific cooperations.

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 2014, 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 “Workshop on Partial Differential Equations and Applications”, held in Pisa in February, the “CIME Course on Partial Differential Equations and Geometric Measure Theory” in Cetraro in June, and the Conference “Méthodes Géométriques et Variationnelles pour des EDPs Non-linéaires” in Lyon in September.



**Fig. 1:** Highlights of the workshop in Pisa

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 crystal dislocations, partial differential equations in anisotropic media, nonlocal diffusion equations, partial differential equations in spaces of infinite dimensions, and density estimates for some nonlocal phase transition equations.

In particular, in [1] the nonlocal heat equation is considered, and a uniqueness and representation theorem is provided for positive solutions. It is consistent with the physical interpretation of the equation, in which the solution represents an absolute temperature, which is positive due to the so-called *third principle of thermodynamics*.

In [3], a problem of atom dislocation in crystals is considered. It is proved that, at a macroscopic space and time scale, the dislocations have the tendency to concentrate at single points of the crystal, where the size of the slip coincides with the natural periodicity of the medium, and the motion of the dislocation points is governed by a repulsive potential that is superposed to an elastic reaction to the external stress. The strongly nonlocal character of the problem provides in this case additional mathematical complications.

In [6], the minimization problem of the nonlocal Allen–Cahn equation is considered. It is proved that the interface of minimizers locally divides the space in nontrivial regions in the sense of measure: that is, both the phases have positive density in the vicinity of the interface. Also, sharp energy estimates are obtained. The quantitative form of the result depends explicitly on the fractional exponent of the operator: in a sense, the smaller the degree of the operator, the larger the energy contribution in a given ball, due to the long-range particle interaction.

In [2] and [5], some partial differential equations in anisotropic media are considered, and some pointwise gradient bounds are provided. These bounds are the natural extension of the Conservation of Energy Principle, as discovered by L. Modica. Also, as a consequence, some rigidity results follow that reduce the solution to a one-dimensional function. The cases of singular and degenerate equations are also taken into account, and a study of the Wulff shape is performed.

Furthermore, Enrico Valdinoci acted as an advisor for the Ph.D. students Claudia Bucur, Alessio Fiscella, Nicola Abatangelo, and Matteo Cozzi, and for the masters student Luca Lombardini.

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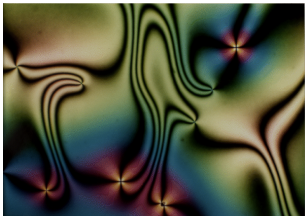
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## 4.12 ERC Group 2 “Entropy Formulation of Evolutionary Phase Transitions”

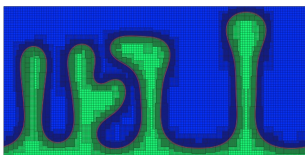
The group is meant to collect the results obtained in the ERC-StG Grant EntroPhase “Entropy Formulation of Evolutionary Phase Transitions” funded by the European Union in April 2011 and lasting five years. The group members are Elisabetta Rocca (PI) and Sergio Frigeri (PostDoc). The main group aim is to get relevant mathematical results in order to get further insight into new models for phase transitions and special materials and the corresponding evolution partial differential equation (PDE) systems. The new approach developed in the project turns out to be particularly helpful within the investigation of issues like existence, uniqueness, control, and long-time behavior of the solutions for such evolutionary PDEs.



**Fig. 1:** Binary mixtures of incompressible fluids



**Fig. 2:** Nematic liquid crystals



**Fig. 3:** Tumor growth

The importance of applying this new theory to phase transitions lies in the fact that such phenomena arise in a variety of applied problems like, e.g., melting and freezing in solid-liquid mixtures, phase changes in solids, liquid crystals flows, soil freezing, damage in elastic materials, plasticity, food conservation, collisions, and tumor growth models.

In particular, the group mainly focused on the following subjects in 2014:

- Control problems related to a nonlocal version of a model of phase separation in binary mixtures of incompressible fluids (cf., e.g. [4, 7]; see Figure 1)
- Entropic formulations for models for phase transitions in viscoelastic material, damaging phenomena, and two-phase fluids, including temperature dependence (cf., e.g. [1, 5, 6])
- Evolution and long-time behavior of liquid crystal flows (cf., e.g. [2]; see Figure 2)
- Models for tumor growth (cf., e.g., [3]; see Figure 3)

### The key idea

The key idea consists in building up new notions of solution, the so-called *entropic* solutions, reinterpreting the concept of weak solution satisfying a suitable energy conservation and entropy inequality—recently introduced by Eduard Feireisl (Prague) for a problem of heat conduction in fluids. These ideas turn out to be particularly useful in the analysis of highly nonlinear PDE systems arising from different applications and were already successfully applied in [6] and in [2], where phase transitions in thermoviscoelastic materials and liquid crystals dynamics were studied, respectively.

The models are consistent with the general principles of thermodynamics and mathematically tractable. The a priori estimates for the associated system of evolutionary partial differential equations are identified and global-in-time *entropic* solutions for arbitrary physically relevant initial data are constructed.

## Further activities

Knowledge transfer was developed via the organization of international workshops and the participation of the group members in international conferences and workshops, but also by cooperating with international experts visiting WIAS like Pavel Krejčí (Prague) on February 10–12 and May 5–10, 2014, Eduard Feireisl (Prague) and Maria Schonbek (California) on March 24–28, 2014, Flaviana Iurlano (Bonn) on March 30 – April 4, 2014, and Gabriela Marinoschi (Bucharest) on May 14–16, 2014.

### Main International Meetings and Sessions organized in 2014

- Special Session “Variational Energy and Entropy Approaches in Non-smooth Thermomechanics” of the 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, July 7–11, 2014, Madrid, organized jointly with Elena Bonetti (Pavia)
- “RIPE60 – Rate Independent Processes and Evolution” (Workshop on the occasion of Pavel Krejčí’s 60th birthday), Mathematical Institute of the Academy of Sciences of the Czech Republic, Prague, June 24–26, 2014, organized jointly with Eduard Feireisl (Prague)
- International Conference “Two Days Workshop on LC-flows”, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, March 24–25, 2014, organized jointly with Antonio Segatti (Pavia)

## References

- [1] M. ELEUTERI, E. ROCCA, G. SCHIMPERNA, *Existence of solutions to a two-dimensional model for nonisothermal two-phase flows of incompressible fluids*, WIAS Preprint no. 1966, 2014, submitted.
- [2] M. DAI, E. FEIREISL, E. ROCCA, G. SCHIMPERNA, M. SCHONBEK, *On asymptotic isotropy for a hydrodynamic model of liquid crystals*, WIAS Preprint no. 2021, 2014, submitted.
- [3] S. FRIGERI, M. GRASSELLI, E. ROCCA, *On a diffuse interface model of tumor growth*, WIAS Preprint no. 1956, 2014, submitted.
- [4] S. FRIGERI, E. ROCCA, J. SPREKELS, *Optimal distributed control of a nonlocal Cahn–Hilliard/Navier–Stokes system in 2D*, WIAS Preprint no. 2036, 2014, submitted.
- [5] C. HEINEMANN, E. ROCCA, *Damage processes in thermoviscoelastic materials with damage-dependent thermal expansion coefficients*, WIAS Preprint no. 1937, 2014, to appear in: Math. Methods Appl. Sci.
- [6] E. ROCCA, R. ROSSI, *“Entropic” solutions to a thermodynamically consistent PDE system for phase transitions and damage*, WIAS Preprint no. 1931, 2014, submitted.
- [7] E. ROCCA, J. SPREKELS, *Optimal distributed control of a nonlocal convective Cahn–Hilliard equation by the velocity in 3D*, WIAS Preprint no. 1942, 2014, submitted.



**Fig. 4:** Two Days Workshop on LC-flows, March 24–25, 2014





# 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
- Membership in Organizing Committees (non-WIAS)
- Publications
- Preprints, Reports
- Talks, Posters, and Contributions to Exhibitions
- Visits to other Institutions
- Academic Teaching
- Weierstrass Postdoctoral Fellowship Program
- Visiting Scientists
- Guest Talks
- Software

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

### A.1.1 Calls

1. CH. BAYER, Senior lectureship, December 17, Linköping University, Department of Mathematics.
2. TH. DICKHAUS, W2 professorship, November 10, Technische Hochschule Wildau, Fachbereich Wirtschaft, Informatik, Recht.
3. ———, W3 professorship, September 22, Universität Bremen, Fachbereich Mathematik/Informatik.
4. ST. NEUKAMM, W2 professorship, July 29, Technische Universität Dresden, Fakultät Mathematik und Naturwissenschaften.

### A.1.2 Awards and Distinctions

1. R. HILDEBRAND, 2013 *Optimization Letters Best Paper Award* for the paper “Scaling relationship between the copositive cone and Parrilo’s first level approximation”, jointly authored with Peter J.C. Dickinson, Mirjam Duer, and Luuk Gijben, and published in *Optim. Lett.*, 7:8 (2013), December 1.
2. D. KNEES, Vice chair of the GAMM Activity Group “Analysis of Partial Differential Equations”, Gesellschaft für Angewandte Mathematik und Mechanik.
3. A. MIELKE, Head of the Secretariat of the International Mathematical Union (IMU).
4. ———, Member of the IMU Berlin Einstein Foundation Program Committee.
5. ———, Treasurer of IMU.
6. ST. NEUKAMM, ISIMM Junior Prize, September 8, 2014.
7. E. ROCCA, ISIMM Junior Prize, September 8, 2014.
8. J. SPREKELS, International Member of the Physical Sciences, Mathematics and Engineering Panel (Main Panel B) in the Research Excellence Framework (REF2014) of Great Britain, 2014.
9. ———, Member of the Scientific Advisory Committee of the Centrum Wiskunde & Informatica (CWI, Amsterdam), 2014.
10. M. THOMAS, GAMM Junior, Gesellschaft für Angewandte Mathematik und Mechanik, 2013–2015.

### A.1.3 Habilitations

1. O. KLEIN, *Darstellung von Hysterese-Operatoren mit stückweise monotaffinen Input-Funktionen durch Funktionen auf Strings*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, February 10.
2. E. ROCCA, qualified as Full Professor in Mathematical Analysis at the Abilitazione Scientifica Nazionale (National Scientific Qualification), Italy, November 14.

### A.1.4 Ph.D. Theses

1. S. BECKER, *The Propagation-Separation Approach*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. P. Mathé, May 8.
2. K. CHOUK, *Three controlled paths*, Dauphine Université Paris, Research Centre in Mathematics of Decision, supervisor: Prof. Dr. P. Friz, January 20.
3. A. FIEBACH, *A dissipative finite volume scheme for reaction-diffusion systems in heterogeneous materials*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, June 12.
4. A. FISCELLA, *Variational problems involving non-local elliptic operators*, Università degli Studi di Milano, Facoltà di Scienze Matematiche, Fisiche e Naturali, supervisor: Prof. Dr. E. Valdinoci, December 12.
5. C. PATZ, *On dynamics of Hamiltonian systems on infinite lattices*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, February 24.
6. N. TOGOBYTSKA, *Multiphase steels: Modelling parameter identification and optimal control*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 19.
7. TH. ARNOLD, *Scattering of plane waves by rough surfaces in the sense of Born approximation*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, March 10.
8. B. BUGERT, *On integral equation methods for electromagnetic scattering by bi-periodic structures*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, June 2.
9. A. CIPRIANI, *High points of a Gaussian free field and a Gaussian membrane model and limit shape of Young diagrams for random permutations*, Universität Zürich, Mathematisch-naturwissenschaftliche Fakultät, supervisor: Prof. Dr. E. Bolthausen, January 14.
10. C. GUHLKE, *Theorie der elektrochemischen Grenzfläche*, Technische Universität Berlin, Fakultät V – Verkehrs- und Maschinensysteme, supervisor: Prof. Dr. W. Dreyer, November 7.
11. H. HANKE, *Rigorous derivation of two-scale and effective damage models based on microstructure evolution*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, August 25.
12. CH. HIRSCH, *Connectivity and percolation properties of stochastic networks*, Universität Ulm, Fakultät Mathematik und Wirtschaftswissenschaften, supervisor: Prof. Dr. V. Schmidt, December 16.
13. S. JACHALSKI, *Derivation and analysis of lubrication models for two-layer thin-films*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. B. Wagner, May 26.
14. TH. PETZOLD, *Modelling, analysis and simulation of multifrequency induction hardening*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, May 19.
15. K. STURM, *On shape optimization with non-linear partial differential equations*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, October 9.

### A.1.5 Undergraduate-degree Supervision

1. L. BLANK, *On divergence-free finite element methods for the Stokes equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, September 24.

2. M. BRAND, *Modellierung der Bahnplanung für einen polygonalen Roboter* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 20.
3. L. BRUST, *Das Sekretärinnenproblem mit erweiterten Wahlmöglichkeiten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 4.
4. A. BUSA, *The Leray- $\alpha$  model of turbulence* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, August 21.
5. J. BUSHE, *Fluktuationen im Random-Energy-Modell* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 4.
6. F. CLAUSS, *Abweichungen für die normierten Lokalzeiten einer Irrfahrt mit zufälligen Leitfähigkeiten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 15.
7. P. CRAJA, *Stochastische Analyse des Sekretärinnenproblems* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 11.
8. L. EBERMANN, *Langzeitverhalten von Selbstüberschneidungslokalzeiten ergodischer Markovketten in stetiger Zeit* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 26.
9. TH. FRENZEL, *Von Swift-Hohenberg nach Ginzburg-Landau mit evolutionärer Gamma-Konvergenz* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, December 3.
10. A. HARTMANN, *Die Odds-Strategie im Sekretärinnenproblem* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 6.
11. L. HOFFMANN, *Die Schrödingergleichung und Verzweigungsprozesse* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 19.
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, July 17.
13. S. JACHNIK, *Konnektivität im Boole'schen Modell zu einem Gitter bei beschränkter Reichweite* (bachelor's thesis), Technische Universität Berlin, Fakultät II—Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 31.
14. K. KAISER, *Finite element methods for the incompressible Stokes equations with non-constant viscosity* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, June 7.
15. M. KODDENBROCK, *Effizienz und Genauigkeit einer divergenzfreien Diskretisierung für die stationären inkompressiblen Navier-Stokes-Gleichungen* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Linke, June 7.
16. M. KRÄMER, *Punktprozesskonvergenz für Eigenwerte zufälliger heavy-tailed Matrizen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 17.
17. 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, July 17.
18. M. MARQUARDT, *Die Ratenfunktion im Prinzip großer Abweichungen für das Random Waypoint Model* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 15.

19. M. MARSHALL, *Subballistizität der selbstvermeidenden Irrfahrt* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 15.
20. P. MASCHER, *A powerful goodness-of-fit test with locally uniform calibration* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, August 11.
21. ST. MELCHIONNA, *L'Equazione di Cahn–Hilliard nonlocale con reazione: Esistenza unicità e regolarità* (master's thesis), Università di Milano, Dipartimento di Matematica, supervisor: Prof. Dr. E. Rocca, September 24.
22. M. MITTENZWEIG, *Entropy production inequalities for heat equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. A. Mielke, Priv.-Doz. P. Gurevich, December 26.
23. A.B. NASRALLAH, *Mischeigenschaften des Random Way-Point Modells* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 1.
24. K. NOWORYTA, *Verzweigungsprozesse in zufälligen Medien auf einem vollständigen Graphen* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 18.
25. M. ORLT, *Verzweigungsprozesse in zufälligen Medien auf einem endlichen Graphen* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 8.
26. K.H. PHI, *Konvergenzgeschwindigkeiten in der Extremwerttheorie* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 10.
27. E. QUEIROLO, *Isogeometric analysis for Navier–Stokes equations (jointly with Luca Dedé)* (master's thesis), Ecole Polytechnique Fédérale de Lausanne, Section de Mathématiques, supervisor: Prof. Dr. V. John, July 17.
28. T. RENKER, *Extremwerttheorie und Copulas* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 15.
29. E. ROLLY, *Maxima von unabhängigen, nicht identisch verteilten Gauß'schen Vektoren* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 13.
30. M.H. SANCO RICO, *Ein zufälliges Polymer in stetiger Zeit mit Wand und Drift* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 22.
31. J. SCHMIDT, *Maxima von Summen unabhängiger identisch verteilter Zufallsgrößen* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, November 30.
32. J. SCHUBERT, *Extremwertstatistik für mischende stationäre Prozesse* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 30.
33. C. SCHUNKE, *Ein zufälliges Polymer mit Attraktion in zufälligem Medium* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 25.
34. S. STACHELHAUS, *Ein zufälliges Polymer in stetiger Zeit mit Attraktion zur Null* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 23.

35. L. VESTWEBER, *Über den semiklassischen Grenzwert der Schrödingergleichung mit unstetigem Potential* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, May 30.



## A.2 Grants<sup>1</sup>

### 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

#### ■ KMU-innovativ (Program for innovative small and medium-sized enterprises)

“Verbundprojekt EPILYZE: DNA Methylierungs-Signaturen als innovative Biomarker für die quantitative und qualitative Analyse von Immunzellen” (Joint project EPILYZE: DNA methylation signatures as innovative biomarkers for the quantitative and qualitative analysis of immune cells; in RG 6)

#### ■ 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)

“Professionalisierung und Verstetigung des Verwertungskonzeptes am Weierstraß-Institut für Angewandte Analysis und Stochastik – WIAS” (Professionalization and implementation of dissemination strategies at WIAS)

#### ■ 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)

<sup>1</sup>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, until May 31, 2014**

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)

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/Transregio (TRR) 154, Friedrich-Alexander-Universität Erlangen-Nürnberg**

**“Mathematische Modellierung, Simulation und Optimierung am Beispiel von Gasnetzwerken” (Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks)**

“Nichtlineare Wahrscheinlichkeitsrestriktionen in Gastransportproblemen” (Nonlinear chance constraints in problems of gas transportation; in RG 4)

■ **Collaborative Research Center (SFB) 649, Humboldt-Universität zu Berlin**

**“Ökonomisches Risiko” (Economic Risk)**

B5: “Structural methods in risk modeling” (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)
- **Collaborative Research Center (SFB) 1114**, Freie Universität Berlin  
**“Skalenkaskaden in komplexen Systemen” (Scaling Cascades in Complex Systems)**  
 B01: “Störungszonennetzwerke und Skaleneigenschaften von Deformationsakkumulation” (Fault networks and scaling properties of deformation accumulation; in RG 1)  
 C05: “Effektive Modelle für mikroskopisch strukturierte Trennflächen” (Effective models for interfaces with many scales; in RG 1)  
 C08: “Stochastische räumliche koagulierende Partikelprozesse” (Stochastic spatial coagulation particle processes; in RG 5)
- **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 1506: “Fluide Grenzflächen” (Transport Processes at Fluidic Interfaces)**, Technische Universität Darmstadt and Rheinisch-Westfälische Technische Universität Aachen  
 “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 environment with 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)

- **Priority Program SPP 1748: “Zuverlässige Simulationstechniken in der Festkörpermechanik – Entwicklung nichtkonventioneller Diskretisierungsverfahren, mechanische und mathematische Analyse” (Reliable Simulation Techniques in Solid Mechanics – Development of Non-standard Discretisation Methods, Mechanical and Mathematical Analysis)**, Universität Duisburg-Essen

“Finite-Elemente-Approximation von Funktionen beschränkter Variation mit Anwendungen in der Modellierung von Schädigung, Rissen und Plastizität” (Finite element approximation of functions of bounded variation and application to models of damage, fracture, and plasticity; in RG 1)

- **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

“Multiple testing under unspecified dependency structure” (in RG 6)

“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)

“Inferenzstatistische Methoden für Verhaltensgenetik und Neuroökonomie” (Statistical inference methods for behavioral genetics and neuroeconomics; in RG 6)

“Zufälliger Massenfluss durch zufälliges Potential” (Random mass flow through random potential; in RG 5)

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

“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)

“Inverse Fluid-Solid-Kopplungsprobleme” (Inverse fluid-solid interaction problems; 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”)**

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

“Probabilistische Methoden für Kommunikationsnetzwerke mit mobilen Relais” (Probabilistic methods for communication networks with mobile relays; in LG 4)

### Einstein Stiftung Berlin (Einstein Foundation Berlin)

#### ■ Einstein-Zentrum für Mathematik Berlin (Einstein Center for Mathematics Berlin)

Research Center MATHEON with the projects (started June 1, 2014):

OT1: “Mathematical modeling, analysis, and optimization of strained germanium microbridges” (in RG 1)

OT2: “Turbulence and extreme events in nonlinear optics” (in RG 2)

SE2: “Electrothermal modeling of large-area OLEDs” (in RG 1)

SE4: “Mathematical modeling, analysis and novel numerical concepts for anisotropic nanostructured materials” (in RG 7 and YSG)

SE7: “Optimizing strategies in energy and storage markets” (in RG 6)

SE8: “Stochastic methods for the analysis of lithium-ion batteries” (in RG 6 and RG 7)

SE13: “Topology optimization of wind turbines under uncertainties” (in RG 4)

#### ■ Two scholarship holders of the IMU Berlin Einstein Foundation Program (in RG 1); see page 187

### Investitionsbank Berlin

#### ■ Programm zur Förderung von Forschung, Innovationen und Technologien (*Pro FIT*) (Support program for research, innovation and technology)

“Erforschung effizienter mathematischer Methoden zur Modellkalibrierung und Unbestimmtheitsabschätzung in Umweltsituationen (MUSI)” (Efficient mathematical methods for model calibration and uncertainty estimation in environmental simulations; in RG 3 and RG 4)

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

#### ■ A Humboldt Research Fellowship holder (in RG 3); see page 187

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

#### ■ A Leibniz-DAAD Research Fellowship holder (in RG 3); see page 187

### International projects

#### ■ 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 $\text{CuInS}_2$ -Chalkopyrit” (2D and 3D simulations of the particular thin-film solar-cell models based on $\text{CuInS}_2$ chalcopyrite; in RG 1)

#### ■ Max Planck Institute for Physics, Munich, and Max Planck Institute for Extraterrestrial Physics, Garching: Simulation of semiconductor devices for radiation detectors (in RG 3)

#### ■ TOTAL E&P RECHERCHE DEVELOPPEMENT, Courbevoie, France: “Improved algorithms and software for hybrid volumetric meshing based on Voronoi diagrams for geological models” (in RG 3)

### A.3 Membership in Editorial Boards<sup>2</sup>

1. TH. DICKHAUS, Editorial Board, Annals of the Institute of Statistical Mathematics, Springer-Verlag, Heidelberg.
2. ———, Editorial Board, Statistics, Taylor & Francis, Berlin.
3. P. FRIZ, Editorial Board, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
4. ———, Editorial Board, Monatshefte der Mathematik, Springer-Verlag, Berlin.
5. ———, Editorial Board, Stochastic Processes and Applications, Elsevier, Oxford, UK.
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, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
18. ———, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
19. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
20. ———, Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
21. H. NEIDHARDT, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
22. ———, Editorial Board, Journal of Operators, Hindawi Publishing Corporation, New York, USA.

<sup>2</sup>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.



23. ———, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russia.
24. J. POLZEHL, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
25. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
26. J.G.M. SCHOENMAKERS, Editorial Board, Applied Mathematical Finance, Taylor & Francis, Oxford, UK.
27. ———, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
28. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
29. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
30. V. SPOKOINY, Editor, Theory of Probability and its Applications, SIAM, Philadelphia, Pennsylvania, USA.
31. J. SPREKELS, Editor, Advances in Mathematical Sciences and Applications, Gakkōtoshō, Tokyo, Japan.
32. ———, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
33. ———, Editorial Board, Applied Mathematics and Optimization, Springer-Verlag, New York, USA.
34. ———, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
35. W. WAGNER, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.

## A.4 Conferences, Colloquia, and Workshops

### A.4.1 WIAS Conferences, Colloquia, and Workshops

MURPHYS-HSFS-2014 — “7TH INTERNATIONAL WORKSHOP ON MULTI-RATE PROCESSES & HYSTERESIS” IN CONJUNCTION WITH “2ND INTERNATIONAL WORKSHOP ON HYSTERESIS AND SLOW-FAST SYSTEMS”

Berlin, April 7–11

Organized by: WIAS (RG 7 and YSG), Freie Universität Berlin, Stefan cel Mare University (Suceava, Romania), University College Cork (Ireland)

Supported by: DFG Research Center MATHEON, DFG Collaborative Research Center 910 “Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, WIAS

The 7th International Workshop on Multi-Rate Processes & Hysteresis continued a series of biennial conferences and was held in conjunction with the 2nd International Workshop on Hysteresis and Slow-Fast Systems, being the follow-up of the HSFS workshop organized in Lutherstadt Wittenberg in 2011. It was organized by Olaf Klein (RG 7), jointly with Mihai Dimian (Suceava), Pavel Gurevich (Berlin), Dorothee Knees, (WIAS/Kassel), Dmitrii Rachinskii (Dallas), and Sergey Tikhomirov (Leipzig).

The joint workshop was devoted to the mathematical theory and applications of systems with hysteresis and multiple temporal and spatial scales. More than 60 scientists from nine European countries and from the USA participated in the workshop. The program featured 49 talks, including 15 main lectures and 15 invited talks on the mathematical theory and applications of systems with hysteresis for multiple temporal and spatial scales. Recent mathematical results for systems with hysteresis operators, rate-independent systems, systems with energetic solutions, singularly perturbed systems, and systems with stochastic effects were presented. The applications included magnetization dynamics, biological systems, smart materials, networks, ferroelectric and ferroelastic hysteresis, fatigue in materials, market models with hysteresis, bio-medical applications, chemical reactions, noise-induced phenomena, partially saturated soils, colloidal films, and the evaporation of automotive fuel droplets.

FIRST BERLIN SINGAPORE WORKSHOP ON QUANTITATIVE FINANCE & FINANCIAL RISK

Berlin, May 21–24

Organized by: WIAS (RG 6), HU Berlin, TU Berlin, NUS Singapore

Supported by: Berlin Mathematical School, Quantitative Finance Laboratory (Singapore)

This workshop was the first of a series with the aim of establishing a sustainable cooperation between Singapore and Berlin. It was a collaboration between Humboldt Universität (HU) Berlin, Technische Universität (TU) Berlin, WIAS, and the Center for Quantitative Finance at the National University of Singapore (NUS).

The workshop was held at WIAS on May 21–22 and at HU Berlin on May 23–24. Four plenary lectures, 19 invited and 6 contributed talks were delivered, and there were more than 60 participants.

KOMSO CHALLENGE WORKSHOP “MATH FOR THE DIGITAL FACTORY”

Berlin, May 7–9

Organized by: WIAS (RG 4)

Supported by: ECMI, Committee for Mathematical Modeling, Simulation and Optimization (KoMSO), Research Center MATHEON, WIAS

The workshop was the kick-off meeting for the new Special Interest Group on digital manufacturing of the European Consortium for Mathematics in Industry (ECMI). Participants from 10 European countries and Japan, 41 from academia and 10 from industry, discussed scientific challenges related to digital manufacturing. In 22 talks, participants discussed topics like multibody and partial differential equation systems of production processes, discrete and continuous models of production planning as well as aspects of energy efficiency related to machine tools and more complex production systems.

## NONLINEAR DYNAMICS IN SEMICONDUCTOR LASERS (NDSL14)

Berlin, May 12–14

Organized by: WIAS (RG 2)

Supported by: Research Center MATHEON, DFG Collaborative Research Centre 787 “Semiconductor Nanophotonics: Materials, Models, Devices”, Marie Curie Initial Training Network PROPHET, WIAS

The aim of the workshop was to bring together applied mathematicians and scientists from semiconductor physics and to give them the opportunity to exchange experience in the field of nonlinear phenomena in semiconductor lasers. The main topics of the workshop were

- Bifurcation theory, analytical and numerical methods in optoelectronics
- Quantum dot and quantum dash lasers
- Mode-locked lasers
- Dynamics of ring and multisection lasers
- Dynamics of lasers with delayed feedback
- High-power tapered and broad-area lasers and amplifiers

The workshop was attended by more than 66 participants from 11 countries. 36 talks and 7 posters were presented.

## FVCA7 – THE INTERNATIONAL SYMPOSIUM OF FINITE VOLUMES FOR COMPLEX APPLICATIONS VII

Berlin, June 15–20

Organized by: WIAS (RG 1 and RG 3), Universität Heidelberg, Université Paris-Est, Czech Technical University (CTU) Prague, Freie Universität Berlin, Westfälische Wilhelms-Universität (WWU) Münster, Universität Stuttgart

Supported by: Stuttgart Research Centre for Simulation Technology, CTU Prague, DFG, DFG Priority Program 1276 “MetStröm – Multiple Scales in Fluid Mechanics and Meteorology”, WWU Münster, WIAS

The triennial series of International Symposia on Finite Volumes for Complex Applications – Problems and Perspectives brings together mathematicians, physicists, and engineers interested in physically motivated discretizations, with a special emphasis on finite volume methods. Previous conferences of this series were held in Rouen (1996), Duisburg (1999), Porquerolles (2002), Marrakech (2005), Aussois (2008), and Prague (2011). FVCA7 was held in Berlin on June 15–20, 2014, at the conference center of the Berlin Brandenburg Academy of Sciences.

The conference had 147 participants from 17 countries, among them 7 invited speakers. All conference contributions were published in a two-volume edition of the „Springer Proceedings in Mathematics and Statistics“.

## BMS-WIAS SUMMER SCHOOL “APPLIED ANALYSIS FOR MATERIALS”

Berlin, August 25 – September 5

Organized by: WIAS (RG 5), BMS, MASDOC (Warwick)

Supported by: BMS, MASDOC, WIAS

The annual Summer School of the Berlin Mathematical School (BMS) in 2014 was devoted to one of the core subjects of WIAS: to applied analysis for the description of materials. The head of RG 5, Wolfgang König, took the scientific organization into his hands, and a number of WIAS members gave lecture series in some of their core topics, among them the heads of RG 1, RG 2, RG 4, and the YSG. This summer school was organized jointly with the Mathematics and Statistics Centre for Doctoral Training (MASDOC) of the University of Warwick, who contributed also some internationally well-known speakers. The local organization by the BMS staff was extremely efficient, as always. About 60 young people from all over the world attended the school. The two-week event was complemented by a welcome party and a closing event, such that also social contacts benefited. The school was an excellent opportunity for the WIAS researchers to get into close contact with highly interested and gifted young people.

## ELECTROCHEMICAL INTERFACES: RECENT TOPICS AND OPEN QUESTIONS

Berlin, September 30 – October 2

Organized by: WIAS (LG 3 and RG 3)

Supported by: Research Initiative Energy Storage Systems of the German Federal Government, Leibniz Association, Research Center MATHEON, WIAS

The international and interdisciplinary workshop “Electrochemical Interfaces: Recent Topics and Open Questions” organized by the Leibniz Group LG 3 *Mathematical Models for Lithium-ion Batteries* jointly with Jürgen Fuhrmann from the Research Group RG 3 *Numerical Mathematics and Scientific Computing* took place at WIAS on September 30 – October 2, 2014. The workshop provided a platform to discuss the latest findings and open problems particularly related to the modeling of electrochemical interfaces. It brought together 47 scientists from eight countries. Important topics were the role of continuum models, analysis, and simulations in cooperation with experimentalists and industrial people. The relationships between different modeling approaches like atomistic versus continuum models and homogenized models were intensively discussed.

## COLLECTIVE DYNAMICS IN COUPLED OSCILLATOR SYSTEMS

Berlin, November 24–26

Organized by: WIAS (RG 2), HU Berlin

Supported by: Collaborative Research Center 910 “Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, WIAS

Recent research showed that systems of coupled oscillators can exhibit a huge variety of collective behavior and complex dynamical regimes. The understanding of such phenomena, as ,e.g., the emergence of various types of coherence incoherence patterns, sometimes called *chimera states*, implicates intriguing questions from various fields of mathematics. The workshop was organized by Matthias Wolfrum (RG 2) and Serhiy Yanchuk (Humboldt-Universität (HU) zu Berlin) to discuss approaches including dynamical systems theory, statistical physics, stochastic phenomena, applications, and experiments. It brought together 75 scientists from 10 countries.

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

## SADCO-WIAS YOUNG RESEARCHER WORKSHOP

Berlin, January 29–31

Organized by: WIAS, Universität Bayreuth, Imperial College London

Supported by: EU (7th Framework Program “FP7-PEOPLE-2010-ITN”)

Organized by Jürgen Sprekels (RG 7), Roberto Guglielmi (Universität Bayreuth), and Michele Palladino (Imperial College London), the second edition of the Young Researcher Workshop intended to gather current and past fellows of the Initial Training Network “Sensitivity Analysis for Deterministic Controller Design” (SADCO) with contributions from WIAS researchers, in order to share overviews and backgrounds on subjects related to the optimal control of partial and ordinary differential equations. The topics discussed included necessary and sufficient optimality conditions, sensitivity analysis, model predictive control, large scale systems, system stabilization, game theory, the Hamilton Jacobi–Bellman equation, numerical methods for optimal control, optimal control of PDEs, and stochastic control. About 35 young researchers participated in the workshop. 14 talks were given.

### YOUNG EUROPEAN PROBABILISTS (YEP) XI: MASS TRANSPORT IN ANALYSIS AND PROBABILITY

Eindhoven, March 10–14

Organized by: WIAS (RG 1), Universität Leipzig, University of Bath

Supported by: Stochastics – Theoretical and Applied Research (Dutch research cluster), ESF (Random Geometry of Large Interacting Systems and Statistical Physics)

The field of optimal transport has recently seen a major boost of activity with many different focal points, including: geometry in discrete/continuous and general metric spaces, Sobolev inequalities and gradient flows, random measures, hydrodynamic limits and large deviations of particle systems, and applications to financial mathematics, kinetic theory and quantum mechanics. This year's YEP workshop aimed at bringing together promising young European researchers from both analysis and probability to expose them to some of the most recent developments in optimal transport, and to provide a forum for the exchange of ideas and a starting point for future intradisciplinary collaborations.

The workshop consisted of four mini-courses by eminent researchers in the field (Nicola Gigli, Université de Nice, Mathias Beiglböck, Universität Wien and Universität Bonn, Jan Maas, Universität Bonn, and Gero Friesecke, Technische Universität München), augmented with presentations of sixteen young researchers, who talked about their own research topic. In total, there were 42 participants, which was more than envisaged. Both the facilities and the informal format lead to active participation and stimulating cross-community interactions.

### TWO DAYS WORKSHOP ON LC FLOWS

Pavia, March 24–25

Organized by: WIAS (ERC 2), Istituto di Matematica Applicata e Tecnologie Informatiche Enrico Magenes (CNR, Pavia)

Supported by: ERC Starting Grant “EntroPhase”, National Group for Mathematical Analysis, Probability and Related Applications of Italian National Institute of Higher Mathematics “F. Severi”

The aim of the workshop was to bring together young researchers and leading experts in the analysis and modeling of liquid crystals and to promote stimulating discussions on the most recent advances in the field. The program featured 13 invited lectures, and the workshop was attended by 30 participants.

### BERLIN – PADOVA YOUNG RESEARCHERS MEETING “STOCHASTIC ANALYSIS AND APPLICATIONS IN BIOLOGY, FINANCE AND PHYSICS”

Berlin, October 23–25

Organized by: DFG RTN 1845 “Stochastic Analysis with Applications in Biology, Finance and Physics”

Supported by: TU Berlin, Universität Potsdam, Einstein Center for Mathematics Berlin, Berlin Mathematical School, University of Padua, WIAS

The aim of this workshop was to bring together young researchers in probability, and let them present their recent results in a stimulating environment for the exchange of ideas. The workshop took place at three different locations, among them WIAS. It was one of the activities of the DFG Graduate School in Stochastic Processes, jointly with its strategic partner, the University of Padua, to which there exist a lot of fruitful connections. Three distinguished speakers gave survey lectures. Apart from these, a large number of short talks were given by young participants from Berlin and Padua, but also from other German cities. About 60 participants enjoyed the talks and the relaxed atmosphere provided by the WIAS premises and organization.

### WORKSHOP ON RECENT ADVANCES IN HIGH-FREQUENCY STATISTICS

Berlin, November 20–21

Organized by: WIAS (RG 6), Humboldt-Universität (HU) zu Berlin

Supported by: DFG Collaborative Research Center 649 “Economic Risk”, International Research Training Group 1792 “High Dimensional Non Stationary Time Series”, DFG Research Unit 1735 “Structural Inference in Statistics: Adaptation and Efficiency”

From November 20 to 21, the “Workshop on Recent Advances in High-Frequency Statistics” took place at the Weierstrass Institute. Distinguished speakers presented their recent research projects related to the field in

an open inspiring atmosphere and discussed perspectives for future developments. The organizing committee Markus Bibinger (HU), Nikolaus Hautsch (Vienna), Marc Hoffmann (Paris), Markus Reiß (HU), and Vladimir Spokoiny (RG 6) invited as speakers Torben Andersen (Evanston), Emmanuel Bacry (Palaiseau), Peter Hansen (Florence), Marc Hoffmann (Paris/Berlin), Jean Jacod (Paris), Nour Meddahi (Toulouse), Per Mykland (Chicago), Mark Podolskij (Aarhus), Mathieu Rosenbaum (Paris), Viktor Todorov (Evanston), and Mathias Vetter (Marburg) to gather experts currently working on important topics related to high-frequency financial data, both on empirical and methodological aspects. Almost sixty interested participants from twenty different institutions were present in the audience. A poster session provided a platform for young researchers working in this area, including members of the organizing institutions and as well foreign guests, to present their research and get in touch with the participants and invited speakers.

#### EXTREMA OF BRANCHING PROCESSES AND GAUSSIAN FREE FIELDS

Berlin, November 28–29

Organized by: WIAS (RG 5), TU Berlin

Supported by: Einstein Foundation Berlin, Berlin Mathematical School, TU Berlin, WIAS

The aim of this event was to bring together distinguished researchers in the field of branching processes and Gaussian free fields, and give them a stimulating environment for the exchange of ideas and the presentation of their latest results. The workshop took place at two different locations, among them WIAS. It managed to gather together 10 of the most prominent researchers in the area, among whom Ofer Zeitouni (Rehovot), Jian Ding (Chicago), and Remi Rhodes (Paris). The attendance was of about 40 participants coming mainly from Germany, but also from France, the UK, and outside Europe. The joint organization of WIAS and Technische Universität (TU) Berlin managed to enhance the scientific aspect of the workshop with a friendly and relaxed atmosphere.

### A.4.3 Oberwolfach Workshops co-organized by WIAS

#### WORKSHOP “VARIATIONAL METHODS FOR EVOLUTION”

Mathematisches Forschungsinstitut Oberwolfach, December 15–20

Organized by: Luigi Ambrosio (Pisa), Alexander Mielke (RG 1), Mark Peletier (Eindhoven), Giuseppe Savaré (Pavia)

About 50 pure and applied mathematicians discussed a wide range of topics in the field of evolutionary equations. This included large deviation and variational principles, rate-independent evolution and gradient flows, heat flows in metric-measure spaces, applications of optimal transport and entropy-entropy dissipation methods for Markov processes, and many more. The main goal of the workshop, the systematic encouragement of intense discussions between researchers in the fields of analysis and stochastics, was achieved to a high extent.

## A.5 Membership in Organizing Committees of non-WIAS Meetings<sup>3</sup>

1. U. BANDELOW, head of the Award Committee, *International Nano-Optoelectronics Workshop (iNOW 2014)*, Luga and St. Petersburg, Russia, August 10–22.
2. CH. BAYER, co-organizer, *Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis*, University of Oxford, Oxford-Man Institute of Quantitative Finance, UK, July 1–2.
3. M. EIGEL, co-organizer of the minisymposium “Low-Rank and Sparse Representation Methods for Uncertainty Quantification”, *SIAM Conference on Uncertainty Quantification (UQ14)*, Savannah, USA, March 31 – April 3.
4. P. FRIZ, co-organizer, *Rough Paths: Theory and Applications*, University of California Los Angeles, Institute for Pure and Applied Mathematics, USA, January 27–31.
5. ———, organizer, *11th German Probability and Statistics Days 2014*, Universität Ulm, March 4–7.
6. ———, co-organizer, *Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis*, University of Oxford, Oxford-Man Institute of Quantitative Finance, UK, July 1–2.
7. ———, organizer of the invited session “Rough Paths”, *Australian Statistical Conference in conjunction with the Institute of Mathematical Statistics Annual Meeting*, The University of Sydney, School of Mathematics and Statistics, Australia, July 7–11.
8. ———, co-organizer, *IHP Trimester “Geometry, Analysis and Dynamics on Sub-Riemannian Manifolds”*, Institut Henri Poincaré, Paris, France, October 6–10.
9. A. GLITZKY, co-organizer, *Kick-Off Meeting of the ECMI Special Interest Group “Sustainable Energy” on Nanostructures for Photovoltaics and Energy Storage*, Technische Universität Berlin, Institut für Mathematik, December 8–9.
10. D. HÖMBERG, organizer of the minisymposium “Simulation and Control of Hot-Rolling”, *The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014)*, Taormina, Italy, June 9–13.
11. TH. KOPRUCKI, co-organizer, *Kick-Off Meeting of the ECMI Special Interest Group “Sustainable Energy” on Nanostructures for Photovoltaics and Energy Storage*, Technische Universität Berlin, Institut für Mathematik, December 8–9.
12. A. MIELKE, co-organizer, *13th GAMM Seminar on Microstructures*, Ruhr-Universität Bochum, Lehrstuhl für Mechanik – Materialtheorie, January 17–18.
13. TH. PETZOLD, organizer of the minisymposium “Recent Trends in Modeling, Analysis, and Simulation of Induction Heat Treatments”, *The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014)*, Taormina, Italy, June 9–13.
14. E. ROCCA, co-organizer, *RIPE60 – Rate Independent Processes and Evolution Workshop*, Prague, Czech Republic, June 24–26.
15. ———, co-organizer of the special session 31 “Variational Energy and Entropy Approaches in Non-Smooth Thermomechanics”, *The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications*, Madrid, Spain, July 7–11.
16. V. SPOKOINY, organizer, *International Workshop “Advances in Optimization and Statistics”*, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, May 15–16.

<sup>3</sup>Membership in organizing committees of non-WIAS meetings by guests during their long-term stay at WIAS have been listed in front of those by the WIAS staff members.



17. ———, member of the Program Committee, *Information Technologies and Systems (ITaS2014)*, Russian Academy of Sciences, Institute for Information Transmission Problems, Nizhny Novgorod, September 1–5.
18. ———, member of the Program Committee, *International Scientific Conference “Science of the Future”*, Ministry of Education and Science of the Russian Federation, St. Petersburg, September 17–20.
19. ———, co-organizer, *Stochastics, Statistics, Financial Mathematics*, Russian Academy of Sciences, Steklov Mathematical Institute, Moscow, October 13–15.
20. E. VALDINOCI, co-organizer, *Méthodes Géométriques et Variationnelles pour des EDPs Non-linéaires*, Université Lyon 1, Institut C. Jordan, France, September 1–5.
21. B. WAGNER, organizer of the minisymposium 39 “Models of Drift-Diffusion for Concentrated Solutions”, *The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014)*, Taormina, Italy, June 9–13.
22. ———, organizer of the minisymposium 40 “Mathematical Modeling of Photovoltaic Devices”, *The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014)*, Taormina, Italy, June 9–13.
23. ———, co-organizer, *Kick-Off Meeting of the ECMI Special Interest Group “Sustainable Energy” on Nanostructures for Photovoltaics and Energy Storage*, Technische Universität Berlin, Institut für Mathematik, December 8–9.

## A.6 Publications

### A.6.1 Monographs

- [1] TH. DICKHAUS, *Simultaneous Statistical Inference*, Springer, Berlin et al., 2014, 180 pages.
- [2] P. FRIZ, M. HAIRER, *A Course on Rough Paths: With an Introduction to Regularity Structures*, Universitext, Springer, Berlin et al., 2014, 251 pages.
- [3] CH. HEINEMANN, CH. KRAUS, *Phase Separation Coupled with Damage Processes: Analysis of Phase Field Models in Elastic Media*, Springer Fachmedien, Wiesbaden, 2014, 173 pages.
- [4] M. EHRHARDT, TH. KOPRUCKI, eds., *Multi-Band Effective Mass Approximations — Advanced Mathematical Models and Numerical Techniques*, vol. 94 of Lecture Notes in Computational Science and Engineering, Springer, Cham et al., 2014, xvi+318 pages.

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### A.7.2 Preprints/Reports in other Institutions

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## A.8 Talks, Posters, and Contributions to Exhibitions

### A.8.1 Main and Plenary Talks

1. W. DREYER, *Modeling of the non-local and non-linear behavior of many-particle electrodes*, MORE Conference “Modeling, Analysis and Computing in Nonlinear PDEs”, September 21–26, Chateau Liblice, Czech Republic, September 24.
2. P. FRIZ, *Rough integration with jumps*, Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis, July 1–2, University of Oxford, Oxford-Man Institute of Quantitative Finance, UK, July 2.
3. R. HENRION, *Calmness as a constraint qualification for MPECs*, German Polish Conference on Optimization Methods and Applications, February 28 – March 4, Wittenberg, March 1.
4. ———, *Nonlinear programming for solving chance constrained optimization problems: Application to renewable energies*, Winter School on Stochastic Programming with Applications in Energy, Finance and Insurance, March 23–28, Bad Hofgastein, Austria, March 25.
5. ———, *Probabilistic constraints in hydro reservoir management*, XIII Symposium of Specialists in Electric Operational and Expansion Planning (SEPOPE), May 18–21, Foz do Iguassu, Brazil, May 19.
6. ———, *Probabilistic constraints via nonlinear programming: Application to energy management problems*, Euro Mini Conference on Stochastic Programming and Energy Applications (EuroCSP2014), September 24–26, Institut Henri Poincaré, Paris, France, September 25.
7. ———, *Gradient formulae in probabilistic programming*, Conference on Optimization & Practices in Industry (PGMO-COP14), October 28–31, Ecole Polytechnique, Paris, France, October 29.
8. L. KAMENSKI, *How a non-convergent Hessian recovery works in mesh adaptation*, 2014 AARMS-CRM Workshop on Adaptive Methods for PDEs, August 17–22, Memorial University of Newfoundland, Canada, August 20.
9. A. LINKE, *On the role of the Helmholtz decomposition in incompressible flows and a new variational crime*, NonLinear PDE and Applications: Theoretical and Numerical Study, May 5–7, Abdelmalek Essadi University, Tanger, Morocco, May 6.
10. A. MIELKE, *Modeling jumps in rate-independent systems using balanced-viscosity solutions*, 7th International Workshop on Multi-Rate Processes & Hysteresis, 2nd International Workshop on Hysteresis and Slow-Fast Systems (MURPHYS-HSFS-2014), April 7–11, WIAS Berlin, April 8.
11. M. RADZIUNAS, *Modeling and simulations of beam quality improvement in broad area semiconductor devices*, 19th International Conference Mathematical Modelling and Analysis, May 26–29, Druskininkai, Lithuania, May 26.
12. J. SPREKELS, *A deep quench approach to the optimal control of an Allen–Cahn system with dynamic boundary conditions and double-obstacle potentials*, 7th International Workshop on Multi-Rate Processes & Hysteresis, 2nd International Workshop on Hysteresis and Slow-Fast Systems (MURPHYS-HSFS-2014), April 7–11, WIAS Berlin, April 10.
13. A.G. VLADIMIROV, *Delay differential equation models of multimode laser dynamics*, III Dynamics Days South America 2014, November 3–7, Vina del Mar, Chile, November 5.
14. B. WAGNER, *Unsteady non-uniform base states and their stability*, International Conference on Free Boundary Problems: Theory and Applications, June 23–27, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, June 23.



## A.8.2 Scientific Talks (Invited)

1. F. DASSI, *Curvature-adapted remeshing of CAD surfaces*, 23rd International Meshing Roundtable, October 12–15, London, UK, October 14.
2. G. HU, *Corners and edges always scatter*, Distinguished Lectures on Inverse Problems 2014, August 4–8, University of Helsinki, Finland, August 5.
3. ———, *Mathematical problems in time-harmonic wave scattering from bounded and unbounded obstacles*, South University of Science and Technology of China (SUSTC), Department of Financial Mathematics and Financial Engineering, Shenzhen, November 3.
4. ———, *Mathematical problems in time-harmonic wave scattering*, Shandong Normal University, Department of Mathematics, Jinan, China, November 11.
5. R. ALLEZ, *Random matrices at high temperature*, Stochastic Analysis Seminar Series, Oxford-Man Institute, UK, January 20.
6. ———, *Random matrices at high temperature*, Probability series, University of Cambridge, UK, February 11.
7. ———, *Les ensembles beta invariants*, Séminaire de l'équipe Probas/Stats, Institut Élie Cartan de Lorraine, Équipe Probabilités et Statistiques, Nancy, France, May 22.
8. ———, *Invariant beta ensembles and beyond*, Seminar Mathematische Physik, Universität Bielefeld, Mathematical Physics Group, June 11.
9. S. AMIRANASHVILI, *Elementary processes behind turbulent states in optical fibers*, Weak Chaos and Weak Turbulence, February 3–7, Max-Planck-Institut für Physik komplexer Systeme, Dresden, February 5.
10. ———, *Extreme waves in optical fibers*, Wave Interaction (WIN-2014), April 23–26, Johannes Kepler University, Linz, Austria, April 24.
11. ———, *Solitons who do not want to be too short*, Workshop on Abnormal Wave Events (W-AWE2014), June 5–6, Nice, France, June 5.
12. ———, *Recent progress in theory of pulse propagation in optical fibers*, 14th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2014), September 1–5, Palma de Mallorca, Spain, September 2.
13. A. ANDRESEN, *Finite sample analysis of maximum likelihood estimators*, Kolloquium über Mathematische Statistik und Stochastische Prozesse, Universität Hamburg, April 22.
14. ———, *Finite sample analysis of M-estimators*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
15. U. BANDELOW, *Analytical rogue wave solutions in extended NLS-type equations*, International Workshop “Rogue Waves, Dissipative Solitons, Plasmonics, Supercontinuum and Special Fibres”, July 25–26, Barcelona, Spain, July 25.
16. ———, *Dynamics of classical optical fields in semiconductor lasers*, International Nano-Optoelectronics Workshop (iNOW 2014), August 10–22, Luga and St. Petersburg, Russia, August 11.
17. ———, *Dynamics of Semiconductor Lasers*, 4 talks, Autumn School on Laser Dynamics, September 24–28, University of Szeged, Bolyai Institute, Hungary, September 24–28.
18. CH. BAYER, *Asymptotics beats Monte Carlo: The case of correlated local vol baskets*, Stochastic Analysis Seminar Series, Oxford-Man Institute, UK, January 27.

19. ———, *From rough path estimates to multilevel Monte Carlo*, Eleventh International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing, April 6–11, Catholic University of Leuven, Department of Computer Science, Belgium, April 7.
20. ———, *Asymptotics beats Monte Carlo: The case of correlated local vol baskets*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
21. ———, *The forward-reverse method for conditional diffusion processes*, Numerical Analysis Seminar, Royal Institute of Technology Stockholm, Department of Mathematics, Sweden, October 10.
22. ———, *Asymptotics beats Monte Carlo: The case of correlated local vol baskets*, Workshop on Stochastic and Quantitative Finance, November 28–29, Imperial College London, UK, November 29.
23. ———, *Simulation of forward-reverse stochastic representations for conditional diffusions*, Foundations of Computational Mathematics Conference 2014, December 11–20, Universidad de la República, Facultad de Ingeniería, Montevideo, Uruguay, December 19.
24. C. BRÉE, M. HOFMANN, *On the optical response of atomic gases and solids*, Universität Hannover, Institut für Quantenoptik, February 27.
25. A. CAIAZZO, *Multiscale modeling of weakly compressible elastic materials in harmonic regime*, University of Ghent, Department of Electrical Energy, Systems and Automation, Belgium, April 22.
26. ———, *Efficient blood flow simulations for the design of stented valve size reducer in enlarged ventricular outflow tracts*, 4th International Conference on Engineering Frontiers in Pediatric and Congenital Heart Disease, May 21–22, INRIA Research Centre Paris – Rocquencourt, France, May 22.
27. ———, *Multiscale modeling of weakly compressible elastic materials in harmonic regime*, Université de Franche-Comté, Laboratoire de Mathématiques de Besançon, France, July 1.
28. ———, *Multiscale modeling of palisade formation in glioblastoma multiforme*, Instituto de Matemática Aplicada a la Ciencia y Ingeniería, Applied Mathematics Group, Ciudad Real, Spain, December 4.
29. A. CIPRIANI, *Thick points for generalized Gaussian fields with different cut-offs*, Berlin-Padova Young Researchers Meeting, October 23–25, Technische Universität Berlin, October 24.
30. TH. DICKHAUS, *Simultaneous Bayesian analysis of contingency tables in genetic association studies*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 15.
31. K. DISSER, *Parabolic equations with mixed boundary conditions, degenerate diffusion and diffusion on Lipschitz interfaces*, International Conference “Vorticity, Rotations and Symmetry (III)—Approaching Limiting Cases of Fluid Flow”, May 5–9, Centre International de Rencontres Mathématiques (CIRM), Luminy, Marseille, France.
32. ———, *Asymptotic behaviour of a rigid body with a cavity filled by a viscous liquid*, Autumn School and Workshop on Mathematical Fluid Dynamics, October 27–30, Universität Darmstadt, International Research Training Group 1529, Bad Boll, October 28.
33. D.H. DOAN, *On modifications of the Scharfetter–Gummel scheme for drift-diffusion equations with Fermi-like distribution functions*, Kick-Off Meeting of the ECMI Special Interest Group “Sustainable Energy” on Nanostructures for Photovoltaics and Energy Storage, December 8–9, Technische Universität Berlin, Institut für Mathematik, December 8.
34. W. DREYER, *Mathematical modelling of electrolytes in the context of battery research*, Institute’s Seminar, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, January 16.
35. ———, *Coupling of reaction-diffusion equations with the momentum balance in the context of electrolytes*, Workshop “Maxwell–Stefan meets Navier–Stokes/Modeling and Analysis of Reactive Multi-Component Flows”, March 31 – April 2, Universität Halle, April 1.

36. P.-E. DRUET, *Optimization of crystal growth using magnetic fields: Some mathematical aspects*, The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014), Minisymposium 36: Recent Trends in Modeling, Analysis, and Simulation of Induction Heat Treatments, June 9–14, Taormina, Italy, June 13.
37. M. EIGEL, *Guaranteed a posteriori error control with adaptive stochastic Galerkin FEM*, SIAM Conference on Uncertainty Quantification (UQ14), March 31 – April 3, Savannah, USA, April 1.
38. ———, *Adaptive spectral methods for stochastic optimisation problems*, Technische Universität Berlin, Institut für Mathematik, May 22.
39. ———, *Adaptive stochastic FEM*, Universität Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen (IWR), June 5.
40. M.H. FARSHBAF SHAKER, *Relating phase field and sharp interface approaches to structural topology optimization*, SADCOWIAS Young Researcher Workshop, January 29–31, WIAS, January 31.
41. ———, *A deep quench approach to the optimal control of an Allen–Cahn equation with dynamic boundary conditions and double obstacles*, Conference on Partial Differential Equations, May 28–31, Novacella, Italy, May 29.
42. S.P. FRIGERI, *Cahn–Hilliard–Navier–Stokes system with nonlocal interactions and optimal control*, RIPE60 – Rate Independent Processes and Evolution Workshop, June 24–26, Prague, Czech Republic, June 24.
43. ———, *A diffuse interface model related to tumor dynamics*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 39: Interfaces in Fluid Mechanics, July 7–11, Madrid, Spain, July 11.
44. P. FRIZ, *Gaussian rough paths with applications to SPDEs*, SPDE Meeting, January 6–10, Centro Internazionale per la Ricerca Matematica (CIRM), Levico Terme, Italy, January 6.
45. ———, *Signatures, rough paths and related topics*, Colloquium “Rough Paths”, Universität Potsdam, Institut für Mathematik, February 5.
46. ———, *Rough path and stochastic analysis*, 2 talks, Trimester Partial Differential Equations & Probability, Week on Rough Paths and PDE, February 10–15, Centre International de Mathématiques et Informatique de Toulouse, France, February 10–12.
47. ———, *Signatures, rough paths and probability*, BMS Days 2014, February 17–18, The Berlin Mathematical School, February 17.
48. ———, *Implied, local and stochastic volatility: Analytical results in Heston and Stein Stein*, Thematic Cycle on Robust Management in Finance, Workshop “Model Approximation and Numerical Methods” (February – March 2014), Institut Louis Bachelier, Paris, France, March 14.
49. ———, *Basic of rough paths*, Workshop “Stochastic Analysis: Around the KPZ Universality Class”, June 1–7, Mathematisches Forschungsinstitut Oberwolfach, June 2.
50. ———, *Fully-nonlinear SPDEs with rough path dependence*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 109: Stochastic Partial Differential Equations, July 7 – August 11, Madrid, Spain, July 7.
51. ———, *Rough Paths (minicourse)*, 2 talks, IHP Trimester “Geometry, Analysis and Dynamics on Sub-Riemannian Manifolds”, October 6–10, Institut Henri Poincaré, Paris, France, October 6–7.
52. ———, *Rough paths, with jumps*, Probability Seminar, The University of Edinburgh, School of Mathematics, UK, October 10.
53. J. FUHRMANN, *Numerical approaches to Nernst–Planck–Poisson systems with volume constraints*, Workshop “Frei, porös, reaktiv! – Mathematik reaktiver Transportprozesse in porösen Medien”, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, June 12.

54. ———, *Divergence free coupling of fluid flow and solute transport*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, July 10.
55. ———, *Well-balanced Voronoi finite volume schemes for generalized Nernst–Planck–Poisson systems*, MoMaS (Modélisations Mathématiques et Simulations numériques liées aux problèmes de gestion des déchets nucléaires) 2014 Conference, November 17–20, International Center for Mathematical Meetings (CIRM), Marseille, France, November 19.
56. K. GÄRTNER, *From silicon detectors to organic triodes — a generalized Scharfetter–Gummel scheme*, Technische Universität München, Lehrstuhl für Technische Elektrophysik, January 13.
57. A. GLITZKY, *Drift-diffusion models for heterostructures in photovoltaics*, 8th European Conference on Elliptic and Parabolic Problems, Minisymposium “Qualitative Properties of Nonlinear Elliptic and Parabolic Equations”, May 26–30, Universität Zürich, Institut für Mathematik, organized in Gaeta, Italy, May 27.
58. O. GÜN, *Stochastic encounter-mating models*, University of Leiden, Mathematical Institute, The Netherlands, September 4.
59. CH. HEINEMANN, *Phase separation coupled with complete damage processes*, Applied Mathematics Seminar, Institute for Applied Mathematics and Information Technologies “Enrico Magenes” of the National Research Council of Italy, Pavia, January 14.
60. ———, *Analysis of coupled phase-field models describing damage phenomena*, International Conference on Free Boundary Problems: Theory and Applications, June 23–27, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, June 26.
61. R. HENRION, *Application of chance constraints in a coupled model of hydro-wind energy production*, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, March 6.
62. ———, *Calmness as a constraint qualification for MPECs*, 6th Seminar on Optimization and Variational Analysis, University of Elche, Spain, June 3.
63. ———, *Conditioning of linear-quadratic two-stage stochastic optimization problems*, 5th Conference on Optimization Theory and its Applications (ALEL 2014), June 5–7, Universidad de Sevilla, Spain, June 6.
64. ———, *Probabilistic constraints: A structure-oriented introduction*, Optimization and Applications Seminar, Eidgenössische Technische Hochschule Zürich, Switzerland, September 29.
65. ———, *Application of probabilistic constraints to problems of energy management under uncertainty*, Eidgenössische Technische Hochschule Zürich, Power Systems Laboratory, Switzerland, September 30.
66. ———, *Nichtlineare Optimierung bei unsicheren Nebenbedingungen*, 1. Arbeitstreffen zur Initiative “Biokybernetik”, November 20–21, Großkarlbach, November 20.
67. ———, *Gradient formulae in probabilistic programming*, Université Paul Sabatier, Laboratoire d’analyse et d’architecture des systèmes, Toulouse, France, December 8.
68. ———, *Problèmes d’optimisation sous contraintes en probabilité: une initiation*, 3 talks, Université Paul Sabatier, Institut de Mathématiques de Toulouse, France, December 9–10.
69. M. HESSE, *Asymptotic growth of a branching random walk in a random environment on the hypercube*, Third Bath–Paris Branching Structures Meeting, June 9–11, University of Bath, UK, June 9.
70. ———, *Branching Brownian motion in a strip: Survival near criticality*, University of Leiden, Mathematical Institute, The Netherlands, September 4.
71. ———, *Asymptotic growth of a branching random walk in a random environment on the hypercube*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, December 4.
72. R. HILDEBRAND, *Spectrahedral cones generated by rank 1 matrices*, Workshop “Real Algebraic Geometry With A View Toward Systems Control and Free Positivity”, April 6–12, Mathematisches Forschungsinstitut Oberwolfach, April 11.

73. CH. HIRSCH, *From heavy-tailed Boolean models to scale-free Gilbert graphs*, Karlsruher Institut für Technologie, Institut für Stochastik, November 14.
74. M. HOFMANN, *Intense laser-matter interaction in atomic gases and crystalline solids*, Leibniz-Universität Hannover, Institut für Quantenoptik, February 27.
75. D. HÖMBERG, *Multifrequency induction hardening — Modelling, analysis, and simulation*, Fudan University, School of Mathematical Sciences, Shanghai, China, March 4.
76. ———, *Modelling and simulation of multi-frequency induction hardening*, Ecole Polytechnique, Laboratoire de Mécanique des Solides, Palaiseau, France, March 13.
77. ———, *Nucleation, growth, and grain size evolution in dual phase steels*, Workshop “Recent Developments and Challenges in Interface and Free Boundary Problems”, March 25–28, University of Warwick, UK, March 26.
78. ———, *Nucleation, growth, and grain size evolution in dual phase steels*, The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014), Minisymposium 37: Simulation and Control of Hot-rolling, June 9–13, Taormina, Italy, June 9.
79. ———, *Models of induction hardening – An FK limited approach*, RIPE60 – Rate Independent Processes and Evolution Workshop, June 24–26, Prague, Czech Republic, June 25.
80. ———, *Nucleation, growth, and grain size evolution in dual phase steels*, Wrocław University of Technology, Institute of Mathematics and Computer Science, Poland, July 1.
81. ———, *Variational calculus and optimal control*, 13 talks, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, October 13–31.
82. ———, *Modelling, analysis and simulation of multifrequency induction hardening*, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, October 21.
83. ———, *Modelling, simulation and control of surface heat treatments*, Norwegian University of Science and Technology, Department of Physics, Trondheim, October 31.
84. ———, *Oberflächenbearbeitung mit Mathematik*, Opel Innovation Day, Rüsselsheim, November 7.
85. S. JACHALSKI, *Weak solutions to lubrication systems describing the evolution of bilayer thin films*, Joint Meeting 2014 of the German Mathematical Society (DMV) and the Polish Mathematical Society (PTM), September 17–20, Adam Mickiewicz University, Faculty of Mathematics and Computer Science, Poznan, Poland, September 18.
86. V. JOHN, *Numerical methods for convection-dominated equations*, 2nd Workshop “Populationsbilanzen” of the DFG Priority Program SPP 1679 “Dyn-Sim-FP – Dynamic Simulation of Interconnected Solids Processes”, May 6–7, Technische Universität Hamburg-Harburg, May 6.
87. ———, *Turbulent flows and their numerical simulation*, Humboldt Kolleg on Interdisciplinary Science: Catalyst for Sustainable Progress, September 4–6, Indian Institute of Science, Numerical Mathematics & Scientific Computing, Bangalore, September 5.
88. ———, *Finite element methods for incompressible flow problems*, 4 talks, Indian National Program on Differential Equations – Theory, Computation, and Applications (NPDE-TCA) Advanced Workshop on Finite Element Methods for Navier–Stokes Equations, September 8–12, Indian Institute of Science, Numerical Mathematics & Scientific Computing, Bangalore, September 9–10.
89. ———, *On the simulation of mantle convection*, Symposium on Simulation and Optimization of Extreme Fluids, November 10–12, Internationales Wissenschaftsforum Heidelberg, November 12.
90. O. KLEIN, *Classification of hysteresis operators for vector-valued inputs by using their representation as functions on strings*, RIPE60 – Rate Independent Processes and Evolution Workshop, June 24–26, Prague, Czech Republic, June 24.

91. D. KNEES, *A quasilinear differential inclusion for viscous and rate-independent damage systems in non-smooth domains*, Analysis & Stochastics Seminar, Technische Universität Dresden, Institut für Analysis, January 16.
92. W. KÖNIG, *Von der Binomialverteilung zur Normalverteilung*, 11th German Probability and Statistics Days 2014, March 4–7, Ulm, March 6.
93. ———, *A variational formula for the free energy of a many-Boson system*, IKERBASQUE, Basque Foundation for Science, Bilbao, Spain, May 29.
94. ———, *Cluster-size distributions in a classical many-body system*, Workshop “Mathematical Facets of Crystallization”, September 9–12, Lorentz Center, Leiden, The Netherlands, September 9.
95. ———, *A variational formula for the free energy of an interacting many-body system*, Columbia Probability Seminar, University of Columbia, Department of Mathematics, New York, USA, December 5.
96. ———, *Cluster size distribution in classical many-body systems with Lennard–Jones potential*, Universität Ulm, Institut für Stochastik, December 17.
97. C. KREISBECK, *Thin-film limits of functionals on A-free vector fields and applications*, Oberseminar “Mathematik in den Naturwissenschaften”, Universität Würzburg, Institut für Mathematik, July 16.
98. ———, *Thin-film limits of functionals on A-free vector fields and applications*, Workshop on Trends in Non-Linear Analysis 2014, July 31 – August 1, Instituto Superior Técnico, Departamento de Matemática, Lisbon, Portugal, August 1.
99. M. LADKAU, *Brownian motion approach for spatial PDEs with stochastic data*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
100. M. LANDSTORFER, *A new interpretation of the Stern layer*, Fourth Annual Electrochemistry Workshop, July 6–9, Monterey Bay, USA, July 8.
101. ———, *Structure of the space charge layer in electrolytic solutions based on modern continuum thermodynamics*, Institute’s Seminar, Max-Planck-Institut für Festkörperforschung, Stuttgart, November 24.
102. ———, *Structure of the space charge layer in electrolytic solutions based on modern continuum thermodynamics*, Seminar “Modellierung in der Elektrochemie” der Arbeitsgemeinschaft Elektrochemischer Forschungsinstitutionen, Universität Duisburg-Essen, Fakultät für Chemie, Essen, December 9.
103. M. LIERO, *On dissipation distances for reaction-diffusion equations — The Hellinger–Kantorovich distance*, RIPE60 – Rate Independent Processes and Evolution Workshop, June 24–26, Prague, Czech Republic, June 24.
104. ———, *On dissipation distances for reaction-diffusion equations — The Hellinger–Kantorovich distance*, Workshop “Entropy Methods, PDEs, Functional Inequalities, and Applications”, June 30 – July 4, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Canada, July 1.
105. ———, *Electrothermal modeling of large-area OLEDs*, Kick-Off Meeting of the ECMI Special Interest Group “Sustainable Energy” on Nanostructures for Photovoltaics and Energy Storage, December 8–9, Technische Universität Berlin, Institut für Mathematik, December 8.
106. A. LINKE, *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, January 7.
107. ———, *On the role of the Helmholtz decomposition in mixed methods for incompressible flows and a new variational crime*, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, April 2.
108. ———, *Ein neues Konstruktionsprinzip zur divergenzfreien Diskretisierung der inkompressiblen Navier-Stokes-Gleichungen*, Ruhr-Universität Bochum, Fakultät für Mathematik, July 17.

109. ———, *On the role of the Helmholtz decomposition in mixed methods for incompressible flows and a new variational crime*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fachbereich Mathematik, November 20.
110. ———, *On the role of the Helmholtz decomposition in mixed methods for incompressible flows and a new variational crime*, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, December 9.
111. H. MAI, *Pathwise stability of likelihood estimators for diffusions via rough paths*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
112. ———, *Robustness and pathwise stability of maximum likelihood estimators for jump diffusions*, Universidad de Buenos Aires, Instituto de Calculo, Argentina, August 8.
113. ———, *Robustness of likelihood estimators for diffusions via rough paths*, Advances in Stochastic Analysis, September 3–5, National Research University – Higher School of Economics, Laboratory of Stochastic Analysis and its Applications, Moscow, Russia, September 3.
114. P. MATHÉ, *Oracle-type posterior contraction rates in Bayesian inverse problems*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
115. ———, *Convergence of Bayesian schemes in inverse problems*, Kolloquium über Angewandte Mathematik, Georg-August-Universität Göttingen, Fakultät für Mathematik und Informatik, June 10.
116. ———, *Merging regularization theory into Bayesian inverse problems*, Chemnitz Symposium on Inverse Problems, September 15–19, Universität Chemnitz, Fachbereich Mathematik, September 18.
117. ———, *Bayesian analysis of statistical inverse problems*, Colloquium of the Faculty of Mathematics and Computer Science, University of Tartu, Estonia, October 13.
118. ———, *A random surfer in the internet*, German-Estonian Academic Week “Academica”, October 13–15, University of Tartu, Faculty of Mathematics and Computer Science, Estonia, October 14.
119. ———, *Smoothness beyond differentiability*, Seminar for Doctoral Candidates, University of Tartu, Faculty of Mathematics and Computer Science, Estonia, October 15.
120. ———, *Bayesian regularization of statistical inverse problems*, Rencontres de Statistique Mathématique: Nouvelles Procédures pour Nouvelles Données, December 15–19, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 17.
121. A. MIELKE, *How thermodynamics induces geometry structures for reaction-diffusion systems*, Gemeinsames Mathematisches Kolloquium der Universitäten Gießen und Marburg, Universität Gießen, Mathematisches Institut, January 15.
122. ———, *On gradient structures for reaction-diffusion systems*, Joint Analysis Seminar, Rheinisch-Westfälische Technische Hochschule Aachen (RWTH), Institut für Mathematik, February 4.
123. ———, *Gradient structures and dissipation distances for reaction-diffusion systems*, Seminar “Analysis of Fluids and Related Topics”, Princeton University, Department of Mechanical and Aerospace Engineering, Princeton, NJ, USA, March 6.
124. ———, *Gradient structures and dissipation distances for reaction-diffusion systems*, Workshop “Advances in Nonlinear PDEs: Analysis, Numerics, Stochastics, Applications”, June 2–3, Vienna University of Technology and University of Vienna, Austria, June 2.
125. ———, *Generalized gradient structures for reaction-diffusion systems*, Applied Mathematics Seminar, Università di Pavia, Dipartimento di Matematica, Italy, June 17.



126. ———, *On gradient structures and dissipation distances for reaction-diffusion systems*, Kolloquium “Angewandte Mathematik”, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, July 3.
127. ———, *On gradient-flow structure for thermoplasticity*, IUTAM Symposium on Innovative Numerical Approaches for Materials and Structures in Multi-field and Multi-scale Problems, September 1–4, Universität Siegen, Institut für Mechanik und Regelungstechnik, organized at Burg Schnellenberg near Cologne, September 3.
128. ———, *On the microscopic origin of generalized gradient structures for reaction-diffusion systems*, XIX International Symposium on Trends in Applications of Mathematics to Mechanics (STAMM 2014), September 8–11, The International Society for the Interaction of Mechanics and Mathematics (ISIMM), Poitiers, France, September 11.
129. ———, *Homogenization of parabolic gradient systems via evolutionary  $\Gamma$ -convergence*, Second Workshop of the GAMM Activity Group on “Analysis of Partial Differential Equations”, September 29 – October 1, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, September 30.
130. ———, *A reaction-diffusion equation as a Hellinger–Kantorovich gradient flow*, ERC Workshop on Optimal Transportation and Applications, October 27–31, Centro di Ricerca Matematica “Ennio De Giorgi”, Pisa, Italy, October 29.
131. ———, *On a metric and geometric approach to reaction-diffusion systems as gradient systems*, Mathematics Colloquium, Jacobs University Bremen, School of Engineering and Science, December 1.
132. H.-J. MUCHA, *Variable selection in cluster analysis by means of bootstrapping*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
133. ———, *From univariate to multivariate clustering with application to P-ED-XRF data*, Workshop “Application of Portable Energy-dispersive X-ray Fluorescence to the Analysis of Archaeological Ceramics”, June 20–21, Excellence Cluster TOPOI, Berlin, June 21.
134. H. NEIDHARDT, *Landauer–Büttiker formula applied to photon emitting and absorbing system*, Workshop “Mathematical Challenge of Quantum Transport in Nanosystems” (Pierre Duclos Workshop), September 23–26, Saint Petersburg National Research University of Informational Technologies, Mechanics, and Optics, Russia, September 24.
135. ST. NEUKAMM, *Characterization and approximation of macroscopic properties with homogenization*, 4th British-German Frontiers of Science Symposium, March 6–9, Alexander von Humboldt-Stiftung, Potsdam, March 7.
136. ———, *Homogenization of nonlinear bending plates*, Workshop “Relaxation, Homogenization, and Dimensional Reduction in Hyperelasticity”, March 25–27, Université Paris-Nord, France, March 26.
137. ———, *Stochastic homogenization: An optimal quantitative two-scale expansion*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 27: Mathematical Problems in Economics, Materials and Life Science: Analysis and Simulation of Nonlinear Multiscale Dynamics, July 7–10, Madrid, Spain, July 9.
138. J. NEUMANN, *Stochastic bounds for quantities of interest in groundwater flow with uncertain data*, Université Paris-Sud, Laboratoire d’Analyse Numérique, Orsay, France, October 9.
139. O. OMEL’CHENKO, *Bifurcation analysis of chimera states*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 13: Nonlocally Coupled Dynamical Systems: Analysis and Applications, July 7–11, Madrid, Spain, July 7.
140. ———, *Spike solutions to singularly perturbed elliptic problems*, Workshop “Modern Problems of Mathematical Physics”, November 28–29, Lomonosov Moscow State University, Russia, November 28.

141. ST. PATRIZI, *On a long range segregation problem*, The Seventh International Conference on Differential and Functional Differential Equations, August 22–29, Moscow, Russia, August 26.
142. ———, *Crystal dislocations with different orientation and collisions*, Program “Homogenization and Random Phenomenon”, October 1–31, Institut Mittag-Leffler, Stockholm, Sweden, October 9.
143. ———, *On a long range segregation problem*, Università degli Studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, November 11.
144. R.I.A. PATTERSON, *Statistical error analysis for coagulation-advection simulations*, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, May 1.
145. ———, *Stochastic numerical methods for coagulating particles*, Seminar “Geophysical Fluid Dynamics”, Freie Universität Berlin, Institut für Mathematik, June 4.
146. ———, *Convergence of coagulation-advection simulations*, Workshop on Particle Transport with Emphasis on Stochastics, November 6–7, Aarhus University, Denmark, November 6.
147. J. PELLERIN, *Toward mixed-element meshing based on restricted Voronoi diagrams*, 23rd International Meshing Roundtable, October 12–15, London, UK, October 14.
148. TH. PETZOLD, *Modelling and simulation of multifrequency induction hardening for gear components*, The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014), Minisymposium “Recent Trends in Modelling, Analysis, and Simulation of Induction Heat Treatments”, June 9–13, Taormina, Italy, June 13.
149. ———, *Finite element simulations and experiments for multifrequency induction hardening*, IUTAM Symposium on Thermomechanical-Electromagnetic Coupling in Solids: Microstructural and Stability Aspect, June 16–18, Paris, France, June 18.
150. ———, *Modellierung, Simulation und Optimierung in angewandter Mathematik am Weierstraß-Institut*, Innovation Days 2014, December 1–2, München, December 2.
151. A. PIMENOV, *Population models and the effects of hysteresis*, CRM Applied Mathematical and Physics (CAMP) Seminar, Centre de Recerca Matemàtica, Barcelona, Spain, July 24.
152. J. POLZEHL, *Quantification of noise in MR experiments*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
153. ———, *Quantification of noise in MR experiments*, Statistical Challenges in Neuroscience, September 3–5, University of Warwick, Centre for Research in Statistical Methodology, UK, September 4.
154. ———, *Statistical problems in diffusion weighted MR*, CoSy Seminar, University of Uppsala, Department of Mathematics, Sweden, November 11.
155. M. RADZIUNAS, *Simulation and analysis of the external cavity diode lasers with LDSL-tool*, Research Seminar, Technical University of Moldova, Department of Physics, Chisinau, June 4.
156. ———, *Simulations and analysis of beam shaping in spatially modulated broad area edge-emitting devices*, 24th International Semiconductor Laser Conference (ISLC 14), September 7–10, Palma de Mallorca, Spain, September 7.
157. ———, *Computation and analysis of optical modes in multisection ring and edge-emitting semiconductor lasers*, International Symposium “Advances in Nonlinear Photonics”, September 29 – October 3, Minsk, Belarus, September 30.
158. ———, *Modeling and simulations of beam quality improvement in broad area semiconductor devices*, Research Seminar of DONLL (Nonlinear Dynamics, Nonlinear Optics and Lasers), Universitat Politècnica de Catalunya, Department of Physics, Terrassa, Spain, November 20.

159. J. REHBERG, *Optimal Sobolev regularity for second order divergence operators*, 85th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2014), Session on Applied Operator Theory, March 10–14, Friedrich-Alexander Universität Erlangen-Nürnberg, March 13.
160. ———, *On non-smooth parabolic equations*, Workshop “Maxwell–Stefan meets Navier–Stokes/Modeling and Analysis of Reactive Multi-Component Flows”, March 31 – April 2, Universität Halle, April 1.
161. ———, *Maximal parabolic regularity on strange geometries and applications*, Joint Meeting 2014 of the German Mathematical Society (DMV) and the Polish Mathematical Society (PTM), September 17–20, Adam Mickiewicz University, Faculty of Mathematics and Computer Science, Poznan, Poland, September 18.
162. S. REICHELT, *Two-scale homogenization of reaction-diffusion systems with small diffusion*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 8: Emergence and Dynamics of Patterns in Nonlinear Partial Differential Equations from Mathematical Science, July 7–11, Madrid, Spain, July 8.
163. ———, *Two-scale homogenization of nonlinear reaction-diffusion systems involving different diffusion length scales*, MATHEON Multiscale Seminar, Technische Universität Berlin, Institut für Mathematik, December 3.
164. D.R.M. RENGIER, *Connecting particle systems to entropy-driven gradient flows*, Oberseminar “Stochastische und Geometrische Analysis”, Universität Bonn, Institut für Angewandte Mathematik, May 28.
165. ———, *Connecting particle systems to entropy-driven gradient flows*, Conference on Nonlinearity, Transport, Physics, and Patterns, October 6–10, Fields Institute for Research in Mathematical Sciences, Toronto, Canada, October 9.
166. E. ROCCA, *Non-isothermal two phase flows of incompressible fluids*, 9th DFG-CNRS Workshop Two-Phase Fluid Flows. Modeling, Analysis and Computational Methods, February 25–27, Université Pierre et Marie Curie, Paris, France, February 26.
167. J.G.M. SCHOENMAKERS, *Multilevel dual evaluation and multilevel policy iteration for optimal stopping/American options*, Advances in Financial Mathematics, January 7–10, l'Institut Louis Bachelier, Paris, France, January 9.
168. ———, *Affine LIBOR models with multiple curves: Theory, examples and calibration*, 11th German Probability and Statistics Days 2014, March 5–7, Universität Ulm, March 6.
169. H. SI, *Towards anisotropic quality tetrahedral mesh generation*, Politecnico di Milano, Dipartimento di Matematica “F. Brioschi”, Italy, February 26.
170. ———, *Introduction to Delaunay-based tetrahedral mesh generation*, 23rd International Meshing Roundtable, October 12–15, London, UK, October 12.
171. ———, *TetGen, a Delaunay-based quality tetrahedral mesh generator*, OpenGeoSys Community Meeting 2014, November 20–21, Helmholtz Centre for Environmental Research, Leipzig, November 20.
172. R. SOARES DOS SANTOS, *Quenched CLT for ballistic random walks in non-uniformly elliptic random environments*, December 8–10, Technische Universität München.
173. V. SPOKOINY, *Modern Parametric Statistics*, 6 talks, Independent University of Moscow, Russia, February 10–25.
174. ———, *Fisher and Wilks expansions and critical dimension*, Workshop “Adaptive Statistical Inference”, March 9–14, Mathematisches Forschungsinstitut Oberwolfach, March 13.
175. ———, *Fisher and Wilks expansions and their applications to statistical inference*, 4 talks, Spring School 2014 of Research Unit FOR 1735 “Structural Inference in Statistics: Adaptation and Efficiency”, March 17–21, Königs Wusterhausen, March 17–21.

176. ———, *Statistical methods in medical imaging and pharmacokinetics*, IV Annual International Conference PhystechBio “Northern” BioPharmCluster at MIPT, May 29–30, Moscow Institute of Physics and Technology, Russia, May 30.
177. ———, *Bernstein–von Mises theorem for a quasi-posterior*, International Symposium on Financial Engineering and Risk Management 2014, June 27–28, Central University of Finance and Economics, Beijing, China, June 27.
178. ———, *Semiparametric approach to error-in-variables regression*, The 3rd Institute of Mathematical Statistics Asia Pacific Rim Meeting, June 29 – July 3, Taipei, Taiwan, June 29.
179. ———, *Construction of the sharp confidence bands using multiplier bootstrap*, Advances in Stochastic Analysis, September 3–5, National Research University – Higher School of Economics, Laboratory of Stochastic Analysis and its Applications, Moscow, Russia, September 5.
180. ———, *Bootstrap confidence sets under a model misspecification*, Workshop “New Horizons in Statistical Decision Theory”, September 7–13, Mathematisches Forschungsinstitut Oberwolfach, September 8.
181. ———, *Statistical methods in medical imaging*, International Scientific Conference “Science of the Future”, September 17–20, Ministry of Education and Science of the Russian Federation, St. Petersburg, Russia, September 19.
182. ———, *From lambda-convergence to Fisher and Wilks expansions*, Stochastics, Statistics, Financial Mathematics, October 13–15, Russian Academy of Sciences, Steklov Mathematical Institute, Moscow, Russia, October 13.
183. J. STANGE, *Computation of an effective number of simultaneous  $\chi^2$  tests*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 15.
184. H. STEPHAN, *Ungleichungen I und II, Zahlenfolgen I und II*, 4 talks, Internationales Mathe-Sommercamp der Humboldt-Universität zu Berlin für junge Mathe-Asse, Europäische Jugenderholungs- und Begegnungsstätte, Joachimsthal, August 28–29.
185. ———, *Zahlentheorie und Geometrie*, Herbsttagung der Mathematischen Gesellschaft in Hamburg, November 14–15, Universität Hamburg, Fachbereich Mathematik, November 15.
186. K. STURM, *The volume expression of the shape derivative: Geometrical interpretation and numerics*, Workshop on Numerical Methods for Optimal Control and Inverse Problems, March 3–5, Technische Universität München, March 3.
187. ———, *A new approach to the differentiability of a minimax function*, DK-RICAM Workshop on PDE-Constrained Optimization, March 6–7, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, March 6.
188. ———, *The volume expression of the shape derivative: Geometrical interpretation and numerics*, 85th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2014), Young Researchers’ Minisymposia, March 10–14, Friedrich-Alexander Universität Erlangen-Nürnberg, March 11.
189. K. TABELOW, *High-resolution diffusion MRI by msPOAS*, Statistical Challenges in Neuroscience, September 3–5, University of Warwick, Centre for Research in Statistical Methodology, UK, September 4.
190. M. THOMAS, *Existence and stability results for rate-independent processes in viscoelastic materials*, Women in Partial Differential Equations & Calculus of Variations Workshop, March 6–8, University of Oxford, Mathematical Institute, UK, March 6.
191. ———, *Existence & stability results for rate-independent processes in viscoelastic materials*, Applied Mathematics Seminar, Università di Pavia, Dipartimento di Matematica, Italy, March 18.

192. ———, *A stress-driven local-solution approach to quasistatic brittle delamination*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 91: Variational Methods for Evolution Equations, July 7–11, Madrid, Spain, July 7.
193. ———, *Thermomechanical modeling of dissipative processes in elastic media via energy and entropy*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 8: Emergence and Dynamics of Patterns in Nonlinear Partial Differential Equations from Mathematical Science, July 7–11, Madrid, Spain, July 8.
194. ———, *Rate-independent, partial damage in thermo-viscoelastic materials with inertia*, International Workshop “Variational Modeling in Solid Mechanics”, September 22–24, University of Udine, Department of Mathematics and Informatics, Italy, September 23.
195. ———, *Rate-independent, partial damage in thermo-viscoelastic materials with inertia*, Oberseminar “Analysis und Angewandte Mathematik”, Universität Kassel, Institut für Mathematik, December 1.
196. ———, *Rate-independent systems with viscosity and inertia: Existence and evolutionary Gamma-convergence*, Workshop “Variational Methods for Evolution”, December 14–20, Mathematisches Forschungsinstitut Oberwolfach, December 18.
197. N. TOGOBYTSKA, *Optimal control approach for production of multiphase steels*, The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014), Minisymposium 37: Simulation and Control of Hot-rolling, June 9–13, Taormina, Italy, June 9.
198. E. VALDINOCI, *(Non)local interfaces and minimal surfaces*, International Conference on “Nonlinear Phenomena in Biology”, March 5–7, Helmholtz Zentrum München – Deutsches Forschungszentrum für Gesundheit und Umwelt, March 5.
199. ———, *Nonlinear PDEs*, 3 talks, Spring School on Nonlinear PDEs, March 24–27, INdAM Istituto Nazionale d’Alta Matematica, Sapienza – Università di Roma, Italy, March 24–26.
200. ———, *Dislocation dynamics in crystals*, Geometry and Analysis Seminar, Columbia University, Department of Mathematics, New York City, USA, April 3.
201. ———, *Concentration solutions for a nonlocal Schroedinger equation*, Kinetics, Non Standard Diffusion and the Mathematics of Networks: Emerging Challenges in the Sciences, May 7–16, The University of Texas at Austin, Department of Mathematics, USA, May 14.
202. ———, *Nonlocal minimal surfaces and free boundary problems*, Geometric Aspects of Semilinear Elliptic and Parabolic Equations: Recent Advances and Future Perspectives, May 25–30, Banff International Research Station for Mathematical Innovation and Discovery, Calgary, Canada, May 27.
203. ———, *Concentrating solutions for a nonlocal Schroedinger equation*, Nonlinear Partial Differential Equations and Stochastic Methods, June 7–11, University of Jyväskylä, Finland, June 10.
204. ———, *Dislocation dynamics in crystals*, Recent Advances in Non-local and Non-linear Analysis: Theory and Applications, June 10–14, FIM – Institute for Mathematical Research, ETH Zuerich, Switzerland, June 13.
205. ———, *Gradient estimates and symmetry results in anisotropic media*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 76: Viscosity, Nonlinearity and Maximum Principle, July 7–11, Madrid, Spain, July 8.
206. ———, *Nonlocal minimal surfaces*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 96: Geometric Variational Problems with Associated Stability Estimates, July 7–11, Madrid, Spain, July 8.
207. ———, *Concentration phenomena for nonlocal equation*, Méthodes Géométriques et Variationnelles pour des EDPs Non-linéaires, September 1–5, Université C. Bernard, Lyon 1, Institut C. Jordan, France, September 2.

208. ———, *Dislocation dynamics and fractional equations*, Analysis Seminar, Heriot-Watt University of Edinburgh, London, UK, October 31.
209. ———, *Dislocation dynamics and fractional equations*, Analysis Seminar, University of Texas at Austin Mathematics, USA, November 5.
210. ———, *Nonlocal equations and applications*, Seminario de Ecuaciones Diferenciales, Universidad de Granada, IEMath-Granada, Spain, November 28.
211. ———, *Nonlocal problems in analysis and geometry*, 5 talks, Universidad Autonoma de Madrid, Departamento de Matemáticas, Spain, December 1–5.
212. ———, *Dislocation dynamics in crystals*, Seminari di Analisi Matematica, Università di Torino, Dipartimento di Matematica “Giuseppe Peano”, Italy, December 18.
213. A.G. VLADIMIROV, *Modeling of multimode laser dynamics by means of delay differential equations*, 14th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2014), September 1–4, Palma de Mallorca, Spain, September 3.
214. ———, *Delay differential equation models of multimode lasers*, International Symposium “Advances in Nonlinear Photonics”, September 29 – October 3, Minsk, Belarus, October 30.
215. ———, *Delay differential equations in laser dynamics*, International Conference-School Hamiltonian Dynamics, Nonautonomous Systems, and Patterns in PDE’s, December 10–15, Nishni Novgorod, Russia, December 14.
216. B. WAGNER, *The wavelength of the contact line instability in dewetting rims*, 8th European Conference on Elliptic and Parabolic Problems, Minisymposium “Pattern Formation in Nonlinear Evolution Equations”, May 25–30, Universität Zürich, Institut für Mathematik, organized in Gaeta, Italy, May 29.
217. W. WAGNER, *Heat generation in the electrothermal Monte Carlo method*, The 18th European Conference on Mathematics for Industry 2014 (ECMI 2014), Minisymposium “Semiclassical and Quantum Transport in Semiconductors and Low Dimensional Materials”, June 9–13, Taormina, Italy, June 11.
218. ———, *Random cloud models for the Schrödinger equation*, Sapienza – Università di Roma, Dipartimento di Matematica, Italy, October 9.
219. N. WILLRICH, *Model selection by Lepski’s method for penalized likelihood*, International Workshop “Advances in Optimization and Statistics”, May 15–16, Russian Academy of Sciences, Institute of Information Transmission Problems (Kharkevich Institute), Moscow, May 16.
220. M. WOLFRUM, *Stabilizing chimera states by feedback control*, Colloquium “Applications of Dynamical Networks” of the Collaborative Research Center 910, Technische Universität Berlin, June 20.
221. ———, *The Turing bifurcation in network systems: Snaking branches of localized patterns*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 122: Dynamics of Networks in Biology and Chemistry, July 7–11, Madrid, Spain, July 8.
222. ———, *Amplitude equations for DDEs with large delay*, The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 5: Differential Delay Equations, July 7–11, Madrid, Spain, July 9.
223. ———, *Delay-differential equations for semiconductor lasers*, 3 talks, Autumn School on Laser Dynamics, September 24–28, University of Szeged, Bolyai Institute, Hungary, September 24–28.
224. ———, *Chimera states: Patterns of coherence and incoherence in coupled oscillator systems*, Institut Non Linéaire de Nice – Sophia Antipolis, France, October 10.
225. M. ZHILOVA, *Uniform confidence bands for generalized regression via multiplier bootstrap*, International Symposium on Financial Engineering and Risk Management 2014, June 27–28, Central University of Finance and Economics, Beijing, China, June 27.

226. ———, *Uniform confidence bands in generalized regression via multiplier bootstrap*, The 3rd Institute of Mathematical Statistics Asia Pacific Rim Meeting, June 29 – July 3, Taipei, Taiwan, July 1.

### A.8.3 Talks for a More General Public

1. C. BARTSCH, *Zur Kopplung atomistischer und kontinuierlicher Modelle*, Dies Mathematicus, Technische Universität Berlin, November 21.
2. W. DREYER, *Luftballons, Lithium-Ionen-Batterien und Wasserstoffautos – Ein Fall für die Mathematik*, MATHEON Rent the Center, Technische Universität Berlin, Berlin, October 28.
3. P. GAJEWSKI, *Der Weg ins Chaos: Die logistische Abbildung*, 19. Berliner Tag der Mathematik (19th Berlin Day of Mathematics), Technische Universität Berlin, May 17.
4. W. KÖNIG, *Von der Binominalverteilung zur Normalverteilung*, Tag der Wissenschaften 2014, Weinberg-Gymnasium Kleinmachnow, November 13.
5. TH. KOPRUCKI, *Organische LEDs (OLEDs) – eine heiße Sache*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2014, WIAS at Leibniz Association Headquarters, Berlin, May 10.
6. M. LADKAU, *Volumenberechnung durch Würfeln*, MathInside – Mathematik ist überall, Urania, Berlin, March 11.
7. M. LANDSTORFER, *Career Stories – Mathematiker/-innen berichten aus ihrem Berufsalltag*, 40-Jahres-Feier des Studienganges Mathematik, Ostbayerische Technische Hochschule Regensburg, April 8.
8. M. LIERO, *Mit Mathematik und dem richtigen “Mittel” von Mikro zu Makro*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2014, WIAS at Leibniz Association Headquarters, Berlin, May 10.
9. G. REINHARDT, *Das Luzifer-Rätsel*, 19. Berliner Tag der Mathematik (19th Berlin Day of Mathematics), Technische Universität Berlin, May 17.
10. D.R.M. RENGIER, *Unendlichkeit*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2014, WIAS at Leibniz Association Headquarters, Berlin, May 10.
11. ———, *Die Entropie einer unendlichen Anzahl von Molekülen*, 19. Berliner Tag der Mathematik (19th Berlin Day of Mathematics), Technische Universität Berlin, May 17.
12. ———, *Infinity: Imagining the unimaginable*, Nerd Nite Amsterdam, University of Amsterdam, Department of Mathematics, The Netherlands, June 6.
13. H. STEPHAN, *Nichts als die mathematische Wahrheit*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2014, WIAS at Leibniz Association Headquarters, Berlin, May 10.
14. ———, *Geometrie und Zahlentheorie. Ganzzahlige geometrische Objekte*, 19. Berliner Tag der Mathematik (19th Berlin Day of Mathematics), Technische Universität Berlin, May 17.
15. K. TABELOW, *Magnet-Resonanz-Tomographie – Einblicke in das lebende Gehirn*, 19. Berliner Tag der Mathematik (19th Berlin Day of Mathematics), Technische Universität Berlin, May 17.

### A.8.4 Posters

1. R.M. ARKHIPOV, *Pulse repetition-frequency multiplication of passively mode-locked semiconductor lasers coupling to an external passive cavity*, “SPIE Photonics Europe”, Brussels, Belgium, April 14–17.
2. ———, *Theoretical investigation of a passively mode-locked semiconductor laser with external periodic forcing*, “SPIE Photonics Europe”, Brussels, Belgium, April 14–17.



3. ———, *Theoretical analysis of coherent passive and self mode-locking in lasers*, 16th International Conference “Laser Optics”, June 30 – July 4, 2014, St. Petersburg, Russia, June 29 – July 6.
4. R.M. ARKHIPOV, M.V. ARKHIPOV, *Mode-locking in two section and single section lasers due to coherent interaction of light and matter in the gain and absorbing media*, XIV School Seminar “Wave Phenomena In Inhomogeneous Media” (Waves 2014), Moscow, Russia, May 26–31.
5. C. BRÉE, M. KRETSCHMAR, T. NAGY, M. HOFMANN, A. DEMIRCAN, U. MORGNER, M. KOVACEV, *Fingerprint of self-compression in the high harmonic spectrum from a filament*, High-Intensity Lasers and High-Field Phenomena (HILAS), Berlin, March 18–20.
6. J. FUHRMANN, *Activity based finite volume methods for generalised Nernst–Planck–Poisson systems*, The International Symposium of Finite Volumes for Complex Applications VII (FVCA 7), Berlin-Brandenburgische Akademie der Wissenschaften, June 15–20.
7. J. FUHRMANN, A. LINKE, CH. MERDON, *Coupling of fluid flow and solute transport using a divergence-free reconstruction of the Crouzeix–Raviart element*, The International Symposium of Finite Volumes for Complex Applications VII (FVCA 7), Berlin-Brandenburgische Akademie der Wissenschaften, June 15–20.
8. J. FUHRMANN, A. LINKE, CH. MERDON, M. KHODAYARI, H. BALTRUSCHAT, *Detection of solubility, transport and reaction coefficients from experimental data by inverse modeling of thin layer flow cells*, 65th Annual Meeting of the International Society of Electrochemistry, Lausanne, Switzerland, August 31 – September 5.
9. J. FUHRMANN, CH. MERDON, *Activity based finite volume methods for generalised Nernst–Planck–Poisson systems*, 65th Annual Meeting of the International Society of Electrochemistry, Lausanne, Switzerland, August 31 – September 5.
10. A. FIEBACH, A. GLITZKY, *Uniform estimate of the relative free energy by the dissipation rate for finite volume discretized reaction-diffusion systems*, The International Symposium of Finite Volumes for Complex Applications VII (FVCA 7), Berlin, June 15–20.
11. V. JOHN, S. ROCKEL, ST. SOBOLEV, *Viscoelastic mantle flow*, 3rd Annual GEOSIM Workshop, Potsdam, November 13–14.
12. M. KANTNER, TH. KOPRUCKI, H.-J. WÜNSCHE, *Numerical simulation and optimization of electrical resistance in GaAs/Al(x)Ga(1-x)As-based distributed Bragg reflectors*, International Nano-Optoelectronics Workshop (iNOW 2014), St. Petersburg, Russia, August 9–23.
13. J. DAUBE, H. ABELS, CH. KRAUS, D. KRÖNER, *Sharp interface limit for the Navier-Stokes-Korteweg model*, International Conference on Free Boundary Problems: Theory and Applications, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, June 23–27.
14. M. LANDSTORFER, *What are the Helmholtz planes? New insights from continuum thermodynamics*, 65th Annual Meeting of the International Society of Electrochemistry, Lausanne, Switzerland, September 1–4.
15. A. LINKE, CH. MERDON, *Optimal and pressure-independent  $L^2$  velocity error estimates for a modified Crouzeix–Raviart element with BDM reconstructions*, The International Symposium of Finite Volumes for Complex Applications VII (FVCA 7), Berlin-Brandenburgische Akademie der Wissenschaften, June 15–20.
16. H. MAI, *Pathwise stability of likelihood estimators for diffusions via rough paths*, 37th Conference on Stochastic Processes and their Applications, Buenos Aires, Argentina, July 28 – August 1.
17. A. MIELKE, S. REICHEL, M. THOMAS, *Pattern formation in systems with multiple scales*, Evaluation of the DFG Collaborative Research Center 910 “Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, Berlin, June 30 – July 1.
18. ST. NEUKAMM, *Characterization and approximation of macroscopic properties in elasticity with homogenization*, 4th British-German Frontiers of Science Symposium, Potsdam, March 6–9.
19. ———, *Homogenization of slender structures in small-strain regimes*, 14th Dresden Polymer Discussion, Meißen, May 25–28.

20. N. ANGENSTEIN, J. POLZEHL, K. TABELOW, A. BRECHMANN, *Categorical versus sequential processing of sound duration*, 20th Annual Meeting of the Organization for Human Brain Mapping, Hamburg, June 8–12.
21. K. SCHILDKNECHT, *A two-stage hierarchical multiple test procedure based on the asymptotically optimal rejection curve*, 60. Biometrisches Kolloquium, Bremen, March 10–13.
22. J. STANGE, *Multiple testing adjustments with copula models*, 27th International Biometric Conference (IBC 2014), Florence, Italy, July 6–11.
23. S. MOHAMMADI, L. RUTHOTTO, K. TABELOW, T. FEIWEIER, J. POLZEHL, N. WEISKOPF, *ACID – A post-processing toolbox for advanced diffusion MRI*, 20th Annual Meeting of the Organization for Human Brain Mapping, Hamburg, June 8–12.
24. K. TABELOW, S. MOHAMMADI, N. WEISKOPF, J. POLZEHL, *Adaptive noise reduction in multi-shell dMRI data with SPM by POAS4SPM*, 20th Annual Meeting of the Organization for Human Brain Mapping, Hamburg, June 8–12.
25. K. TABELOW, H.U. VOSS, J. POLZEHL, *Local estimation of noise standard deviation in MRI images using propagation separation*, 20th Annual Meeting of the Organization for Human Brain Mapping, Hamburg, June 8–12.
26. ———, *Local estimation of the noise level in MRI images using structural adaptation*, 5th Ultra-Highfield MRI Scientific Symposium, Max Delbrück Center, Berlin, June 20.
27. M. THOMAS, *GENERIC for solids with dissipative interface processes*, 85th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2014), GAMM Juniors' Poster Session, Friedrich-Alexander Universität Erlangen-Nürnberg, March 10–14.
28. M. WOLFRUM, *Bifurcations and nonuniversal transitions to synchrony in the Sakaguchi–Kuramoto model*, International Conference on Control of Self-organizing Nonlinear Systems, Rostock-Warnemünde, August 24–28.

### A.8.5 Contributions to Exhibitions

1. TH. PETZOLD, *WIAS-MeFreSim with talk “WIAS-MeFreSim – Simulation des Mehrfrequenz-Induktionshärtens” on April 10 at “tech transfer – Gateway2Innovation Forum”*, Hannover Messe 2014, April 9–11.
2. W. WEISS, *WIAS-MeFreSim*, Hannover Messe 2014, April 7–9.

## A.9 Visits to other Institutions<sup>6</sup>

1. R. ALLEZ, University of Cambridge, Statistical Laboratory, UK, January 2–11.
2. ———, University of Cambridge, Statistical Laboratory, UK, January 22 – February 1.
3. ———, University of Cambridge, Statistical Laboratory, Cambridge, UK, February 10–14.
4. ———, University of Cambridge, Statistical Laboratory, UK, March 3–8.
5. ———, University of Cambridge, Statistical Laboratory, UK, April 15–23.
6. ———, University of Cambridge, Statistical Laboratory, UK, May 9–14.
7. ———, University of Cambridge, Statistical Laboratory, UK, August 22 – September 5.
8. ———, University of Cambridge, Statistical Laboratory, UK, September 26 – October 14.
9. ———, University of Cambridge, Statistical Laboratory, UK, November 1–17.
10. L. AVENA, Università degli Studi di Roma “La Sapienza”, Dipartimento di Matematica, Italy, December 16, 2013 – January 7, 2014.
11. ———, University of Leiden, Mathematical Institute, The Netherlands, April 7–11.
12. ———, Universität Zürich, Institut für Mathematik, Switzerland, April 22–25.
13. N. BALDIN, Moscow Institute of Physics and Technology, PreMoLab, Russia, February 21–27.
14. CH. BAYER, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, January 12–23.
15. ———, University of Texas, Center for Computational Engineering and Sciences, Austin, USA, July 16–26.
16. ———, City University of New York, Department of Mathematics, USA, October 20–25.
17. A. CIPRIANI, Universität Zürich, Institut für Mathematik, Switzerland, April 7–11.
18. M.H. FARSHBAF SHAKER, Universität Regensburg, Fakultät für Mathematik, June 23–27.
19. J. FUHRMANN, Norwegian University of Science and Technology, Department of Physics, Trondheim, January 27–30.
20. ———, Norwegian University of Science and Technology, Department of Physics, Trondheim, November 26–29.
21. O. GÜN, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, February 4–14.
22. ———, University of Leiden, Mathematical Institute, The Netherlands, August 29 – September 4.
23. H. HANKE, Universität Bonn, Institut für Numerische Simulation, November 18–21.
24. ———, Universität Bonn, Institut für Numerische Simulation, November 24–28.
25. CH. HEINEMANN, Università di Pavia, Dipartimento di Matematica, Italy, December 15, 2013 – April 17, 2014.
26. S. HEINZ, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, February 17–21.
27. R. HENRION, Universidad Miguel Hernández de Elche, Instituto Centro de Investigación Operativa, Spain, May 29 – June 4.

<sup>6</sup>Only stays of more than three days are listed.

28. M. HESSE, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, April 28 – May 5.
29. ———, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, June 16–20.
30. ———, University of Leiden, Mathematical Institute, The Netherlands, August 28 – September 4.
31. ———, University of Bath, Department of Mathematical Sciences, UK, October 13–17.
32. D. HÖMBERG, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, January 20–24.
33. ———, Fudan University, School of Mathematical Sciences, Shanghai, China, March 2–7.
34. ———, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, March 31 – April 11.
35. ———, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, October 14–31.
36. V. JOHN, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, December 8–11.
37. L. KAMENSKI, University of Kansas, Department of Mathematics, USA, July 7–15.
38. W. KÖNIG, University of Warwick, Mathematics Institute, Coventry, UK, March 24–27.
39. ———, University of Columbia, Department of Mathematics, New York, USA, December 1–5.
40. CH. KRAUS, Albert-Ludwigs-Universität Freiburg, Mathematisches Institut, January 27–31.
41. C. KREISBECK, Universität Würzburg, Institut für Mathematik, July 14–18.
42. M. LIERO, Technische Universität München, Zentrum Mathematik, February 17–22.
43. H. MAI, Mathematisches Forschungsinstitut Oberwolfach, June 1–24.
44. ———, Universidad de Buenos Aires, Instituto de Calculo, Argentina, August 4–8.
45. M. MAURELLI, Università di Pisa, Dipartimento di Matematica, Italy, December 15–19.
46. CH. MERDON, Norwegian University of Science and Technology, Department of Physics, Trondheim, January 27–30.
47. ———, Norwegian University of Science and Technology, Department of Physics, Trondheim, November 26–29.
48. A. MIELKE, Università di Pavia, Dipartimento di Matematica, Italy, June 16–20.
49. H. NEIDHARDT, Institute Mittag-Leffler, The Royal Swedish Academy of Sciences, Stockholm, Sweden, July 14 – August 2.
50. ST. NEUKAMM, Université Libre de Bruxelles, Département de Mathématique, Belgium, June 4–7.
51. ———, Universität Bonn, Hausdorff Center for Mathematics, July 21–24.
52. J. NEUMANN, Université Paris-Sud, Laboratoire d'Analyse Numérique, Orsay, France, October 6–11.
53. ST. PATRIZI, King Abdullah University of Science and Technology (KAUST), Department of Mathematics, Jeddah, Saudi Arabia, January 27–30.
54. ———, Università degli studi di Milano, Dipartimento di Matematica “F. Enriques”, Italy, November 9–14.
55. R.I.A. PATTERSON, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, December 15–18.

56. D. PESCHKA, University of California, Department of Mathematics, Los Angeles, USA, June 16 – September 12.
57. A. PIMENOV, Centre de Recerca Matemàtica, Barcelona, Spain, July 22 – August 7.
58. J. POLZEHL, University of Minnesota, School of Statistics, Minneapolis, USA, September 26 – October 4.
59. M. RADZIUNAS, Technical University of Moldova, Department of Physics, Chisinau, Moldova, June 2–7.
60. ———, University Politecnica de Catalunya (UPC), Department of Physics, Barcelona, Spain, November 17–21.
61. D.R.M. RENGIER, University of Bath, Department of Mathematical Sciences, UK, February 10–14.
62. ———, Universität Bonn, Institut für Angewandte Mathematik, May 25–28.
63. ———, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), and Delft University of Technology, Faculty Electrical Engineering, Mathematics and Computer Science, The Netherlands, June 10–13.
64. ———, University of Bath, Department of Mathematical Sciences, UK, August 18–22.
65. H. SI, Politecnico di Milano, Dipartimento di Matematica “F. Brioschi”, Italy, February 24–28.
66. V. SPOKOINY, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Russia, February 5–24.
67. ———, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Russia, May 12–16.
68. ———, Moscow Institute of Physics and Technology, PreMoLab, Russia, June 16–24.
69. J. STANGE, Johannes Gutenberg-Universität Mainz, Gutenberg School of Management & Economics, September 1–19.
70. M. THOMAS, Università di Pavia, Dipartimento di Matematica, Italy, March 17–24.
71. ———, Polytechnic University of Turin, Department of Mathematical Sciences, Italy, May 19–23.
72. ———, International School of Advanced Studies (SISSA), Trieste, Italy, May 25–30.
73. E. VALDINOCI, Columbia University, Columbia Geometry & Analysis Seminar, New York, USA, March 30 – April 14.
74. ———, University of Edinburgh, School of Mathematics, UK, April 15–22.
75. ———, University of Edinburgh, School of Mathematics, UK, May 1–6.
76. ———, Università di Padova, Dipartimento di Matematica, Italy, May 21–25.
77. ———, Universidad de Chile, Departamento de Ingeniería Matemática, Facultad de Ciencias Físicas y Matemáticas, Santiago, July 10 – August 8.
78. ———, Heriot-Watt University of Edinburgh, UK, October 28 – November 2.
79. ———, University of Texas at Austin, Mathematics, USA, November 3–16.
80. ———, Universidad de Granada, IEMath-Granada, Spain, November 27–30.
81. A.G. VLADIMIROV, Imperial College London, Department of Applied Mathematics, UK, June 27 – July 1.
82. M. ZHILOVA, Moscow Institute of Physics and Technology, PreMoLab, Russia, February 17–28.

## A.10 Academic Teaching<sup>7</sup>

### Winter Semester 2013/2014

1. A. CAIAZZO, *Analysis I (lehramtsbezogen)* (seminar), Freie Universität Berlin, 2 SWS.
2. W. DREYER, *Grundlagen der Kontinuumsmechanik II: Kontinuumsphysik* (lecture), Technische Universität Berlin, 4 SWS.
3. M. EIGEL, *Lineare Algebra für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
4. P. FRIZ, *Hairer's Regularity Structures* (lecture), Technische Universität Berlin/Berlin Mathematical School, 4 SWS.
5. ———, *Stochastik und Finanzmathematik* (seminar), Technische Universität Berlin, 2 SWS.
6. D. BECHERER, J. BLATH, P. FRIZ, W. KÖNIG, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), 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. C. CARSTENSEN, P. DEUFLHARD, H. GAJEWSKI, V. JOHN, R. KLEIN, R. KORNUBER, J. SPREKELS, ET AL., *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
11. J. BLATH, W. KÖNIG, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
12. H. GAJEWSKI, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
13. ST. NEUKAMM, *Partielle Differentialgleichungen* (lecture), Ruprecht-Karls-Universität Heidelberg, 4 SWS.
14. ———, *Stochastic Homogenization* (lecture), Ruprecht-Karls-Universität Heidelberg, 2 SWS.
15. ———, *Homogenisierung* (seminar), Ruprecht-Karls-Universität Heidelberg, 2 SWS.
16. D. PESCHKA, *Numerische Mathematik II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
17. V. SPOKOINY, *Methoden der Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
18. ———, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
19. ———, *Methoden der Statistik* (practice), Humboldt-Universität zu Berlin, 2 SWS.
20. V. SPOKOINY, W. HÄRDLE, M. REISS, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
21. J. SPREKELS, *Höhere Analysis I (Funktionalanalysis)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
22. H. STEPHAN, *Mathematische Modellierung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
23. K. TABELOW, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
24. M. WOLFRUM, B. FIEDLER, ST. LIEBSCHER, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

<sup>7</sup>SWS = semester periods per week

25. L. RECKE, H.-J. WÜNSCHE, U. BANDELOW, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.

### Summer Semester 2014

1. L. RECKE, U. BANDELOW, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. CH. BAYER, A. PAPAPANTOLEON, *Computational Finance* (lecture), Technische Universität Berlin, 4 SWS.
3. A. CAIAZZO, *Mathematik für Geowissenschaftler II* (lecture), Freie Universität Berlin, 2 SWS.
4. ———, *Mathematik für berufliche Fachrichtungen* (seminar), Technische Universität Berlin, 2 SWS.
5. TH. DICKHAUS, *Seminar zur simultanen statistischen Inferenz* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
6. M. EIGEL, *Uncertainty Quantification* (lecture), Technische Universität Berlin, 2 SWS.
7. P. FRIZ, *Rough Paths and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
8. D. BECHERER, J. BLATH, P. FRIZ, W. KÖNIG, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (lecture), WIAS Berlin, 2 SWS.
9. A. GLITZKY, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
10. D. HÖMBERG, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
11. V. JOHN, *Numerical Methods for Incompressible Flow Problems I* (lecture), Freie Universität Berlin, 2 SWS.
12. ———, *Numerical Methods for Incompressible Flow Problems I* (practice), Freie Universität Berlin, 2 SWS.
13. W. KÖNIG, *Spezialvorlesung Extremwerttheorie und Punktprozesse* (lecture), Technische Universität Berlin, 2 SWS.
14. ———, *Extremwerttheorie und Punktprozesse* (seminar), Technische Universität Berlin, 2 SWS.
15. J. BLATH, W. KÖNIG, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
16. R. MÜLLER, *Numerische Verfahren für Erhaltungsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. R.I.A. PATTERSON, *Mathematical Tools for Engineering and Management* (lecture), Technische Universität Berlin, 2 SWS.
18. ———, *Mathematical Tools for Engineering and Management* (practice), Technische Universität Berlin, 2 SWS.
19. V. SPOKOINY, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. V. SPOKOINY, W. HÄRDLE, M. REISS, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
21. H. STEPHAN, *Mathematische Modellierung II* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
22. K. TABELOW, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
23. M. WOLFRUM, B. FIEDLER, ST. LIEBSCHER, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.



## Winter Semester 2014/2015

1. L. RECKE, U. BANDELOW, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. A. CAIAZZO, *Analysis II für Physiker* (lecture), Freie Universität Berlin, 4 SWS.
3. TH. DICKHAUS, *Nichtparametrische Testtheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
4. W. DREYER, *Grundlagen der Kontinuumsmechanik I: Tensoranalysis* (lecture), Technische Universität Berlin, 4 SWS.
5. M. EIGEL, *Numerische Mathematik II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
6. M.H. FARSHBAF SHAKER, *Optimalsteuerung bei partiellen Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS.
7. P. FRIZ, *Rough Paths and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
8. ———, *Stochastik und Finanzmathematik* (seminar), Technische Universität Berlin, 2 SWS.
9. D. BECHERER, J. BLATH, P. FRIZ, W. KÖNIG, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. A. GLITZKY, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. A. GLITZKY, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
12. D. HÖMBERG, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
13. V. JOHN, *Numerical Methods for Incompressible Flow Problems II* (lecture), Freie Universität Berlin, 4 SWS.
14. ———, *Numerical Methods for Incompressible Flow Problems II* (practice), Freie Universität Berlin, 2 SWS.
15. J. BLATH, W. KÖNIG, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
16. R.I.A. PATTERSON, *Theorie der Großen Abweichungen* (lecture), Freie Universität Berlin, 2 SWS.
17. V. SPOKOINY, *Nichtparametrische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
18. ———, *Nichtparametrische Statistik* (practice), Humboldt-Universität zu Berlin, 2 SWS.
19. V. SPOKOINY, W. HÄRDLE, M. REISS, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. J. SPREKELS, *Höhere Analysis I* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
21. H. STEPHAN, *Funktionalanalytische Methoden in der klassischen Physik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
22. K. TABELOW, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
23. B. WAGNER, *Asymptotische Analysis I* (lecture), Technische Universität Berlin, 2 SWS.
24. ———, *Dünne Schichten – Freie Randwertprobleme* (seminar), Technische Universität Berlin, 2 SWS.
25. 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 2014, Dr. Heiko Kröner (Universität Tübingen) and Dr. Tigran Nagapetyan (Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern) worked as fellowship holders at WIAS.

  
Weierstrass Institute for  
Applied Analysis and Stochastics

# Weierstrass Postdoctoral Fellowship Program



The Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Leibniz Institute in Forschungsverbund Berlin e.V. (<http://wias-berlin.de>) is a research institute of the Leibniz Association. WIAS engages in project-oriented research in Applied Mathematics and ranks among the leading research institutions worldwide in the study of the mathematical aspects of the following fields:

- 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

**WIAS offers postgraduate fellowships for 2015 and the following years. Their duration is six or twelve months. These fellowships are designed to enable highly-qualified young scientists to participate in the research into the mathematical problems in the above fields, thus furthering their education and training.**

**The fellowships can be started anytime in the year.**

**Application deadlines: February 28 and August 31 of each year. The decision on the applications will be taken within six weeks. The next application deadline is**

August 31, 2015

**Value:** The monthly stipend is **1,828 Euro**. In well-founded cases, travel allowances may be paid if a special application is made.

**Qualifications for application:** Applicants should hold a PhD in a subject relevant to one of the above fields. It is required that the candidates have a good command of the German or English language.

**Documents to be submitted with the application (in German or English):**

- Curriculum vitae
- PhD certificate
- List of publications
- Summary of research activities to date and proposed research program
- Two letters of recommendation to be sent separately to the address given below

**Applications should be sent to:** Director of WIAS, Mohrenstrasse 39, D-10117 Berlin, Germany ([postdoc@wias-berlin.de](mailto:postdoc@wias-berlin.de)).

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## A.12 Visiting Scientists<sup>8</sup>

### A.12.1 Guests

1. D. ABRAMS, Northwestern University, Department of Engineering Sciences and Applied Mathematics, Evanston, USA, November 21–29.
2. ST. ADAMS, University of Warwick, Mathematics Institute, Coventry, UK, October 20–28.
3. S. AGAPIOU, University of Warwick, Mathematics Institute, UK, May 18–23.
4. V. AVANESOV, Russian Academy of Sciences, Institute for System Programming, Moscow, April 15–24.
5. G.R. BARRENECHEA, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, May 24–29.
6. A. BÁTKAI, Eötvös Loránd University, Department of Applied Analysis and Computational Mathematics, Budapest, Hungary, September 10–13.
7. B. BLASZCZYŹYŹYN, Institut National de Recherche en Informatique et en Automatique (INRIA), Research Group DYOGENE, Paris, France, December 8–11.
8. A. BOITSEV, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russia, November 2–8.
9. E. BONETTI, Università degli Studi di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, May 5–9.
10. C. BUCUR, Università degli Studi di Milano, Dipartimento di Matematica, Italy, September 9 – October 9.
11. N. BUZUN, Russian Academy of Sciences, Institute for System Programming, Moscow, April 15–24.
12. D.P. CHALLA, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, February 16–23.
13. V. CHERNOZHUKOV, Massachusetts Institute of Technology, Department of Economics, Cambridge (MA), USA, December 7–14.
14. D. CHETVERIKOV, University of California, Department of Economics, Los Angeles, USA, December 1–4.
15. ———, December 9–13.
16. F. CHRISTOWIAK, Universität Regensburg, Fakultät für Mathematik, July 6–10.
17. R. ČIEGIS, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, October 1–14.
18. E. CINTI, Università degli Studi di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, September 8 – November 30.
19. P. COLLI, Università degli Studi di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, March 2–7.
20. M. COZZI, Università degli Studi di Milano, Dipartimento di Matematica “Federigo Enriques”, Italy, January 27 – February 17.
21. ———, October 13–26.
22. S. DAMES, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, Center for Applied Statistics and Economics, May 8, 2014 – January 31, 2015.
23. F. DASSI, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, September 1–12.

<sup>8</sup>Only stays of more than three days are listed.

24. ———, September 22–30.
25. M. DELFOUR, Université de Montréal, Centre de Recherches Mathématiques, Canada, October 8–11.
26. A.L. DINIZ, CEPEL – Brazilian Electric Energy Research Center, Rio de Janeiro, September 1 – November 30.
27. S. DIPIERRO, University of Edinburgh, School of Mathematics, UK, October 4–9.
28. S. DOVGAL, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, November 27 – December 12.
29. Y. DUGUET, Centre National de la Recherche Scientifique, Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur, Orsay, France, November 23–28.
30. L. DUMAZ, University of Cambridge, Centre for Mathematical Sciences, UK, March 17 – April 10.
31. ———, June 12 – July 10.
32. P. DVURECHENSKII, Moscow Institute of Physics and Technology, PreMoLab, Russia, May 24 – June 7.
33. K. EFIMOV, Moscow Institute of Physics and Technology, PreMoLab, Russia, September 16, 2013 – August 31, 2014.
34. ———, September 24, 2014 – August 31, 2015.
35. K. FILONENKO, University of Southern Denmark, Mads Clausen Institute, Sønderborg, October 6 – December 9.
36. V. GAYRARD, Université d'Aix-Marseille, Institut de Mathématiques, France, December 15–22.
37. J. GIESSELMANN, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, June 10–13.
38. P. GLASSERMAN, Columbia Business School, Decision, Risk, and Operations Division, New York, USA, May 18–22.
39. S. GUREVICH, Wilhelms-Universität Münster, Institut für Theoretische Physik, February 9–14.
40. ———, May 11–17.
41. ———, July 28 – August 1.
42. J. HÄPPÖLÄ, King Abdullah University of Science and Technology (KAUST), Department of Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, June 2–27.
43. J. HASKOVEC, King Abdullah University of Science and Technology, Department of Computer, Electrical and Mathematical Sciences and Engineering, Thuwal, Saudi Arabia, June 22–27.
44. S. HITTMEIR, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, June 22–26.
45. B.R. HODGSON, Département de Mathématiques et de Statistique, Faculté des Sciences et de Génie, Université Laval, Québec, Canada, May 13–21.
46. B. HOFMANN, Technische Universität Chemnitz, Fakultät für Mathematik, March 17–21.
47. W. HUANG, University of Kansas, Department of Mathematics, Lawrence, USA, September 29 – October 4.
48. J. JAVALOYES, University of the Balearic Islands, Department of Physics, Palma de Mallorca, Spain, November 24–29.
49. S. KÄBISCH, University of Surrey, Department of Mathematics, Guildford, UK, May 21–30.
50. Y. KLOCHKOV, Moscow Institute of Physics and Technology, Department of Control Management and Applied Mathematics, Russia, March 23 – April 1.
51. D. KNEES, Universität Kassel, Institut für Mathematik, August 24 – September 5.

52. V. KOLOKOLTSOV, University of Warwick, Department of Statistics, UK, May 26–29.
53. A. KOZIUK, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, November 27 – December 12.
54. M. KRAFT, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, June 23 – August 1.
55. D. KULIKOV, Yaroslavl State University, Institute of Computer Science, Russia, May 15–26.
56. H. LACQIN, Université Paris Dauphine, Centre de Recherche en Mathématiques de la Décision, France, June 9–12.
57. A. LIONNET, University of Oxford, St John's College, UK, November 10–23.
58. Y. LIU, University of Tokyo, Graduate School of Mathematical Sciences, Japan, May 5 – June 5.
59. S. LU, Fudan University, School of Mathematical Sciences, Shanghai, China, July 1–31.
60. M.M. MALAMUD, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Donetsk, Ukraine, March 28 – April 28.
61. M. MALIOUTOV, Northeastern University, Department of Mathematics, Boston, USA, December 8–12.
62. M. MEDINA, Universidad Autonoma de Madrid, Departamento de Matematicas, Spain, September 8 – November 3.
63. G. MONTECINOS, Università degli Studi di Trento, Departmental Area of Civil and Environmental Engineering, Italy, March 10–15.
64. ST. MUIRHEAD, University College London, Department of Mathematics, UK, November 17–21.
65. L.O. MÜLLER, Università degli Studi di Trento, Departmental Area of Civil and Environmental Engineering, Italy, March 10–15.
66. M. MUMINOV, Universiti Teknologi Malaysia, Faculty of Science, Skudai, December 13–19.
67. J. MURA, Pontificia Universidad Catolica de Valparaíso, Department of Civil Engineering, Chile, September 29 – October 9.
68. O. MUSCATO, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, July 27 – August 8.
69. M. NEGRI, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, January 28–31.
70. J. NOVO, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, April 8–11.
71. V. PATILEA, Institut des Sciences Appliquées de Rennes (INSA), Centre des Mathématiques, France, March 30 – April 3.
72. C. PATZ, Robert Bosch GmbH, Stuttgart, February 21–25.
73. J. PELLERIN, Université de Lorraine, Ecole Nationale Supérieure de Géologie, Vandoeuvre-lès-Nancy, France, January 20–24.
74. ———, August 25–29.
75. I. POPOV, St. Petersburg State University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russia, November 2–8.
76. F. PUNZO, Università degli Studi di Milano, Dipartimento di Matematica “Federigo Enriques”, Italy, October 20–24.
77. E. QUEIROLO, École Polytechnique Fédérale de Lausanne, Section de Mathématiques, Switzerland, February 17 – June 20.

78. D. RACHINSKYI, The University of Texas at Dallas, Department of Mathematical Sciences, USA, July 2–12.
79. I. RAMIS-CONDE, Universidad Castilla-La Mancha, Instituto de Matemática Aplicada a la Ciencia e Ingeniería, Cuenca, Spain, March 18–22.
80. L. REBHOLZ, Clemson University, Department of Mathematical Sciences, USA, June 23–29.
81. R. RICHTER, Max-Planck-Institut Halbleiterlabor, München, December 15–18.
82. F. RINDLER, University of Warwick, Mathematics Institute, UK, May 19–23.
83. R. ROSSI, Università di Brescia, Dipartimento di Matematica, Italy, March 24–28.
84. T. ROUBÍČEK, Charles University, Mathematical Institute, Prague, Czech Republic, January 20 – February 20.
85. ———, April 22 – May 22.
86. ———, September 15 – October 15.
87. M. SCHÄFFNER, Universität Würzburg, Institut für Mathematik, June 22–27.
88. A. SEGATTI, Università degli Studi di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, May 5–9.
89. O. SEKULOVIC, University of Montenegro, Department for Mathematics and Computer Science, Podgorica, July 14–18.
90. B. SENGUL, University of Cambridge, Centre for Mathematical Sciences, UK, January 2–7.
91. ———, March 17–28.
92. ———, July 30 – August 12.
93. B. SENGUL, University of Bath, Department of Mathematical Sciences, UK, November 10–21.
94. J. SIEBER, University of Exeter, College of Engineering, Mathematics and Physical Sciences, UK, September 1–11.
95. I. SIM, National Institute for Mathematical Sciences, Numerical Analysis Group, Daejeon, Republic of Korea, December 14–20.
96. U. STEFANELLI, University of Vienna, Faculty of Mathematics, Austria, October 6–10.
97. A. SUVORIKOVA, Moscow Institute of Physics and Technology, PreMoLab, Russia, January 1, 2014 – September 30, 2015.
98. M. THÉRA, Université de Limoges, XLIM, France, April 8–13.
99. E. TOBISCH, Johannes Kepler University, Institute for Analysis, Linz, Austria, October 20–24.
100. G. TOMASSETTI, Università di Roma “Tor Vergata”, Dipartimento di Ingegneria Civile e Ingegneria Informatica, Italy, January 13–17.
101. D. TURAEV, Imperial College London, Department of Mathematics, UK, May 24–31.
102. ———, July 23–31.
103. E. VESALAINEN, University of Jyväskylä, Department of Mathematics, Finland, October 19–25.
104. J. VIANA, Universidade Estadual Paulista “Júlio de Mesquita Filho”, Rio Claro, Brazil, October 15 – November 16.
105. M. YAMAMOTO, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 17–24.
106. ———, May 9–18.
107. ———, May 23 – June 8.

108. ———, September 6 – October 5.
109. ———, November 23–27.
110. N. YAMAZAKI, Kanagawa University, Department of Mathematics, Yokohama, Japan, August 20 – September 16.
111. T. YIN, Chongqing University, College of Mathematics and Statistics, China, October 26, 2013 – October 20, 2014.
112. V. ZAGREBNOV, Université d’Aix-Marseille, Centre de Mathématiques et Informatique, France, October 10–18.
113. J. ZHANG, Technische Universität München, Lehrstuhl für Mathematische Statistik, April 7–12.
114. ———, November 3–8.
115. J. ZINSL, Technische Universität München, Zentrum Mathematik, February 23–28.
116. ———, September 21–26.

### A.12.2 Scholarship Holders

1. F. DASSI, Politecnico di Milano, Italy, Leibniz-DAAD Research Fellowship, October 1, 2014 – September 30, 2015.
2. S. GANESAN, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, Humboldt Research Fellowship, June 17 – July 31.
3. H. KRÖNER, Universität Tübingen, Mathematisches Institut, Weierstrass Postdoctoral Fellowship Program, January 1 – September 30.
4. T. NAGAPETIAN, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, Weierstrass Postdoctoral Fellowship Program, June 1, 2014 – May 31, 2015.
5. CH.V. PHAM, Hanoi University of Science, Faculty of Mathematics, Mechanics and Informatics, Vietnam, IMU Berlin Einstein Foundation Program, September 1 – December 31.
6. T. RASULOV, Bukhara State University, Faculty of Physics and Mathematics, Department of Mathematical Physics and Analysis, Uzbekistan, IMU Berlin Einstein Foundation Program, April 1 – December 31.
7. S. SIMONELLA, Technische Universität München, Zentrum Mathematik, Weierstrass Postdoctoral Fellowship Program, December 1, 2014 – May 31, 2015.

### A.12.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. N. ABATANGELO, Università di Milano, Dipartimento di Matematica, doctoral candidate, January 1 – December 31.
2. N. BALDIN, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
3. C. BUCUR, Università di Milano, Dipartimento di Matematica, doctoral candidate, January 1 – December 31.
4. M. COZZI, Università di Milano, Dipartimento di Matematica, doctoral candidate, January 1 – December 31.
5. K. EFIMOV, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
6. M. PANOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, doctoral candidate, January 1 – December 31.



7. C. PATZ, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, January 1 – February 24.
8. S. ROCKEL, Freie Universität Berlin, Institut für Mathematik, Helmholtz-Kolleg GEOSIM, 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, January 1 – December 31.

## A.13 Guest Talks

1. T. ARENS, Karlsruher Institut für Technologie, Institut für Algebra und Geometrie, *Indicator functions for shape reconstruction related to the linear sampling method*, June 3.
2. V. AVANESOV, Russian Academy of Science, Institute for System Programming, Moscow, *Topic modeling graph clustering and their application to influence measurement*, April 22.
3. M. BARIGOZZI, London School of Economics, Department of Statistics, UK, *Dynamic factor models, cointegration, and error correction mechanisms*, May 7.
4. G.R. BARRENECHEA, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Curing inf-sup deficiencies: Two quick examples*, May 27.
5. C. BERTOGLIO, Technische Universität München, Institut für Numerische Mechanik, *Forward and inverse modeling of the cardiovascular system: How PDE's can help to improve clinical outcomes*, February 18.
6. L. BITTNER, Bergische Universität Wuppertal, Fachbereich C, AG Stochastik, *Optimal reliability in design for fatigue life under cyclic thermomechanic loading*, November 4.
7. E. BONETTI, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, *An experimental, theoretical and numerical investigation of shape memory polymers*, May 7.
8. N. BOTKIN, Technische Universität München, Zentrum Mathematik, *Modeling of polarized radiation transfer: Application to computed tomography*, October 28.
9. A. BÜCHER, Ruhr-Universität Bochum, Fakultät für Mathematik, *When uniform weak convergence fails: Empirical processes for dependence functions via epi- and hypographs*, January 29.
10. G. CAPELLINI, Leibniz-Institut für innovative Mikroelektronik (IHP), Frankfurt/Oder, *A Si CMOS compatible Ge laser source on silicon*, November 10.
11. D.P. CHALLA, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *Wave propagation by small rigid bodies of arbitrary shapes*, February 18.
12. S. CHANDLER-WILDE, University of Reading, Department of Mathematics and Statistics, UK, *Acoustic scattering by screens: Computation and analysis*, March 10.
13. Y. CHANG, Indiana University, Department of Statistics, USA, *Regime switching model with endogenous autoregressive latent factor*, June 11.
14. V. CHERNOZHUKOV, Massachusetts Institute of Technology, Department of Economics, Cambridge (MA), USA, *Gaussian approximations, bootstrap, and z-estimators when  $p \gg n$* , December 10.
15. D. CHETVERIKOV, University of California, Department of Economics, Los Angeles, USA, *Nonparametric instrumental variable estimation under monotonicity*, December 3.
16. M. CHICHIGNOUD, Swiss Federal Institute of Technology Zurich, Department of Mathematics, *On bandwidth selection in empirical risk minimization*, May 28.
17. S. CHRISTIANSEN, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, *Advanced nano-patterned composite materials and their application in energy harvesting and sensing*, December 15.
18. F. CHRISTOWIAK, Universität Regensburg, Fakultät für Mathematik, *Homogenization of layered materials with rigid components in single-slip elasto-plasticity*, July 7.
19. R. ČIEGIS, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, *On adaptive numerical integration methods for systems of ODEs*, October 9.
20. M. CLAUS, Universität Duisburg-Essen, Fachbereich Mathematik, *A representation of a class of stochastic dominance constraints enabling Lipschitzian properties and stability*, January 14.

21. M. DELFOUR, Université de Montréal, Centre de Recherches Mathématiques, Canada, *Differentials and semidifferentials for metric spaces of shapes and geometries*, October 10.
22. M. DEMUTH, Technische Universität Clausthal, Institut für Mathematik, *On the distribution of eigenvalues for non-selfadjoint operators*, June 25.
23. J. DIEHL, Technische Universität Berlin, Institut für Mathematik, *Stochastic partial differential equations: A rough path view*, April 8.
24. A.L. DINIZ, CEPEL – Brazilian Electric Energy Research Center, Rio de Janeiro, *Stochastic Dual Dynamic Programming (SDDP) for power generation planning – Traditional and risk-averse approaches*, November 4.
25. P. DONDL, Durham University, Department of Mathematical Sciences, UK, *Energy estimates, relaxation, and existence for strain gradient plasticity with cross hardening*, July 9.
26. R. DOS SANTOS, Université Claude Bernard Lyon 1, Institut Camille Jordan, France, *Random walk on random walks*, January 31.
27. P. DVURECHENSKII, Moscow Institute of Physics and Technology, PreMoLab, Russia, *Gradient methods for convex problems with stochastic inexact oracle*, June 3.
28. M. EBERTS, Universität Stuttgart, Fachbereich Mathematik, Institut für Stochastik und Anwendungen, *Adaptive rates for support vector machines*, June 25.
29. E. EMMRICH, Technische Universität Berlin, Institut für Mathematik, *Nonlinear evolution equations of second order with damping: Existence and discretization*, February 5.
30. A. FABRI, GeometryFactory, Valbonne, France, *CGAL – The Computational Geometry Algorithms Library*, February 20.
31. A. FIEBACH, Physikalisch-Technische Bundesanstalt Berlin, Modellierung und Simulation, *An introduction to semiconductor device simulation*, June 12.
32. J. FISCHER, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Global existence of renormalized solutions to entropy-dissipating reaction-diffusion systems*, November 5.
33. S.K. GANESAN, Indian Institute of Science, Supercomputer Education and Research Center, Bangalore, *SUPG finite element method for PDEs in time-dependent domains*, July 10.
34. G. GENOVESE, Université Paris Diderot, UFR de Mathématiques, France, *Variational principles for neural networks*, February 4.
35. J. HÄPPÖLÄ, King Abdullah University of Science and Technology (KAUST), Department of Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, *Weak approximation of SDE by a mean square error adaptive multilevel Monte Carlo method*, June 2.
36. J. HASKOVEC, King Abdullah University of Science and Technology, Department of Computer, Electrical and Mathematical Sciences and Engineering, Thuwal, Saudi Arabia, *Mathematical analysis of a system for biological network formation*, June 25.
37. CH. HIRSCH, Universität Ulm, Institut für Stochastik, *Random geometric graphs: Connectivity, shortest paths and applications in telecommunication networks*, February 5.
38. S. HITTEMEIR, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, *Nonlinear diffusion and additional cross-diffusion in the Keller–Segel model*, June 25.
39. H. HOLZMANN, Universität Marburg, Fachbereich Mathematik und Informatik, *Nonparametric identification and estimation in a triangular random coefficient regression model*, April 30.
40. D. HORSTMANN, Universität zu Köln, Institut für Mathematik, *Anmerkungen zu einer Klasse von Reaktions-Diffusionsmodellen mit Kreuzdiffusion und ihren Lyapunov-Funktionalen*, July 14.

41. W. HUANG, University of Kansas, Department of Mathematics, Lawrence, USA, *Computation of eigenvalue problems with anisotropic diffusion operators*, September 30.
42. S. HUMMEL, Technische Universität München, Zentrum Mathematik, *The TASEP speed process*, January 31.
43. B. JAHNEL, Ruhr-Universität Bochum, Fakultät für Mathematik, *A class of nonergodic interacting particle systems with unique invariant measure*, June 16.
44. J. JAVALOYES, University of the Balearic Islands, Department of Physics, Palma de Mallorca, Spain, *Temporal localized structures in vertical-cavity surface-emitting lasers*, November 27.
45. P. KEELER, Institut National de Recherche en Informatique et en Automatique (INRIA), Paris, France, *Studying the SINR process of the typical user in Poisson networks: A factorial moment measure framework*, February 5.
46. D. KNEES, Universität Kassel, Institut für Mathematik, *Series of lectures "Evolutionary variational inequalities in the context of inelastic solids"*, September 3.
47. V. KOCHAROVSKII, Russian Academy of Sciences, Institute of Applied Physics, Moscow, *Dynamical and spectral features of superradiant lasing*, June 24.
48. P. KOKOSCHKA, Colorado State University, Department of Statistics, USA, *Functional framework for high frequency financial data with focus on regression and predictability of intraday price curves*, June 18.
49. V. KOLOKOLTSOV, University of Warwick, Department of Statistics, UK, *Interacting particle systems, nonlinear Markov processes and SDEs driven by nonlinear Levy noise*, May 28.
50. V. KONAROVSKIY, Yuriy Fedkovych Chernivtsi National University, Department of Mathematics and Informatics, Ukraine, presently at Universität Jena, *Mathematical model of coalescing diffusion particles system with variable weights*, April 9.
51. E. KONG, University of Kent at Canterbury, Faculty of Sciences, UK, *An adaptive composite quantile approach to dimension reduction for censored data*, November 5.
52. A. KOZIUK, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, *Linear hypothesis testing for the case with weak instrumental variables*, December 2.
53. M. KRAFT, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, *Stochastic particle methods for a granulation process*, July 29.
54. D. KRISTENSEN, University College London, Department of Economics, UK, *What drives the yield curve?*, June 4.
55. M. KROLL, Universität Duisburg-Essen, Institut für Soziologie, *On contractive anonymization of spatially referenced microdata via Lipschitz embedding*, January 31.
56. D. KULIKOV, Yaroslavl State University, Institute of Computer Science, Russia, *Local bifurcations of the generalized Kuramoto–Sivashinsky equation*, May 20.
57. H. LACON, Université Paris Dauphine, Centre de Recherche en Mathématiques de la Décision, France, *Description of the phase diagram of Gaussian multiplicative chaos*, June 11.
58. J. LANG, Technische Universität Darmstadt, Numerik und Wissenschaftliches Rechnen, *Adaptive moving meshes in large eddy simulation for turbulent flows*, October 2.
59. P. LEDERER, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, *Hybrid discontinuous Galerkin (HDG) methods for the incompressible Navier–Stokes equations*, October 9.
60. U. LEONHARDT, Weizmann Institute of Science, Physics Faculty, Rehovot, Israel, *Transformation optics*, October 16.
61. D. LI, University of York, Department of Mathematics, UK, *Panel data models with interactive fixed effects and multiple structural breaks*, October 29.

62. A. LITVINENKO, King Abdullah University of Science and Technology, Center for Uncertainty Quantification in Computational Science and Engineering, Thuwal, Saudi Arabia, *Computation of the response surface in the tensor train data*, August 26.
63. Y. LIU, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Well-posedness and numerical simulation for multi-term time-fractional diffusion equations with positive constant coefficients*, May 13.
64. S. LU, Fudan University, School of Mathematical Sciences, Shanghai, China, *A recursive algorithm for multi-frequency acoustic source identification*, July 15.
65. T. MAKAI, Technische Universität Graz, Institut für Optimierung und Diskrete Mathematik, Austria, *Various random graph models*, February 5.
66. M.M. MALAMUD, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Donetsk, Ukraine, *One-dimensional Schrödinger operators with  $\delta'$ -interactions on Cantor-type sets*, April 16.
67. M. MALIOUTOV, Northeastern University, Department of Mathematics, Boston, USA, *SCOT modeling, training and homogeneity testing*, December 9.
68. E. MARIUCCI, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, Grenoble, France, *Asymptotic equivalence for discretely or continuously observed Lévy processes and Gaussian white noise*, November 12.
69. H. MATANO, University of Tokyo, Department of Mathematics, Japan, *Propagating terrace for semilinear diffusion equations*, July 16.
70. N. MEINSHAUSEN, Eidgenössische Technische Hochschule Zürich, Departement Mathematik, Switzerland, *Challenges for high-dimensional inference*, January 15.
71. J.-F. MENNEMANN, Universität Wien, Fachbereich Mathematik, Austria, *Simulation of nanoscale electronic devices using the Schrödinger equation with open boundary conditions*, March 26.
72. N. MEYENDORF, Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, Berlin, *Heinrich Barkhausen in Berlin and Dresden – New applications of his ideas for electromagnetic non-destructive evaluation*, October 7.
73. P. MICHAELIS, Technische Universität Braunschweig, Carl-Friedrich-Gauß-Fakultät, *The embedding of ARMA processes in CARMA processes*, January 31.
74. S. MOLNOS, Technische Universität Berlin, Fachbereich Mathematik, *Controlling transversal instabilities of two-dimensional travelling waves in reaction-diffusion systems*, March 27.
75. ST. MUIRHEAD, University College London, Department of Mathematics, UK, *Trap models with slowly-varying tapes*, November 17.
76. L.O. MÜLLER, Università degli Studi di Trento, Departmental Area of Civil and Environmental Engineering, Italy, *Well-balanced finite volume schemes for one-dimensional blood flow models: Application to a closed-loop model for the cardiovascular system*, March 13.
77. M. MUMINOV, Universiti Teknologi Malaysia, Faculty of Science, Skudai, *On the spectral properties of the two-particle discrete Schrödinger operator*, December 17.
78. O. MUSCATO, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, *Transport phenomena in silicon semiconductor devices*, July 29.
79. J. NAUMANN, Humboldt-Universität zu Berlin, Institut für Mathematik, *On the existence of weak solutions to Kolmogorov's two-equation model of turbulence*, April 23.
80. ———, *On the existence of weak solutions to Prandtl's (1945) one-equation model of turbulence*, December 10.
81. M. NEGRI, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, *Quasi-static evolutions by graph parametrization: Existence, approximation and application to fracture*, January 30.

82. J. NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, *Efficient coarse graining of stochastic high-dimensional configuration spaces as fundament for a fully ab initio based materials design*, July 7.
83. R. NEUMAYER, University of Texas Department of Mathematics, Austin, USA, *A stability result for the anisotropic isoperimetric inequality*, June 30.
84. J. NOVO, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, *Stabilization of finite element approximations to the Stokes and Oseen equations*, April 10.
85. V. PATILEA, Institut des Sciences Appliquées de Rennes (INSA), Centre des Mathématiques, France, *Testing for lack of fit in functional regression models*, April 1.
86. J. PELLERIN, Université de Lorraine, Ecole Nationale Supérieure de Géologie, Vandoeuvre-lès-Nancy, France, *Accounting for the geometrical complexity of geological models in meshing methods based on Voronoi diagrams*, January 23.
87. CH.V. PHAM, Hanoi University of Science, Faculty of Mathematics, Mechanics and Informatics, Vietnam, *Homogenization of very rough interfaces*, November 19.
88. J.-F. PIETSCHMANN, Technische Universität Darmstadt, Fachbereich Mathematik, *Motion and size exclusion – Derivation and properties of non-linear cross-diffusion models*, October 23.
89. Ł. PŁOCINICZAK, Wrocław University of Technology, Institute of Mathematics and Computer Science, Poland, *Mathematics of the human eye*, November 18.
90. J. POISAT, University of Leiden, Mathematical Institute, The Netherlands, *Percolation transition for Brownian paths homogeneously distributed in space*, February 4.
91. I. POPOV, St. Petersburg State University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russia, *Spectral problem for chain type nanostructures*, November 5.
92. P. POZZI, Universität Duisburg-Essen, Fakultät für Mathematik, *On anisotropic Willmore flow*, December 8.
93. F. PUNZO, Università degli Studi di Milano, Dipartimento di Matematica “Federigo Enriques”, Italy, *On the asymptotic behavior of solutions to the weighted fractional porous medium equation*, October 20.
94. E. QUEIROLO, École Polytechnique Fédérale de Lausanne, Section de Mathématiques, Switzerland, *Isogeometrical analysis for Navier–Stokes equations*, June 12.
95. I. RAMIS-CONDE, Universidad Castilla-La Mancha, Instituto de Matemática Aplicada a la Ciencia e Ingeniería, Cuenca, Spain, *Multiscale modeling of palisade formation in glioblastoma*, March 20.
96. M. RASETA, Technische Universität Graz, Institut für Statistik, Austria, *From periodic functions with random frequencies to miscellaneous topics in mathematical economics*, February 5.
97. L. REBHOLZ, Clemson University, Department of Mathematical Sciences, USA, *A connection between coupled and penalty projection timestepping schemes with FE spatial discretization*, June 25.
98. L. RECKE, Humboldt-Universität zu Berlin, Institut für Mathematik, *Solution regularity and smooth dependence for abstract equations and applications to PDEs*, January 8.
99. R. ROSSI, Università di Brescia, Dipartimento di Matematica, Italy, *Singular perturbations of infinite-dimensional gradient flows*, March 26.
100. N. ROTUNDO, University of Calabria, Evolutionary Systems Group, Italy, *Coupling and thermal effects in semiconductor devices*, April 29.
101. T. ROUBÍČEK, Charles University, Mathematical Institute, Prague, Czech Republic, *Global versus local minimization in rate-independent evolution systems*, February 12.
102. M. SCHÄFFNER, Universität Würzburg, Institut für Mathematik, *About an analytical approach to a quasicontinuum method via Gamma convergence*, June 26.

103. A. SCHMIDT, Universität Bremen, Institut für Technomathematik, *FEM for phase transitions in melting and welding processes*, May 20.
104. K. SCHMIDT, Technische Universität Berlin, Institut für Mathematik, *Symmetric local absorbing boundary conditions for the Helmholtz equation*, June 11.
105. U. SCHNEIDER, Wirtschaftsuniversität Wien, Department für Sozioökonomie, Austria, *On distributional properties of Lasso-type estimators noise*, November 26.
106. TH. SCHRÖDER, Leibniz-Institut für innovative Mikroelektronik (IHP), Frankfurt/Oder, *Modern materials research for "More than Moore" silicon microelectronics*, November 10.
107. T. SCHWEDES, Universität Heidelberg, Institut für Angewandte Mathematik, *Sojourn time estimation for queuing networks*, February 7.
108. G. SCILLA, Technische Universität München, Zentrum Mathematik, *Motion of interfaces by crystalline curvature*, November 4.
109. A. SEGATTI, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, *Analysis of a variational model for nematic shells*, May 7.
110. I. SIM, National Institute for Mathematical Sciences, Numerical Analysis Group, Daejeon, Republic of Korea, *Multilevel Monte-Carlo method for optimal control problem*, December 16.
111. M. SŁOWIK, Technische Universität Berlin, Institut für Mathematik, *Recent progress in the theory of quenched invariance principles for random conductance models*, January 15.
112. U. STEFANELLI, University of Vienna, Faculty of Mathematics, Austria, *Carbon geometries as optimal configurations*, October 8.
113. CH. TEMMEL, Vrije Universiteit Amsterdam, Department of Mathematics, The Netherlands, *One-independent point processes*, February 4.
114. M. THÉRA, Université de Limoges, XLIM, France, *Estimate for fixed points of composition of multifunctions and application to the global version of the Lusternik–Graves theorem*, April 9.
115. N. TRIANTAFYLIDIS, Ecole Polytechnique, Laboratoire de Mécanique des Solides & Département de Mécanique, Palaiseau, France, *Electromagnetic forming: A new coupled variational formulation and solution algorithms*, November 3.
116. D. TURAEV, Imperial College London, Department of Mathematics, UK, *Exponential and super-exponential growth of the number of periodic orbits in iterated function systems*, May 27.
117. S. VAN DE GEER, Eidgenössische Technische Hochschule Zürich, Departement Mathematik, Switzerland, *Condence intervals using the graphical lasso (joint work with Jana Jankova)*, July 2.
118. M. VÄTH, Freie Universität Berlin, Institut für Mathematik und Informatik, *Instability for a reaction-diffusion system with obstacles*, January 22.
119. A. VERETENNIKOV, University of Leeds, School of Mathematics, UK, *On local mixing conditions for degenerate SDEs*, August 18.
120. E. VESALAINEN, University of Jyväskylä, Department of Mathematics, Finland, *Scattering from corners*, October 21.
121. P. VIEU, Université Paul Sabatier, Institut de Mathématiques de Toulouse, France, *How to deal with dimensionality in functional data analysis?*, April 23.
122. F. VÖLLERING, Universität Göttingen, Institut für Mathematische Stochastik, *Talagrand's inequality, Russo's formula and influences for dependent random variables*, February 4.
123. M.-K. VON RENESSE, Universität Leipzig, Mathematisches Institut, *A Brownian motion on the Wasserstein space*, April 30.

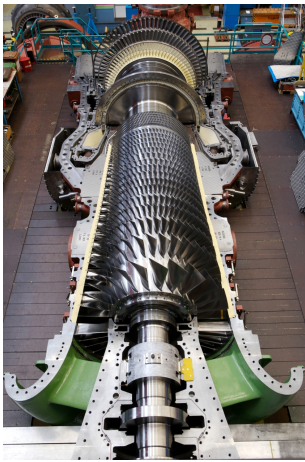


124. M. WEIDNER, University College London, Department of Economics, UK, *Incidental parameter bias in panel quantile regressions*, April 16.
125. D. WIED, Technische Universität Dortmund, Fakultät Statistik, *Detecting relevant changes in time series models*, October 22.
126. P. WINKERT, Technische Universität Berlin, Institut für Mathematik, *Analytical methods for variational inequalities in Sobolev spaces with variable exponents*, November 4.
127. W.B. WU, University of Chicago, Department of Statistics, USA, *An  $L^2$  test theory for nonstationary time series*, May 14.
128. ———, *A sharp strong invariance principle for stationary processes*, May 14.
129. M. YAMAMOTO, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Inverse problem on radioactive soil pollution*, March 18.
130. ———, *Inverse source problems for evolution equations: Detection of stationary and moving sources*, May 27.
131. ———, *Recent results on the forward and inverse problems of fractional diffusion equations*, September 23.
132. N. YAMAZAKI, Kanagawa University, Department of Mathematics, Yokohama, Japan, *Optimal control of phase field system with total variation functional as the interfacial energy*, September 9.
133. T. YIN, Chongqing University, College of Mathematics and Statistics, China, *Variational methods for the fluid-structure interaction problem*, January 28.
134. V. ZAGREBNOV, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, France, *How the spectral theory explains two critical points of Bose condensation*, October 15.
135. Q.M. ZHOU, Simon Fraser University, Department of Statistics and Actuarial Science, Burnaby, Canada, *Goodness-of-fit test for model specification*, December 17.
136. J. ZINSL, Technische Universität München, Zentrum Mathematik, *On existence and equilibration for Keller–Segel-type gradient flow systems*, February 25.
137. ———, *Transport distances and geodesic convexity for systems of degenerate diffusion equations*, September 24.

## 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>).



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Assembly of an Alstom GT26 gas turbine at the Mannheim, Germany, facility

**BOP** (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: juergen.borchardt@wias-berlin.de)

The **Block Oriented Process** 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. So far it has been successfully used for the simulation of several real-life processes in heat-integrated distillation, sewage sludge combustion, or catalytic CO oxidation in automotive oxygen sensors, for example. Currently, it is commercially used for gas turbine simulation.

Detailed information: <http://www.wias-berlin.de/software/BOP>

**ClusCorr98**® (contact: H.-J. Mucha, phone: +49 30/20372-573, e-mail: hans-joachim.mucha@wias-berlin.de)

The statistical software **ClusCorr98**® performs exploratory data analysis with the focus on cluster analysis, classification, and multivariate visualization. A highlight is the pairwise data clustering for finding groups in data. Another highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool based on resampling techniques. It can be considered as a three-level assessment of stability. The first and most general level is decision-making regarding the appropriate number of clusters. The decision is based on well-known measures of correspondence between partitions. Second, the stability of each individual cluster is assessed based on measures of similarity between sets. It makes sense to investigate the (often quite different) specific stability of clusters. In the third and most detailed level of validation, the reliability of the cluster membership of each individual observation can be assessed.

**ClusCorr98**® runs in the host application Excel 2013.

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](mailto: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>

**WIAS-MeFreSim** (contact: T. Petzold, phone: +49 30/20372-498, e-mail: [thomas.petzold@wias-berlin.de](mailto:thomas.petzold@wias-berlin.de))

**WIAS-MeFreSim** allows for the three-dimensional simulation of induction hardening for workpieces made of steel using single- and multifrequency currents. It is the aim of the heat treatment to produce workpieces with hard, wear resistant surface and soft, ductile core. The boundary layer of the workpiece is heated up by induced eddy currents and rapidly cooled down by the subsequent quenching process. The resulting solid-solid phase transitions lead to a hardening of the surface of the workpiece. With the help of simulations, an efficient determination of optimal process parameters for contour hardening of gears is possible, since time- and cost-intensive experiments can be reduced. In addition to the determination of the temperature and the hardening profile, the determination of residual stresses after the quenching process is possible.

For more information see <http://www.wias-berlin.de/software/mefresim>.

**MooNMD** (contact: V. John, phone: +49 30/20372-561, e-mail: [volker.john@wias-berlin.de](mailto:volker.john@wias-berlin.de))

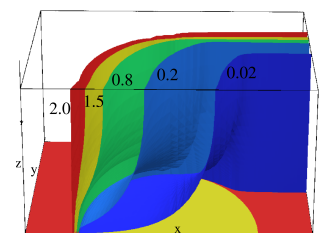
**MooNMD** is a flexible finite element package for the solution of steady-state and time-dependent convection-diffusion-reaction equations, incompressible Navier–Stokes equations, and coupled systems consisting of these types of equations, like population balance systems or systems coupling free flows 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 ( $\theta$ -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](mailto:juergen.fuhrmann@wias-berlin.de))

**pdelib** is a collection of software components that are useful to create simulators and visualization tools for partial differential equations. The main idea of the package is modularity, based on a bottom-up design realized in the C++ programming language. Among others, it provides

- iterative solvers for linear and nonlinear systems of equations

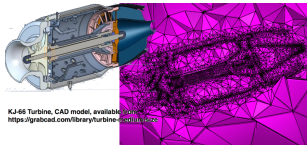


Concentration isosurfaces in a thin-layer flow cell (*pdelib*)

- 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](mailto:hang.si@wias-berlin.de))



*A cut view of a constrained Delaunay tetrahedral mesh of a complex 3D solid generated by TetGen*

TetGen is a mesh generator for three-dimensional simplex meshes as they are used in finite volume and finite element computations. It generates the Delaunay tetrahedralization, Voronoi diagram, and convex hull for three-dimensional point sets. For three-dimensional domains with piecewise linear boundary, it constructs constrained Delaunay tetrahedralizations and quality tetrahedral meshes. Furthermore, it is able to create boundary-conforming Delaunay meshes in a number of cases including all polygonal domains with input angles larger than 70°.

More information is available at <http://www.tetgen.org>.

**WIAS-TeSCA** (contact: R. Nürnberg, phone: +49 30/20372-570, e-mail: [reiner.nuernberg@wias-berlin.de](mailto:reiner.nuernberg@wias-berlin.de))

WIAS-TeSCA is a **Two-** and **three-dimensional Semi-Conductor Analysis** 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](mailto: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](mailto: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/>).

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*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>).