



Weierstrass Institute for  
Applied Analysis and Stochastics

*Intelligent solutions for complex problems*

*Annual Research Report 2016*

Cover figure: Density plot that shows how a pump wave is scattered at an optical soliton, which is then compressed and accelerated.

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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 2016. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2016. Following a 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.

This report marks a special point in the institute's history. After Prof. Jürgen Sprekels's long and successful era as the head of the institute had terminated in Spring 2015, I took on my duties as the new director of WIAS in January 2016 and, after almost one year without a director, the institute and I started to sort out all the promising possibilities for shaping the institute's future.

Soon after my commencement at WIAS, I had the honor and pleasure to welcome the President of the International Mathematical Union (IMU), Prof. Shigefumi Mori, and IMU's Secretary, Prof. Helge Holden, in Berlin. The IMU Secretariat has been permanently based at WIAS since 2011, and its staff, headed by the WIAS Authorized Representative of the Director and IMU Treasurer Prof. Alexander Mielke, has served mathematics and mathematicians all over the world ever since then. Meanwhile, the IMU Secretariat at WIAS has become a well-recognized meeting point of the worldwide mathematical community, which has contributed to the increase of the international visibility of WIAS.

In February, the President of the Leibniz Association, Prof. Matthias Kleiner, came to visit WIAS and its new Director, and on May 19, a WIAS Directorship Transition Ceremony was held in the Leibniz Association's headquarters with greeting addresses from the Federal Ministry of Education and Research, the state of Berlin, IMU, the Leibniz Association, and many others.

As the previous years, 2016 has proven to be a busy and fruitful year for the institute with 159 WIAS Preprints, 148 articles in refereed journals, three monographs, four collected editions, and over three million euros provided by grants. More details on this and more can be found in the facts-and-figures part of this report. All important indicators of scientific productivity and quality remained on an excellent level, continuing WIAS's successful track record.

2016 was also termed the *Leibniz Year*. Indeed, the 370th birthday and the 300th anniversary of the death of the great scientist were celebrated, and WIAS organized, again in Leibniz Headquarters, on November 29 an event for the open public "On Leibniz' Traces in Mathematics" with three mathematical historians speaking about different aspects of Leibniz's mathematical research.

Prof. Dietmar Hömberg, the head of Research Group 4, was appointed President of the European Consortium for Mathematics in Industry (ECMI) for the period 2016–2017. He was also appointed adjunct professor for another three years at the Norwegian University of Science and Technology in Trondheim.

Besides performing more traditional disciplinary research, WIAS is also strongly interested in fostering interdisciplinary research. An excellent example for this cross-fertilization in the sciences, enabled by the nature of applied mathematics as a structural science, is the WIAS-coordinated Leibniz Network "Mathematical Modeling and Simulation (MMS)", where now members of 27 institutes from all sections of the Leibniz Association work together. The first MMS Days bringing all these institutions together in order to shape the future of MMS with the Leibniz Association took



*Prof. Dr. Michael  
Hintermüller, Director*



place in January 2016 at WIAS. In a subsequent topical workshop in September, numerical modeling in Computational Fluid Dynamics (CFD) and Geophysical Fluid Dynamics (GFD) was discussed.

Health technologies benefiting our society are a promising field of research where applied mathematics can contribute with innovative approaches. In July, WIAS joined the Leibniz Research Alliance “Health Technologies” and made *Quantitative Biomedicine* one of its main application areas. WIAS contributes to the alliance’s areas biomarkers, imaging methods, and bioactive boundaries with its expertise in statistical data analysis, medical imaging analysis, numerical models of haemodynamics, and the modeling of multifunctional materials.

Besides its coordinating work in Leibniz associated with MMS, WIAS also serves as the coordinator for the newly established DFG Priority Program SPP 1962 “Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization”. The aim of the SPP is to help solve some of the most challenging problems in the applied sciences that involve nondifferentiable structures as well as partial differential operators, thus leading to nonsmooth distributed parameter systems.

WIAS continues to be successful on the European level. Indeed, in the European Industrial Doctorate (EID) project *MIMESIS – Mathematics and Materials Science for Steel Production and Manufacturing*, which is entirely run by WIAS and headed by Prof. Dietmar Hömberg (RG 4), eight Ph.D. students develop new methods for the production and treatment of steel in close cooperation with industry.

Prof. Peter Friz (WIAS and Technische Universität Berlin) obtained the ERC Consolidator Grant “GPSART – Geometric Aspects in Pathwise Stochastic Analysis and Related Topics”. Here, important problems in stochastic analysis will be examined in the five years to come.

In the Eurostars joint project “HIP-Lasers”, WIAS cooperates with three European commercial enterprises, making an active contribution to promote the transfer of knowledge to industry. The aim of this project is to produce compact high-power laser systems based on edge-emitting diode lasers. WIAS contributes to their modeling, simulation, analysis, and optimization.

The Weierstrass Institute is committed to the implementation of the legally binding German policies and standards to achieve the goal of gender equality. In 2016, the institute defended, for the third year, the “audit berufundfamilie” (audit job and family) quality seal received in December 2013 for three years. In December, WIAS applied for the quality seal for yet another three-year’s term. Two workshops (strategy and re-audition) took place to define new targets to optimize the family friendly arrangements of the institute. The re-audit workshop not only defined new targets in this area, but it also demonstrated the high level of standards of WIAS as an employer paying particular attention to respecting a well-balanced work/life relation.

Besides these important facts and events, WIAS continued its scientific work, further consolidating its leading position in the mathematical community as a center of excellence in the treatment of complex applied problems. Several scientific breakthroughs were achieved, and the reader is cordially invited to follow the Scientific Highlights articles in this report.

WIAS also expanded its scope into new applied problems from medicine, economy, science, and engineering. 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, 61 additional co-workers (+ 8 outside WIAS; Dec. 31, 2016) could be financed from third-party funds.

Seventeen international workshops organized by WIAS evidenced the institute's reputation and its role as an attractive meeting place for international scientific exchange and collaboration. 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. The highlight in this respect was also in 2016 the joint operation of the Research Center MATHEON "Mathematics for key technologies" located at the Technische Universität Berlin and currently funded by the "Einstein Foundation Berlin" in the framework of the "Einstein Center for Mathematics" (ECMath). WIAS is committed to the success of the center by providing considerable financial and personal resources; several members of WIAS play key roles in the scientific administration of the MATHEON. In this respect, the very well-received midterm report of the ECMath and the outlook on yet another funding period of MATHEON/ECMath is a satisfying fact.

Another continuing success for the mathematical community of Berlin is the "Berlin Mathematical School" (BMS), which was extended until 2017 in the framework of the German "Exzellenzinitiative 2012" (competition for excellence). The BMS is a graduate school for advanced mathematical studies that brings together the capacities of all mathematical institutions in Berlin to attract excellent doctoral students from all over the world. Also within the BMS, several WIAS members took long-term responsibilities for the education of the students and the organization of the school.

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. Enjoy reading...

Berlin, in February 2017

M. Hintermüller

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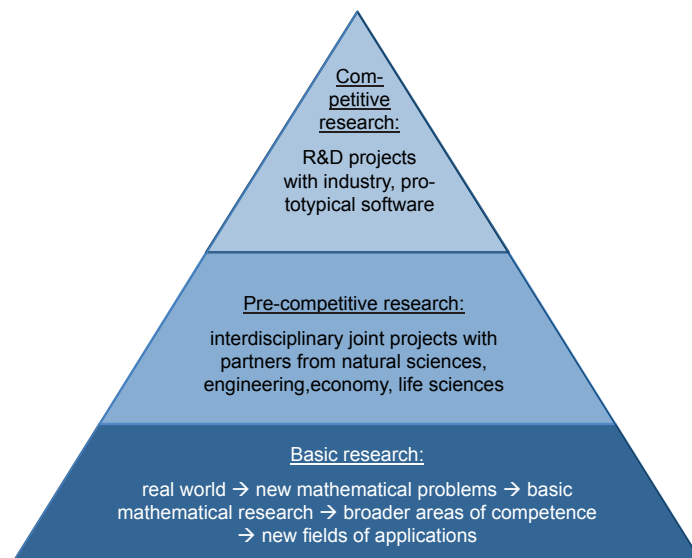
# 1 WIAS in 2016

- Profile
- Structure and Scientific Organization
- Equal Opportunity Activities
- Grants
- Participation in Structured Graduation Programs
- Software



## 1.1 Profile

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



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's successful research concept is based on the above pyramid-shaped structure: Right at the bottom, basic mathematical research dedicated to new mathematical problems resulting from real-world issues as well as research for broadening mathematical areas of competence for developing new, strategically important fields of application. Based on this foundation, precompetitive research, where WIAS cooperates in interdisciplinary joint projects with partners from the natural sciences, engineering, economy, and life sciences. On top, cooperations with industry in R&D projects and the development of prototypical software. Close cooperations with companies and the transfer of knowledge to industry are key issues for WIAS. This is also reflected by the fact that Prof. Dietmar Hömberg, head of a research group at WIAS, has become the President of the *European Consortium for Mathematics in Industry (ECMI)* for the period 2016–2017.



A successful mathematical approach to complex applied problems necessitates a long-term multiply interdisciplinary collaboration in project teams. Besides maintaining the contact to the partners from the applications, which means, in particular, to master their respective technical terminologies, the WIAS members have to combine their different mathematical expertises and software engineering skills. This interdisciplinary teamwork takes full advantage of the possibilities available in a research institute.

The Weierstrass Institute is dedicated to university education on all levels, ranging from the teaching of numerous classes at the Berlin universities and the supervision of theses to the mentoring of postdoctoral researchers and to the preparation of two trainees to become “mathematical technical software developers”.

WIAS promotes the international collaboration in applied mathematics by organizing workshops and running guest and postdoc programs. The institute is embedded in a dense network of scientific partners. In particular, it maintains various connections with Leibniz institutes and actively takes part in the forming and development of strategic networks in its fields. Thus, WIAS coordinates the Leibniz Network “Mathematical Modeling and Simulation (MMS)” connecting twenty-seven partners from all sections of the Leibniz Association. Modern methods of MMS are imperative for progress in science and technology in many research areas. In 2016, the “1st Leibniz MMS Days” (January 27–29) and the “1st Leibniz MMS Mini Workshop on CFD & GFD” (September 8–9) took place at WIAS within this framework.

WIAS has a number of cooperation agreements with universities and is one of the “motors” of the Berlin mathematical research center MATHEON, a cooperation partner of the Einstein Center for Mathematics Berlin, and it supports the Berlin Mathematical School (BMS) through various teaching and supervision activities.

## 1.2 Structure and Scientific Organization

### 1.2.1 Structure

In 2016, WIAS was organized into the following divisions for fulfilling its mission: Seven research groups were complemented by an eighth one headed by the new director of WIAS, Prof. Dr. Michael Hintermüller. Together with the Young Scientists' Group, one Leibniz and two ERC groups<sup>1</sup>, they form the scientific body of the institute. In their mission, they are supported by the departments for technical and administrative services. The Secretariat of the International Mathematical Union (IMU, see page 54), hosted by WIAS, is a supportive institution for the international mathematical community. Moreover, WIAS hosts the German Mathematics Association DMV and the Society of Didactics of Mathematics GDM.

**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**

**RG 8. Nonsmooth Variational Problems and Operator Equations**

**YSG. Modeling of Damage Processes**

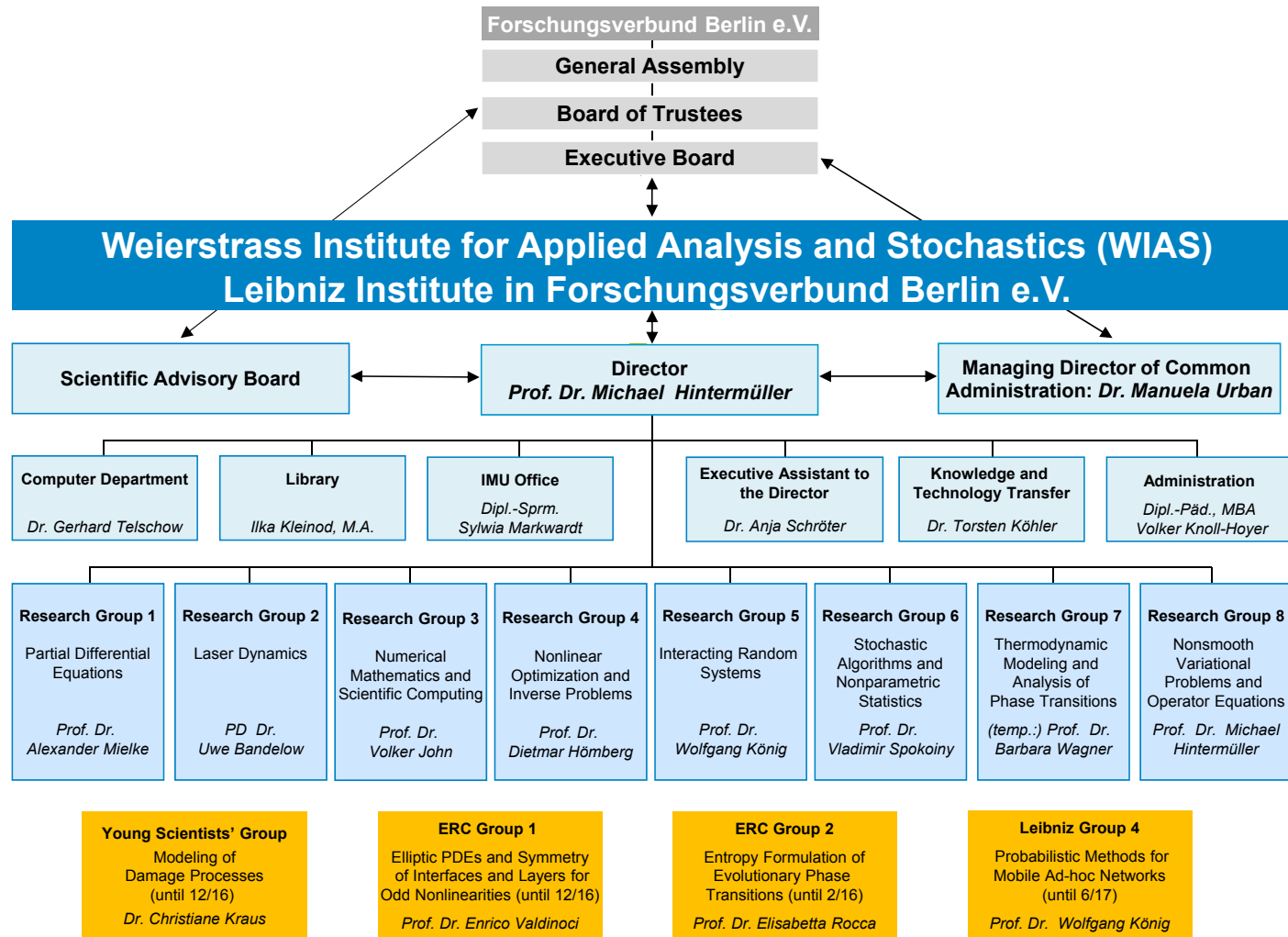
**LG 4. Probabilistic Methods for Mobile Ad-hoc Networks**

**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 2016.

<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”.





### 1.2.2 Main Application Areas

The research at WIAS focused in 2016 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

- **Conversion, Storage, and Distribution of Energy**
- **Flow and Transport**
- **Materials Modeling**
- **Nano- and Optoelectronics**
- **Optimization and Control in Technology and Economy**
- **Quantitative Biomedicine** (new since April, 2016)

To these areas, WIAS made important contributions in the past years that strongly influenced the directions of development of worldwide research.

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

The eight research groups, the Young Scientists' Group, the Leibniz Group, and the two ERC groups form the institute's basis to fully bring to bear and develop the scope and depth of its scientific 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 2016 in the interdisciplinary solution process described above.

Main application areas	RG 1	RG 2	RG 3	RG 4	RG 5	RG 6	RG 7	RG 8	YSG	LG 4	ERC 1	ERC 2
Conversion, Storage, and Distribution of Energy	X		X	X			X	X				
Flow and Transport			X	X	X	X	X	X				X
Materials Modeling	X		X	X	X		X		X		X	X
Nano- and Optoelectronics	X	X	X	X								
Optimization & Control in Technology and Economy	X		X	X	X	X				X		X
Quantitative Biomedicine			X		X	X		X			X	

In the following, special research topics are listed that were addressed in 2016 within the general framework of the main application areas.

#### **Conversion, Storage and Distribution of Energy**

- 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 and RG 7)
- Modeling and analysis of coupled electrochemical processes (fuel cells, batteries, hydrogen storage, soot; in RG 1, RG 3, RG 5, and RG 7)
- Nonlinear chance constraints in problems of gas transportation (in RG 4)
- Parameter identification, sensor localization and quantification of uncertainties in switched PDE systems (in RG 8)

#### **Flow and Transport**

- Treatment of Navier–Stokes equations (in RG 1, RG 3, RG 7, 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, and RG 7)
- Modeling of nanostructures of thin films on crystalline surfaces (fluid films, thin film solar cells; in RG 7)
- 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)
- Transport in random media (in RG 5)
- Trajectories of message flow in mobile ad-hoc communication systems (in LG 4)

#### **Materials Modeling**

- 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 fracture 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)
- Dynamical processes in nonhomogeneous media (in RG 6 and RG 7)
- Material models with stochastic coefficients (in RG 3, RG 4, RG 5, and RG 7)

**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 and OLED lighting (in RG 1 and RG 7)
- Mathematical modeling, analysis, and optimization of strained germanium microbridges (in RG 1 and RG 8)

**Optimization and Control in Technology and Economy**

- Simulation and control in process engineering (in RG 3, RG 4, and RG 6)
- Problems of optimal shape and topology design (in RG 4)
- 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)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6)
- Connectivity problems in large telecommunication networks (in RG 5 and LG 4)
- Optimal control of multiphase fluids and droplets (in RG 8)

**Quantitative Biomedicine**

- Numerical methods for biofluids and biological tissues (in RG 3 and RG 8)
- Branching processes in random media (in RG 5)
- Pairing structures in population models (in RG 5)
- Image processing (in RG 6 and RG 8)
- Dynamics of learning processes in the neurosciences (in RG 6)
- Modeling of high-resolution magnetic resonance experiments (in RG 6)
- Methods of diagnosis of neurodegenerative diseases (in RG 6)
- Hysteresis in the calcium release during muscle cell contraction (in RG 7)

## 1.3 Equal Opportunity Activities

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.

At the beginning of 2016, based on its second annual report, WIAS got the confirmation that the institute met also in 2015 the requirements of the *berufundfamilie audit certificate*, obtained in 2013 for three years. With the certificate, WIAS documents its commitment towards the harmonization of work and family, both internally and externally, and implements central research policy objectives. In May, preparations started for the re-auditing for a re-certification for the years 2017 to 2020. The annual report for the third year was written, containing a status quo on the personnel policy regarding the harmonization of work and family. On this basis, a strategy workshop and a re-auditing workshop took place in November and December, resp., to define objectives to further optimize the family-friendly arrangements.



Besides continuous information by e-mail on equality and work and family topics, the staff members were offered two lectures by external experts about health care proxies and stress and time management, which were well attended.

A new *Plan of Action on Gender Equality* was finalized in 2016. It will be valid until 2019 and contains measures to increase the amount of women working in scientific jobs. Combining work and family life is another central aspect of the plan. In December 2016, WIAS's equal opportunities officer and her substitute held the first women's assembly. They informed the female employees about the manifold aspects of their work and answered questions. In the 2015 staff survey, international WIAS employees asked for German courses. As a result, three language classes started in autumn 2016. On April 25, Franziska Flegel (RG 5) participated in the 2016 Female Ph.D. Students' Seminar of Forschungsverbund Berlin.

In 2016, WIAS again took part in the "Girls' Day – Mädchen Zukunftstag", an initiative of the German Federal Ministry of Family, Senior Citizens, Women and Youth in collaboration with the Federal Ministry of Education and Research. Eight girls aged from 14 to 16 years followed various lectures and asked many questions, mentored by scientists from WIAS.

## 1.4 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 was very successful in 2016, having raised a total of 3.1 million euros, from which 61 additional researchers (+ 8 outside WIAS; Dec. 31, 2016) were financed. In total in 2016, 24.4 percent of the total budget of WIAS and 48.4 percent of its scientific staff originated from grants.

For a detailed account of projects funded by third parties, the reader is referred to the appendix, Section A.2 Grants below on pages 112ff.

## 1.5 Participation in Structured Graduation Programs

### Graduate School *Berlin Mathematical School (BMS)*

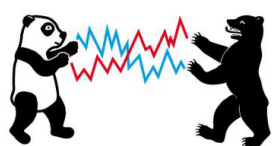


Berlin's mathematicians are proud that, after its successful installation in 2006, a second funding period was granted to this graduate school in Summer 2012 for 2013–2017, for the excellent work done since its inception. The BMS is jointly run by the three major Berlin universities within the framework 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 from all over the world to the city. Many members of WIAS are contributing to the operations of the BMS.

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



This DFG graduate college is located at the 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. The college will be closed at the end of March 2017.




### 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 for 4.5 years. 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.

## 1.6 Software

Scientific software is a tool to evaluate models and algorithms investigated at WIAS. Moreover, software helps to transfer research results to other scientific fields, to industry, and to the general public. The underlying problems often pose very specific and advanced requirements, which cannot be satisfied by standard software that is widely available; hence, the development of algorithms and scientific software belongs to the scientific tasks of WIAS. As a consequence, WIAS is working on the implementation of rules of good scientific practice in the realm of software development. Software-based publications in specific journals and as WIAS Technical Reports are encouraged. The production, dissemination, and sale of software is not part of the core duties of WIAS. Nevertheless, several codes developed at WIAS are distributed outside of WIAS and have earned a good reputation. See page 200ff. for a list of software packages that WIAS makes available. Licensing models depend on the specifics of the corresponding projects. Codes are offered under open source and proprietary licenses as well as combinations thereof.

## 2 Scientific Highlights

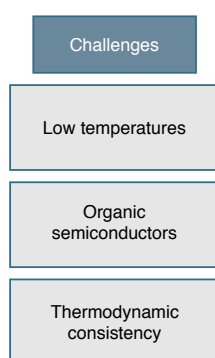
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- New Approaches to Numerical Simulation of Current Flow in Semiconductor Devices
  - Adiabatic Theory of All-optical Switching
  - Towards Pressure-robust Mixed Methods for the Incompressible Navier–Stokes Equations
  - Effective Modeling of Multiscale Phenomena
  - Uncertainty Quantification from Different Perspectives – Methodological Encounters and Inspirations
  - Modeling, Analysis, and Simulation of Damage Processes



## 2.1 New Approaches to Numerical Simulation of Current Flow in Semiconductor Devices

Nella Rotundo, Patricio Farrell, Duy Hai Doan, Jürgen Fuhrmann, Markus Kantner, and Thomas Koprucki

### Challenges for current flow simulation

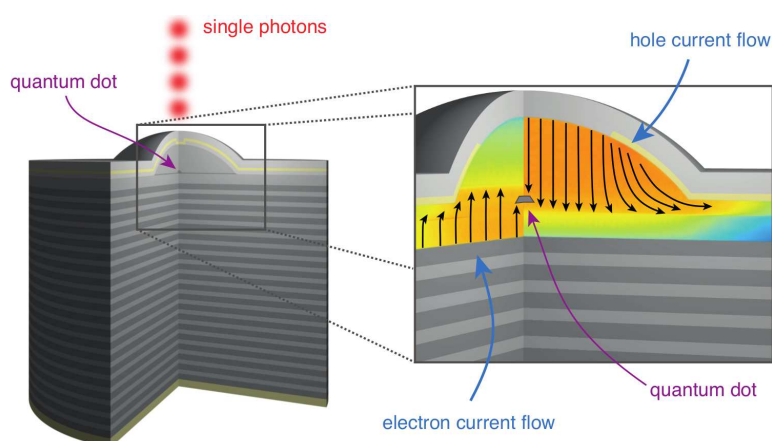


**Fig. 1:** Challenges when simulating currents in semiconductor devices

A world without airplanes, TVs, solar cells, CT scanners, and smartphones would be extremely hard to imagine. All these electronic devices have one thing in common. They contain one of the most important inventions of the 20th century: *transistors*. These electronic devices are composed of semiconductors, i.e., materials which can sometimes act as conductors (like copper) or insulators (like glass) depending on physical factors (temperature or deliberately introduced impurities).

Ever since their successful industrial-scale production in the 1960s, semiconductor devices have been steadily optimized. They have become smaller and their electrical properties improved drastically. In fact, Gordon Moore, one of Intel's co-founders, correctly predicted that the number of transistors on a computer chip would double every couple of years. This exponential rule of thumb is nowadays known as *Moore's law*. Since developing new prototypes is rather costly, such growth would not have been possible without correctly predicting the electric current flow in semiconductor devices. If manufacturers know how charge carriers (electrons and holes) flow in a device *before* building it, they can save a lot of resources. This is why numerical simulation plays an important role in analyzing how these devices work. In the past decades, sound theoretical and numerical methods to model and simulate the current flow in semiconductor devices have been established.

Unfortunately, most of the models and simulation tools do not directly apply to extreme environmental conditions or new materials while still describing consistently a system in equilibrium.



**Fig. 2:** Left: Single-photon source with quantum dot as active region. Right: Computed electron and hole currents. Charge carriers recombine in the quantum dot, emitting single photons

A severe difficulty for current simulations arises, for example, when developing the next generation of secure communication systems. The key idea is to transmit information along optical fibres

using light pulses, where each pulse consists of a single photon (Figure 3). These can neither be copied nor split into smaller particles, making it extremely difficult for an eavesdropper to intercept the communication without being detected. However, to achieve this goal, one has to replace today's lasers in optical communication systems with single photon sources that are capable of emitting single photons at the flick of a switch. One way to realize this objective is to use nanosized semiconductor quantum dots (Figure 2), which operate at extremely low temperatures, ranging from  $-240^{\circ}\text{C}$  down to the absolute zero temperature ( $\approx -273^{\circ}\text{C}$ ). At these cryogenic temperatures, the behavior of electrons and holes in semiconductor devices differs considerably compared to room temperature. Namely, one has to face a phenomenon called *nonlinear diffusion*. Standard simulation techniques are not able to accurately describe electron flow at these temperatures.

Apart from the temperature, also the semiconductor material itself has a tremendous impact on the electric current. For example, so-called *organic* semiconductors have garnered a lot of interest lately. Organic light-emitting diodes (OLEDs) have been used successfully to build digital TV screens (Figure 4) or smart windows that can emit light at night. In the past decade, scientists developed new methods to describe the movement of the electrons and holes, challenging again standard simulation techniques. For organic semiconductors the nonlinear diffusion (often called *diffusion enhancement* in this context) is already prominent at room temperature.

Finally, any numerical simulation scheme should accurately mirror the simplest physical state: (thermodynamic) equilibrium, meaning that, when a device is switched off, the current has to vanish.

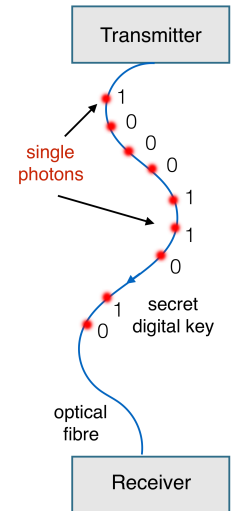
At WIAS, the long-term collaborations with experimental groups on single-photon sources (TU Berlin, funded by DFG CRC 787 *Semiconductor Nanophotonics*) and OLEDs (Dresden Integrated Center for Applied Physics and Photonic Materials, funded by ECMath), stimulated research on novel numerical schemes in order to successfully handle all of the above issues, complementing WIAS's expertise in consistent modeling; see [1, 2, 3]. Our results presented on the next pages are directly incorporated in our new simulation prototype *ddfermi*, which is developed jointly by WIAS Research Groups 1, 2, and 3.

## Electric current and its discretization

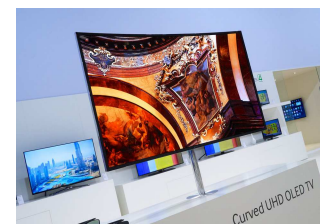
The transport of charge carriers in semiconductors can be modeled by continuity equations. They describe the spatio-temporal evolution of the carrier densities due to current fluxes and recombination processes between charge carriers; see [2]. The driving forces of the currents are the gradients of the quasi-Fermi potentials. For electrons, the current flux is given as

$$\mathbf{j}_n = -q\mu_n n \nabla \varphi_n, \quad (1)$$

where the constant  $q$  represents the elementary charge, the carrier mobility  $\mu_n$  is assumed to be constant. The connection between the electron density  $n$  and the quasi-Fermi potential  $\varphi_n$  is explained in the following. It can easily be seen that for a spatially constant quasi-Fermi potential the flux is zero. This mathematical property corresponds to the fact that the current shall vanish in thermodynamic equilibrium. The numerical method that we present at the end is designed to preserve this property on a discrete level.

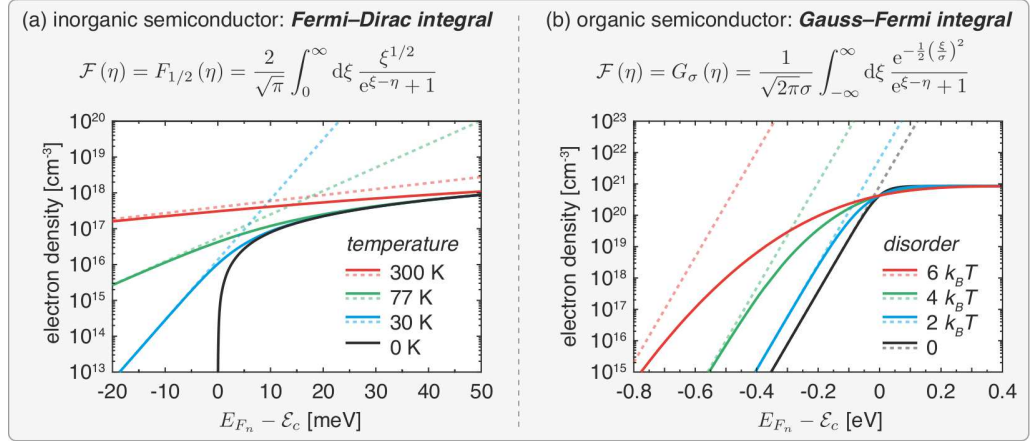


**Fig. 3:** The principle of future secure communication: Secret information is sent through optical fibres via single photons



**Fig. 4:** An OLED TV screen: bright colors and curved. Courtesy Kārlis Dambrāns, no changes, CC BY 2.0

**Fig. 5:** Electron densities according to Eq. (2) in (a) conventional, inorganic semiconductors (GaAs) for different temperatures and in (b) organic semiconductors (PPV) for different values of the disorder parameter  $\sigma$ . Boltzmann approximations are shown as dashed lines

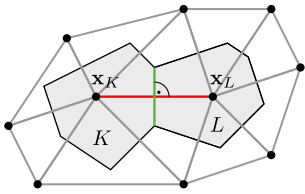


The quasi-Fermi potential and the electron density are related by a state equation that describes the occupation of energy states in the conduction band in a semiconductor, as follows:

$$n = N_c \mathcal{F}(\eta) \quad \text{where} \quad \eta = \eta(\psi, \varphi_n) = \frac{E_{F_n}(\varphi_n) - \mathcal{E}_c(\psi)}{k_B T} \quad (2)$$

with  $E_{F_n} = -q\varphi_n$  and  $\mathcal{E}_c = E_c - q\psi$ . For the applications mentioned above,  $\mathcal{F}$  is either taken to be the Fermi–Dirac integral (cryogenic temperatures) or the Gauss–Fermi integral (organic semiconductors). Both are given in Figure 5. The effective density of states  $N_c$  and the band-edge energy  $E_c$  are material constants,  $k_B$  is the Boltzmann constant, and  $T$  denotes the temperature. The function  $\psi$  represents the electric potential that solves a nonlinear Poisson equation where the right-hand side depends on the electron and hole densities.

Combining continuity equations for electrons and holes with the nonlinear Poisson equation yields the so-called *van Roosbroeck* system. Its solution allows to predict how the electrons, holes and electric field behave in a semiconductor. However, in general, it is not possible to solve the van Roosbroeck system analytically and for this reason one resorts to numerical simulations.



**Fig. 6:** Collocation points  $\mathbf{x}_K$  and  $\mathbf{x}_L$  as well as corresponding control volumes

**Boltzmann approximation and Scharfetter–Gummel scheme.** In many cases, it is common to approximate the complicated functions given in Figure 5 by a simple exponential function  $\mathcal{F}(\eta) \approx e^\eta$  (*Boltzmann approximation*). In this case, the gradient formulation for the current flux (1) can be rewritten in drift-diffusion form by

$$\mathbf{j}_n = q\mu_n [U_T \nabla n - n \nabla \psi]. \quad (3)$$

The first term on the right-hand side describes the diffusion, and the second one describes the drift of the electrons. The thermal voltage  $U_T = k_B T / q$  depends linearly on the temperature and adjusts the ratio of diffusion and drift. Obtaining a stable discretization of the electron continuity equation using the Boltzmann flux (3) is not straightforward and had been a serious problem for almost 20 years. Finally, Scharfetter and Gummel in 1969 [4] derived a local discrete flux expression along the edge  $\overline{\mathbf{x}_K \mathbf{x}_L}$  between two neighboring control volumes with collocation points  $\mathbf{x}_K$  and  $\mathbf{x}_L$ ; see Figure 6.

This Scharfetter–Gummel flux expression is given by

$$j_{n;K,L} = -q\mu_n U_T \left[ B\left(-\frac{\psi_L - \psi_K}{U_T}\right) n_K - B\left(\frac{\psi_L - \psi_K}{U_T}\right) n_L \right], \quad (4)$$

where  $B(x) = x / (\exp x - 1)$  is the Bernoulli function depicted in Figure 7, and the subscripts  $K$  and  $L$  indicate the evaluation of a function at the collocation nodes.

The scheme (4) is numerically stable and preserves several important physical properties of the continuous problem. It guarantees the positivity of carrier densities and correctly mirrors the fact that the flux (3) vanishes in equilibrium (thermodynamic consistency).

**Nonlinear diffusion beyond Boltzmann approximation.** Unfortunately, the Boltzmann approximation is only valid in certain regimes. As a matter of fact, a more accurate description of inorganic semiconductors with parabolic bands is given by the so-called *Fermi–Dirac integral*. For organic materials, however, the Gauss–Fermi integral is the most appropriate choice. These functions are defined and plotted in Figure 5. For large negative arguments all functions  $\mathcal{F}$  coincide with the Boltzmann approximation. However, for large positive arguments this approximation leads to a fatal overestimation of carrier densities.

For a general function  $\mathcal{F}$ , the flux takes the form

$$\mathbf{j}_n = q\mu_n \left[ U_T g\left(\frac{n}{N_c}\right) \nabla n - n \nabla \psi \right], \quad (5)$$

where, in contrast to the Boltzmann case, a density-dependent, nonlinear diffusion factor (or diffusion enhancement) shows up. This factor is given as a function of the nondimensionalized electron density

$$g(x) = x(\mathcal{F}^{-1})'(x) \quad (6)$$

and illustrated for different choices of  $\mathcal{F}$  in Figure 8. Obviously, this factor strongly impacts the diffusion, but is not reflected by the scheme of Scharfetter and Gummel (4).

**Thermodynamically consistent Scharfetter–Gummel scheme for general  $\mathcal{F}$ .** For the Boltzmann approximation the Scharfetter–Gummel scheme works very well. However, we still try to find out how to deal with more general functions  $\mathcal{F}$ . In [5], the thermodynamically consistent discretization for general fluxes

$$j_{n;K,L} = -q\mu_n U_T \bar{g}_{K,L} \left[ B\left(-\frac{\psi_L - \psi_K}{U_T \bar{g}_{K,L}}\right) n_K - B\left(\frac{\psi_L - \psi_K}{U_T \bar{g}_{K,L}}\right) n_L \right] \quad (7)$$

was suggested. The key idea is to properly average the nonlinear diffusion factor on the edge  $\overline{x_K x_L}$ . The explicit expression of this average for a general function  $\mathcal{F}$

$$\bar{g}_{K,L} = \frac{\mathcal{F}^{-1}\left(\frac{n_L}{N_c}\right) - \mathcal{F}^{-1}\left(\frac{n_K}{N_c}\right)}{\log(n_L/N_c) - \log(n_K/N_c)} \quad (8)$$

was given in [1]. This is the only average which yields a thermodynamically consistent discretization of the flux (5).

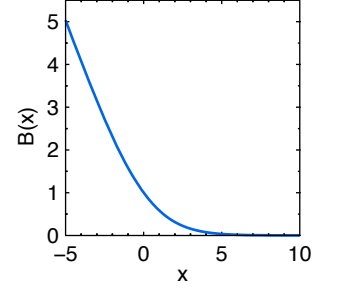


Fig. 7: Bernoulli function

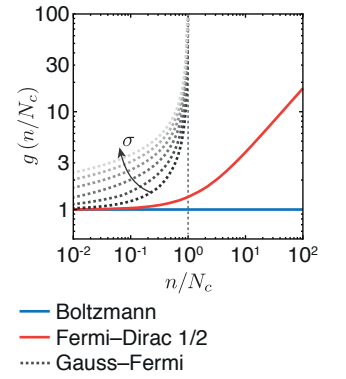
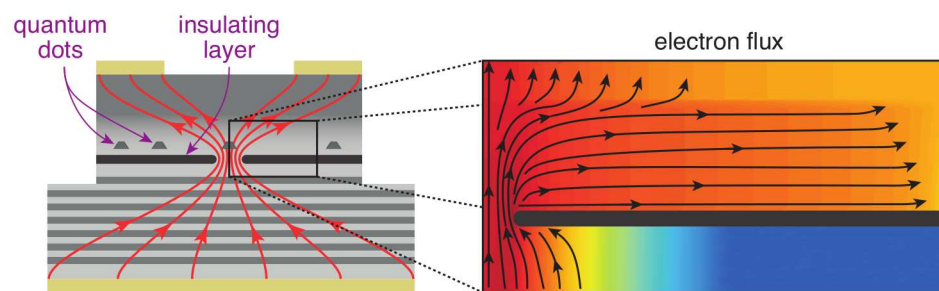


Fig. 8: Nonlinear diffusion factors according to Eq. (6)

**Application: Current flow in a single-photon source at cryogenic temperatures.** We compute the current flux in a single-photon source at extremely low temperatures considering Fermi–Dirac statistics. The device layout is depicted in Figure 9 along with a simulation result of the electron flux. Above an aperture within an insulating layer, a quantum dot is located, which shall be supplied with charge carriers for single-photon generation. However, the specific design supports strong spreading of the electron current above the insulating layer as shown in Figure 9. As a consequence, also parasitic quantum dots located far away from the aperture can generate photons, which impairs the functionality of the device as a single-photon source. In [6], we analyzed this behavior by numerical simulation. Based on our findings, we invented an revised device design to overcome this problem.

**Fig. 9:** Current flow in a single-photon source at an extremely low temperature ( $-243^{\circ}\text{C}$ ). Left: Schematic view of a single-photon source with quantum dots above an insulating layer. Right: Computed electron current flow through a small aperture within the insulating layer



**Conclusions and outlook.** Dealing with nonlinear diffusion in semiconductor device simulation remains a huge challenge. We presented a thermodynamically consistent discretization of the fluxes. In the future, we wish to analyze and compare this scheme with other popular discretizations, helping us to advance the development of our WIAS software prototype `ddfermi`.

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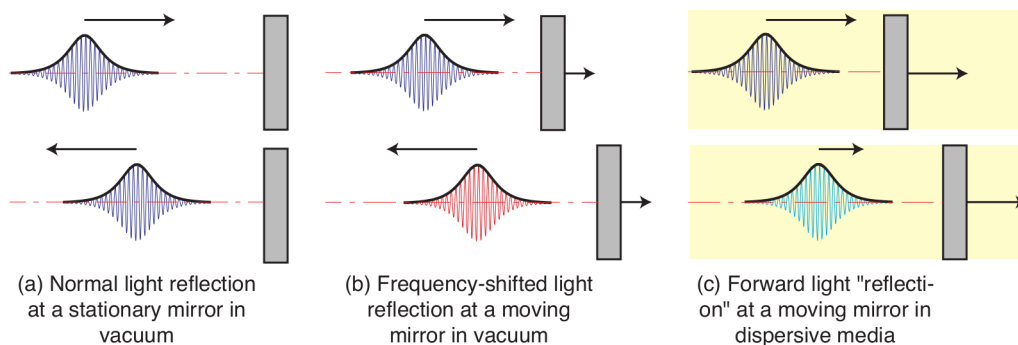
## 2.2 Adiabatic Theory of All-optical Switching

Shalva Amiranashvili, Uwe Bandelow, Sabrina Pickartz, and Matthias Wolfrum

### Introduction

Modern photonic devices show complex dynamics in space and time that originates from the nonlinear interaction of light with matter in often active media with sophisticated geometry. An adequate description of the involved multiscale, high-dimensional behavior requires intensive computations, if it is possible at all with presently available computers. For that reason combined efforts of applied mathematicians and physicists are required when such “brute-force” approaches fail and model reduction on a proper mathematical basis becomes desirable. We shall describe such a reduction that was developed at WIAS and which covers interactions of optical beams with solitons in nonlinear fibers.

Why should one study the scattering of optical beams at solitons? The key issue is control. The future of optoelectronics may well be with devices in which electrons are replaced by photons. A traditional transistor should then be replaced by an *optical transistor*, a device that switches optical signals on and off. The ultimate goal is to reach a so-called *all-optical switching*, i.e., to control light by light itself. But can we really manipulate light pulses? The switching requires a nonlinear self-action of light, and seems to require the use of impractically huge pulses. The scattering of small-amplitude optical beams at solitons is a welcome exception.



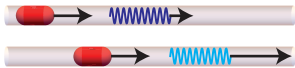
**Fig. 1:** As opposed to the standard case (a), light reflection at a moving mirror in vacuum goes along with a frequency shift (b). In a dispersive medium (c), the frequency-shifted reflected wave may still propagate forward with a decreased velocity.

A monochromatic light beam retains its color as long as nonlinear interactions are not invoked. The beam may be scattered and reflected, focused and defocused, it may produce interference patterns and bend around obstacles, still its color or wave frequency is always the same with only one exception. The situation is different if the beam interacts with a moving object, e.g., when it is reflected by a moving mirror (Figure 1). The modified beam frequency is obtained by (i) transformation to the coordinate frame that moves with the mirror, (ii) deriving the new direction of beam propagation, and (iii) backward transformation to the laboratory frame. Such transformations are the essence of relativity, and it is more than a mere accident that Einstein’s first paper on special relativity “Zur Elektrodynamik bewegter Körper” thoroughly discussed this topic.

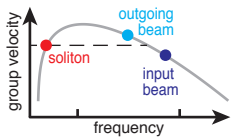


**Fig. 2:** A reconstruction of the first (Russell, 1834) observation of solitons, *Nature* **376**, 373, 1995 <http://www.ma.hw.ac.uk/>

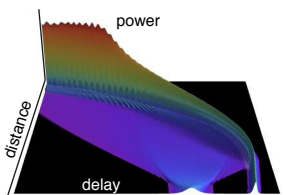




**Fig. 3:** A soliton in an optical fiber can serve as a mirror (shown in red) that overtakes other pulses



**Fig. 4:** In optical fibers, pulses with very different colors (frequencies) may have similar group velocities, cf. Figure 3



**Fig. 5:** A small-amplitude beam can significantly increase the soliton peak power in the course of scattering [3]

Needless to say that traditional mirrors cannot move really fast compared to the speed of light. In any case, they cannot move at all inside optical materials, such as glasses. That is why the fundamental relation between frequency and motion is easier to observe outside electrodynamics and optics; e.g., as Doppler effect for sound waves. However, a traditional mirror can be replaced by an inhomogeneity of material properties, provided that the inhomogeneity effectively scatters optical beams. Rapid recent developments in fiber optics and nonlinear optics provided us with a kind of novel, quickly moving “mirrors” that are created by light itself in the form of optical solitons.

A soliton is a solitary wave that propagates over surprisingly long distances without noticeable changes of its shape. Such behavior cannot be explained within the framework of classical linear wave theory. Solitons were first observed in water channels (Figure 2) and thereafter in nearly all nonlinear systems, including also optical fibers. According to Kerr’s law, an optical pulse induces an inhomogeneity of the material refraction index. This effect is proportional to the intensity of the pulse. In particular, an optical soliton creates a long-living localized inhomogeneity. The soliton acts then as a kind of moving mirror, at which other optical pulses may be scattered.

Optical solitons are very unusual mirrors [1]. First, they are made of light itself and propagate extremely quickly. They can even overtake other optical pulses (Figure 3) due to dispersion, a nontrivial dependence of the pulse velocity on its frequency. Second, as opposed to traditional mirrors, they can propagate inside transparent materials. However, solitons are not that good in reflecting light because even for the most powerful solitons the nonlinear effect is too weak to impose a noticeable reflection of an optical beam. But there is one exception that has been discovered recently and was studied extensively at WIAS. A beam will be almost perfectly reflected if its group velocity is very close to that of the soliton while its frequency is different. Fortunately, many optical fibers allow the propagation of pulses with considerably different frequencies and nearly identical velocities (Figure 4). The similar velocities dramatically increase the interaction time such that even a small nonlinearity can produce large changes. We call this behavior *an extended interaction*. The scattered wave changes its frequency such that energy is either obtained by the soliton or taken from it. An example is shown in Figure 5, where the five-time increase of the soliton peak power is due to an extended interaction with an optical beam that is at least one order of magnitude weaker than the soliton at the moment of scattering.

The first findings of the total beam reflection at a soliton and the induced soliton compression [2, 3] resulted from trial and error. Figure 5 was just one lucky calculation among several dozens of failed attempts. Fortunately, a recently developed theory of all-optical switching presents a breakthrough in our understanding of interactions between solitons and co-propagating optical beams. “Gambler’s luck” is now replaced by exact mathematical knowledge.

## Mathematical modeling

For a mathematical description of short optical pulses (see [4] and references cited therein) it is convenient to replace the real-valued electric field  $E(z, t)$  by a complex-valued analytic signal  $\mathcal{E}(z, t)$  by removing all negative-frequency components from the real-valued field, namely

$$\text{if } E(z, t) = \int_{-\infty}^{\infty} \tilde{E}(z, \omega) e^{-i\omega t} \frac{d\omega}{2\pi}, \quad \text{then } \mathcal{E}(z, t) = \int_0^{\infty} \tilde{E}(z, \omega) e^{-i\omega t} \frac{d\omega}{\pi}.$$

Here,  $\tilde{E}(z, \omega)$  is the Fourier transformed  $E(z, t)$ , and  $z$  is measured along the fiber axis from the beginning of the fiber. It is further convenient to introduce a complex amplitude  $\psi$  of the carrier wave  $\mathcal{E}(z, t) = \psi(z, t)e^{i(\beta_0 z - \omega_0 t)}$ , where the angular frequency  $\omega_0$  and wave vector  $\beta_0$  refer to the soliton carrier wave. Changing to the complex amplitude reflects the multiscale character of pulse propagation. Space-time scales introduced by the carrier wave may considerably differ from the scales for the amplitude  $\psi$ . Furthermore, the wave frequency  $\omega$  and wave vector  $\beta$  are related to each other for any linear wave  $e^{i\beta(\omega)z - i\omega t}$ . The relation is given by a set of the so-called *propagation constants*  $\beta_j = \beta^{(j)}(\omega_0)$ , which are derivatives of  $\beta(\omega)$  calculated for  $j = 0, 1, \dots, J_{\max}$  at the soliton carrier frequency  $\omega_0$ . Finally, it is convenient to change to a moving frame, from  $\psi(z, t)$  to  $\psi(z, \tau)$ , where the delay  $\tau = t - z/V$  is determined by the soliton velocity  $V = 1/\beta_1$ . Positive (negative) delays correspond to pulses that arrive later (earlier) than the reference soliton. Altogether, the dynamics of the envelope is determined by the so-called *Generalized Nonlinear Schrödinger Equation* (GNLSE)

$$i\partial_z \psi + \sum_{j=2}^{J_{\max}} \frac{\beta_j}{j!} (i\partial_\tau)^j \psi + \frac{n_2}{c} (\omega_0 + i\partial_\tau) |\psi|^2 \psi = 0, \quad E(z, t) = \text{Re} \left[ \psi(z, \tau) e^{i(\beta_0 z - \omega_0 t)} \right],$$

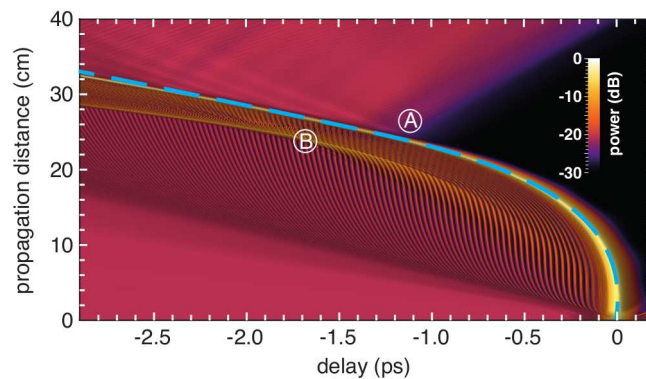
where  $n_2$  is a material parameter,  $c$  is the speed of light, and  $\partial_\tau$  denotes  $\partial/\partial\tau$ .

The GNLSE is one of the most important model equations in nonlinear optics and has analogies in other fields of science, e.g., the Dysthe equation for deep water waves. In the optical context, solutions of the GNLSE show how a temporal signal at the beginning of the fiber ( $z = 0, \tau$ ) is propagating along the fiber. Numerical solutions of the GNLSE can be obtained by the split-step method. For instance, calculation of soliton amplification as shown in Figure 5 takes less than one hour on any modern processor. Parameter search, collecting statistics of extraordinarily large, champion solitons, and numerical optimization of soliton amplification is a different story. Here is where analytical investigations are welcome and where adiabatic theory comes into play.

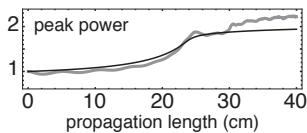
The adiabatic approach introduces two different evolution scales. The first (fast) scale corresponds to the scattering of a small-amplitude wave, the resulting pattern of the transmitted and reflected waves depends only on the current state of the soliton. The scattering problem is similar to that in quantum mechanics, but with the difference that the barrier has a velocity. The second scale corresponds to a slow evolution of the soliton parameters, e.g., the peak power. This evolution can be calculated by the so-called *soliton perturbation theory*. However, standard methods do not cover the case of a change of group velocity with frequency (Figure 4), which happens to be important here. We modified the scattering theory and the soliton perturbation theory to address our needs, and then derived the adiabatic equations in the following steps.

- Two coupled equations are derived to replace the GNLSE, the first equation for the soliton and the second one for the scattered wave.
- The first equation is split in two parts. The main part describes the pure soliton, and the residual part quantifies the influence of the scattered wave on the soliton.
- The solitary solution of the first equation is inserted into the second one, and the scattering theory from quantum mechanics is used to derive the transmission coefficient and waveforms of the transmitted and reflected waves.

- Finally, we return to the first equation and use the just derived waveforms to obtain ordinary differential equations for the soliton parameters in the framework of the soliton perturbation theory.



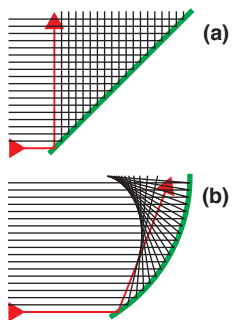
**Fig. 6:** Density plot of the electromagnetic power that results from the full solution of the GNLSE. The adiabatic approach provides only the soliton trajectory (dashed line) but makes the job 1000 times faster [5].



**Fig. 7:** Soliton peak power as derived from the GNLSE (gray) and from the adiabatic equations (black) [5]

The resulting set of adiabatic equations (not shown) looks much more complicated than the original GNLSE. However, we are now dealing with ordinary differential equations providing an accurate description of the soliton evolution. Figure 6 shows a power density plot derived from the original GNLSE. The overimposed dashed line is derived from the adiabatic equations and perfectly reproduces the soliton trajectory. The evolution of the soliton peak power is shown in Figure 7. The agreement is not as perfect as for the trajectory, but still the adiabatic equations give a good quantitative picture of the soliton amplification.

### Final words: optics and geometry

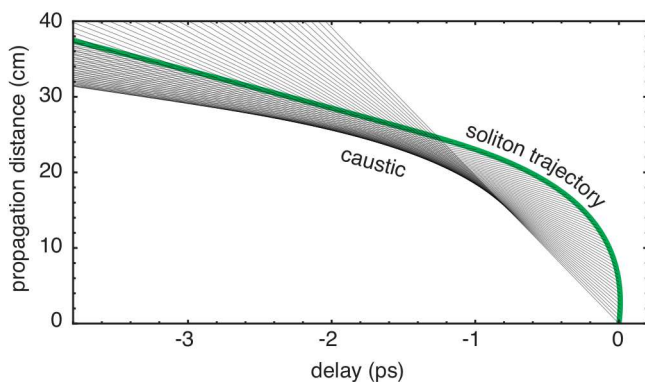


**Fig. 8:** (a) Reflection of light rays from a plane mirror. (b) A curved mirror yields the common envelope or caustic of light rays.

Solving the adiabatic equations is  $\approx 1000$  times faster than the direct solution of the GNLSE. It allows for extensive parameter studies in order to find the optimal pulse parameters for, e.g., (i) the best soliton compression or (ii) the quickest soliton acceleration or (iii) the widest spectrum of the scattered waves. One can even access truly complicated problems, e.g., finding an optimal fiber dispersion profile for the desired effect. Moreover, the adiabatic approach changes the way we think about solitons that scatter optical beams. The solitons, which were described in terms of amplitude and duration, are now described in terms of the transmission coefficient  $\mathfrak{T}$ . One can immediately distinguish between good ( $\mathfrak{T} \ll 1$ ) and bad ( $\mathfrak{T} \approx 1$ ) soliton mirrors. Moreover, one can now follow the evolution of  $\mathfrak{T}$  along the fiber and choose the moment when the soliton becomes transparent for the first beam ( $z \approx 24$  cm, region (A) in Figure 6), and a new beam should be applied for the optimal compression. Last but not least, some effects that were impossible to distinguish or to interpret with the full GNLSE solution become readily accessible from the adiabatic point of view. A nice example of a completely unexpected result is provided by caustic structures.

Caustic structures can be explained by comparing light rays reflected from a plane mirror and from a curved one. While the first picture is quite simple (Figure 8a), the second one (Figure 8b) yields a new geometric structure: a common envelope of rays. In optics, the envelope of light rays reflected or refracted by a curved surface is called *caustic*. Caustics are generic in nature because

all real-world mirrors are more or less curved. Our soliton mirror is not curved as such, however, it follows a curved trajectory. Adiabatic equations provide the frequency of the reflected wave at each point of the soliton trajectory. All these frequencies slightly differ from each other. We have therefore plotted geometric rays for the reflected waves as shown in Figure 9. The caustic structure represents an important feature of the GNLSE calculation; see region (B) in Figure 6. As it appears, we have observed caustic structures during several years starting from [2], but it was only after creating a proper theory [5] that we recognized them.



**Fig. 9:** Reflection of optical rays from a moving soliton produces a caustic structure, cf. region (B) in Figure 6 [5]

**Acknowledgments.** Shalva Amiranashvili, Uwe Bandelow, and Matthias Wolfrum acknowledge the support of the Einstein Foundation Berlin and of the Research Center MATHEON under Project D-OT2 “Turbulence and extreme events in nonlinear optics”.

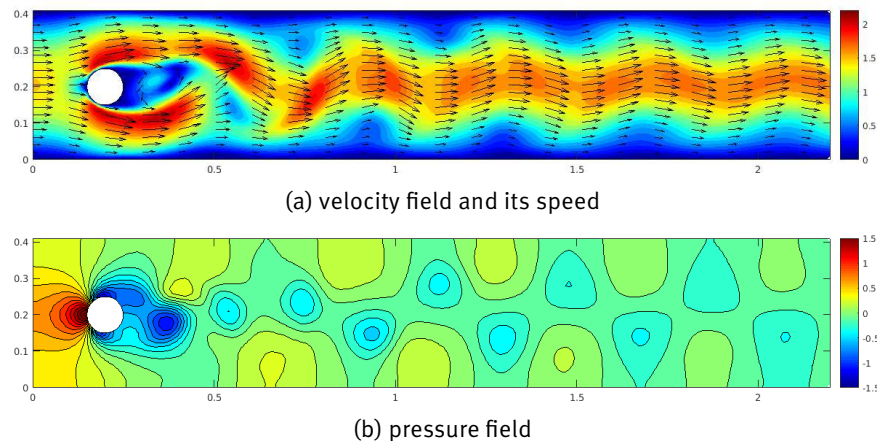
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## 2.3 Towards Pressure-robust Mixed Methods for the Incompressible Navier–Stokes Equations

Alexander Linke and Christian Merdon

With the Navier–Stokes equations (NSE), derived in the first half of the nineteenth century, numerous flow phenomena in nature and engineering can be explained. Among them are the temporal evolution of winds and storms in the atmosphere, the temperature distribution in a cooking pot, the flight of birds, and the air resistance of a car. Therefore, they are an object of study in such different disciplines as physics, biology, meteorology, and engineering. Nowadays, the main tool to solve the NSE is numerical simulation on laptops, work stations, or high performance super computers—depending on the complexity of the flow. The mathematical core of numerical simulations are *discretizations*, i.e., the “art” to approximate the infinite-dimensional NSE by a system of hundreds, thousands, or millions of coupled equations that can be solved automatically by computers. In recent years, research at the Weierstrass Institute has deepened the understanding of a common *discretization issue* of NSE simulators that appears whenever the magnitude of the fluid pressure becomes comparably large to the fluid velocity. Novel *pressure-robust* Navier–Stokes discretizations promise to considerably reduce costs, memory requirements, and simulation times, whenever the fluid pressure is high.



**Fig. 1:** Snapshot of the velocity and pressure fields of a von Kármán vortex street (Reynolds number  $Re = 100$ )

### Mathematics of the incompressible NSE equations

The NSE describe the temporal evolution of mass density, pressure, temperature, and the velocity field of a gas or a liquid; see Figure 1. The velocity field indicates the velocity of the fluid at a certain point in time and space. Mathematically, the NSE build a set of *partial differential equations*, modeling mass conservation, momentum balance, and energy balance. Current research of the WIAS Research Group *Numerical Mathematics and Scientific Computing* focuses on the numerical simulation of the *incompressible NSE*, which are mainly used to model liquids. For the incompressible NSE the density of the fluid is constant and mass conservation in the fluid reduces to a geometric

constraint on the velocity field: it is *divergence free*, i.e., all the flow entering an arbitrary point in space from a certain direction has to leave the point in space again, possibly in a different direction; see Figure 2.

### Numerical simulation of the incompressible NSE, discretization and the challenges

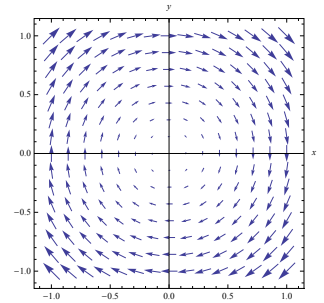
Thousands of scientists are engaged worldwide in the numerical simulation of the incompressible NSE. In the last decades, major progress has been achieved, and the simulation of many flow problems, which seemed to be untractable half a century ago, is nowadays possible. The ultimate goal is the construction of a *black-box solver*: Given an arbitrary, physically reasonable flow problem, the numerical simulation should deliver a reasonably accurate approximation of the real flow situation in a reasonable time and under reasonable costs.

**Different physical regimes as a challenge.** A major challenge for a *black-box solver* is the richness of the solution set of the incompressible NSE. The NSE are physically fundamental, and their solutions belong to several physical regimes with a diversity of properties. The NSE describe the physics of

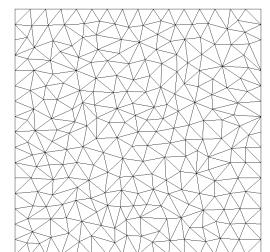
- hydrostatics, where there is no flow, since exterior forces are balanced by the pressure gradient,
- laminar flows, which occur, e.g., in microfluidics and where the friction force is dominant,
- potential flows, which model, e.g., the flow far away from an airfoil,
- turbulent flows, where the friction force is nearly negligible,
- quasi-geostrophic flows in oceanography like the gulf stream with a dominant Coriolis force.

Different physical regimes correspond to certain forces in the Navier–Stokes momentum balance that are approximately negligible. In such cases, essential aspects of the flow can be described by simplified equations: A Poisson equation describes hydrostatics and potential flows, the Stokes equations describe microfluidics, the Euler equations approximate turbulent flows, and the *geostrophic equations* describe quasi-geostrophic flows. *Black-box solvers* for the NSE are needed whenever a flow problem possesses different physical regimes. The challenge for constructing a good *black-box solver* for the NSE is, in a sense, to construct simultaneously a good solver for the Poisson, Stokes, Euler, and geostrophic equations.

**Discretization and triangulation.** The mathematical core of numerical simulations are *discretizations*, i.e., the approximation of the infinite-dimensional NSE by a finite—but potentially very large—system of coupled equations that can be solved automatically by computers. For example, in a finite volume discretization, these equations describe the velocity and the pressure at a finite number of different locations in the *flow domain* and are called the *degrees of freedom (DoF)*. The choice of the DoF is made by the flow solver and can be adapted to the physics of the flow: Wherever the flow is difficult, more DoF can be spent. For example, in Figure 3, a triangulation of a quadratic flow domain is shown. For the Bernardi–Raugel mixed finite element method (Bernardi–Raugel element) [5, 4], the pressure DoF are assigned to the triangles, and the velocity DoF are assigned to the vertices and to the edge midpoints of the triangulation. As a rule of thumb, time



**Fig. 2:** A divergence-free vector field



**Fig. 3:** Triangulation of a quadratic flow domain



and memory consumption increase at least proportionally to the number of DoF in the discretization. Therefore, good discretizations aim at achieving a reasonable accuracy with a reasonably small number of DoF.

**The discrete physics induced by a discretization.** Approximating the NSE by a discretization introduces not only *discrete pressures and velocities* (the DoF to be solved), but induces also a certain kind of *discrete physics*. In the discretization, the *continuous NSE momentum balance* and the *continuous NSE mass conservation* are replaced by a *discrete momentum balance* and a *discrete mass conservation*. In fact, for the continuous NSE several mathematical and physical properties hold at the same time, like conservation of mass, kinetic energy, momentum, and angular momentum. Unfortunately, not all these mathematical and physical properties can be simultaneously preserved in a discretization. Some of them are approximated, but not exactly fulfilled, a potential source of so-called *discretization errors* for flow solvers, which can lead to inaccurate flow simulations.

**Classical mixed methods and the divergence constraint in solvers for the incompressible NSE.**

At the end of the 1960ies, the establishment of the theory of *mixed methods* represented a major breakthrough for discretizations of the incompressible NSE. These classical mixed methods relax the divergence constraint in order to achieve another fundamental mathematical property, the so-called *discrete inf-sup stability*. Subsequently, numerical analysts were able to construct dozens of different flow solvers with different advantages and disadvantages, which are *provably convergent*, i.e., one can prove for this type of discretizations that simulation results with any desired accuracy can be reached if only the number of DoF in the discretization is high enough. This breakthrough enabled major progress in the simulation of the NSE. However, for difficult flows the necessary number of DoF for a reasonable accuracy can be extremely (and prohibitively) high. Simultaneously, the computational fluid dynamics (CFD) community became widely convinced that the accuracy risks from relaxing the divergence constraint for the discretization accuracy are more or less manageable.

**Divergence-free mixed methods for the incompressible NSE.** Nevertheless, some—in a certain sense—seemingly exotic *divergence-free* mixed methods for the incompressible NSE (from the so-called *Scott–Vogelius* finite element family) showed that classical mixed methods, which relax the divergence constraint, are—from a qualitative viewpoint of discretization theory—only the *second-best* ones possible [1]: For the incompressible Stokes equations, which model, e.g., flows in microfluidics and which are embedded in the full NSE model, classical mixed methods deliver an accurate velocity field whenever the continuous velocity and the continuous pressure can simultaneously well be *represented* on a given triangulation. But these exotic *divergence-free mixed methods* deliver an accurate velocity field whenever only the continuous velocity can well be approximated on a triangulation, i.e., the pressure field may be arbitrarily difficult, but this problem does not affect the accuracy of the *velocity field* of *divergence-free* flow solvers [1, 3, 6].

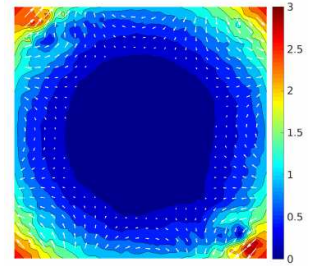
**WIAS research on poor mass conservation.** At WIAS, the first author asked in his PhD thesis in 2007 in which benchmarks the exotic *divergence-free Scott–Vogelius mixed methods* for the incompressible NSE outperform classical mixed methods. Surprisingly, this happens for the easiest flows possible: hydrostatics, where there is no flow at all, and where an exterior (irrotational) force

is completely balanced by the pressure gradient [6]. Since a velocity field  $\mathbf{u} \equiv \mathbf{0}$  can be represented on every triangulation, divergence-free mixed methods deliver the exact answer. On the other hand, the velocity field of *classical mixed methods* may deliver arbitrarily large discretization errors if the *continuous pressure* is large and if it is not contained in the *discrete pressure space*. Though several authors had observed this discretization issue before—sometimes called *poor mass conservation*—, a *systematic research* was started at WIAS for the first time [1, 3, 6]. This research shows that dramatic discretization errors by *poor mass conservation* can be triggered in several flow regimes. Among them are (quasi-)hydrostatic flows, potential flows (see Figure 4), and (quasi-)geostrophic flows [6, 5]. All these flow regimes have in common that the *pressure gradient* is orders of magnitudes larger than other forces in the NSE momentum balance, e.g., the friction force [1].

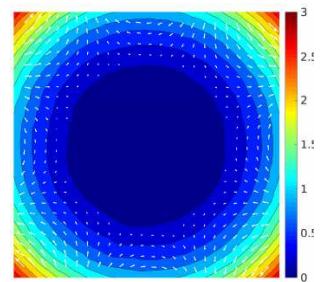
### Novel pressure-robust WIAS NSE solvers for the incompressible NSE that are not divergence free

The WIAS research on *poor mass conservation* revealed that the most important property of the seemingly exotic *divergence-free mixed methods* is that they deliver a reasonably small discretization error for the velocity if only the velocity field can well be *approximated* on a given triangulation, i.e., the velocity error is independent of the pressure. Recently, we called this property *pressure-robustness* [1, 5] and asked whether there exist *pressure-robust* mixed methods for the incompressible NSE that are not divergence free (and considerably less exotic). Looking at the problem in more detail, one recognizes that relaxing the divergence constraint in the *velocity trial functions* is indeed harmless, but relaxing the divergence constraint in the *velocity test functions* is potentially dangerous, since certain *discretely divergence-free* velocity test functions, which are not *exactly divergence free*, are not orthogonal to *arbitrary* gradient fields in the  $L^2$  inner product, though their continuous counterparts would be orthogonal [3, 1]. In a series of papers [3, 4, 2], we exploited this improved understanding and showed that for the most important popular (inf-sup stable) classical mixed finite element methods and also for some Hybrid Discontinuous Galerkin and finite volume methods, the discrete  $L^2$  vector product can be efficiently repaired such that these slightly modified mixed methods become *pressure robust*. In the case of the incompressible Stokes equations, only the right-hand side has to be discretized differently. For this approach, some *velocity reconstruction operators* are constructed that map *discretely divergence-free* to *divergence-free* test functions [3, 4, 2].

**Large speedups for the novel pressure-robust modifications in certain benchmarks.** Our research on poor mass conservation enabled us to construct benchmarks where the novel modified pressure-robust mixed methods outperform their classical counterparts dramatically. Indeed, if one wants to construct an (academic) benchmark for the incompressible Stokes equations, where the modified method is a thousand times, a million times, or a billion times faster, such a benchmark can always be constructed [1, 3, 2]. Searching for practically relevant, non-academic benchmarks, we showed recently that for high Reynolds number potential flows, a similar modification in the nonlinear convection term delivers dramatic speedups, too [5, 1]. These speedups are especially large for first-order methods, and are higher for three- than for two-dimensional flows. In 3D, for the first-order Bernardi–Raugel element we constructed benchmarks with speedups up to



**Fig. 4:** Velocity field and absolute velocity of a cubic potential flow. A classical Bernardi–Raugel mixed method shows large discretization errors.



**Fig. 5:** A novel modified Bernardi–Raugel mixed method [4] is pressure-robust [1, 5], which reduces the discretization error compared to Figure 4.

16 million (!) [5], more precisely, the classical Bernardi–Raugel element needed 16 million times more DoF, in order to achieve the same accuracy as the new modified pressure-robust modification. In two space dimensions, we got speedups with Bernardi–Raugel up to 4096, and for the second-order  $P_2^{\text{bubble}} - P_1^{\text{disc}}$  element we got speedups up to 64 [5].

### Conclusions and outlook

For more than thirty years it was thought that efficient pressure-robust mixed methods for the three-dimensional incompressible NSE, whose velocity error is pressure-independent, were practically impossible to construct. However, recent research at WIAS showed that it is rather easy to slightly modify many classical inf-sup stable mixed methods in order to make them pressure robust [3, 4, 2, 1]. This modification was applied to conforming and nonconforming finite element methods, Hybrid Discontinuous Galerkin and finite volume methods and can probably be applied to all kinds of inf-sup stable mixed flow discretizations. While this modification seems to reduce the accuracy in the *worst case* only marginally, it promises potentially dramatic speedups whenever the pressure is large in magnitude compared to the velocity. Further research has to investigate in which physical regimes such flows arise in practice. Preliminary investigations show that at least flows with a large Coriolis force and potential flows with high Reynolds numbers belong to this class [6, 5, 1]. We also plan to cooperate with developers of flow simulators that allow simulations on massively parallel computing platforms, in order to test the modification for real-world flows at high Reynolds numbers. Besides that, the theoretical understanding of the novel modification has to be deepened. Last but not least, we plan to extend the new insight how to discretize the incompressible NSE to the compressible NSE.

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## 2.4 Effective Modeling of Multiscale Phenomena

Franziska Flegel, Martin Heida, and Sina Reichelt

Artificial materials such as plywood, concrete, and alloys as well as natural materials such as soil, plant tissue, and skin have one thing in common: They reveal different structures at a huge range of length scales. So, how can we effectively model the macroscopic behavior of such materials? What are the relevant scales, i.e., the scales that affect macroscopic properties of the materials? How do the microscopic scales interact with the macroscopic one?

These questions lead us to the theory of asymptotic homogenization, which applies to a variety of situations where heterogeneous microstructures are involved. Usually, mathematicians focus on the interaction of only two distinct scales. In case of more than two scales, if they can be ordered into a hierarchy, they successively study the interaction of each scale with the next higher scale. A typical mathematical problem, which is also interesting to both physicists and engineers, is the Poisson equation

$$-\operatorname{div}(a_\varepsilon \nabla u_\varepsilon) = f, \quad (1)$$

where the coefficients  $a_\varepsilon$  oscillate rapidly at small length scales. The positive parameter  $\varepsilon$  determines the ratio between the characteristic microscopic length scale and the characteristic macroscopic length scale. Equation (1) arises, for instance, when we want to determine the stationary temperature profile  $u_\varepsilon$  given a certain heat source density  $f$  and a thermal (space-dependent) conductivity tensor  $a_\varepsilon$ . Alternatively, we could interpret  $f$  as the rate at which free charges are inserted into a system. Then  $u_\varepsilon$  would be the resulting stationary electric potential given the electric conductivity tensor  $a_\varepsilon$  of the underlying material.

If  $a_\varepsilon$  displays a laminar structure as indicated by the yellow and green layers in Figure 2, then  $\varepsilon$  corresponds to the inverse of the number of layers. In this case, the solution  $u_\varepsilon$  might fluctuate rapidly in the  $x_1$ -direction as in Figure 2.

The question is: When  $\varepsilon$  tends to zero, does the solution  $u_\varepsilon$  converge to the solution of an effective equation

$$-\operatorname{div}(a_{\text{eff}} \nabla u) = f, \quad (2)$$

and how can we characterize the effective conductivity  $a_{\text{eff}}$ ? It is one of the subjects of homogenization theory to answer this question. What does  $a_{\text{eff}}$  look like in the specific example in Figure 2? In this case, we can characterize  $a_{\text{eff}}$  quite intuitively: When we look along the  $x_1$ -axis, we see that the different layers are connected in series, and thus the effective conductivity is the harmonic mean of the individual conductivities. On the other hand, when we look along the  $x_2$ -axis, the layers are connected in parallel, and, therefore, the effective conductivity is the arithmetic mean of the individual conductivities. It follows that the effective conductivity tensor  $a_{\text{eff}}$  is anisotropic.

For general coefficients  $a_\varepsilon$ , it can be very difficult to determine whether the effective quantity  $a_{\text{eff}}$  exists. If it exists, it is the unique solution of a minimization problem, which can be computed numerically.



Fig. 1: Plywood

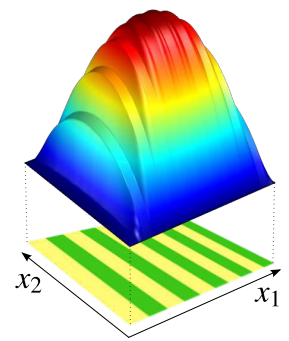


Fig. 2: Solution  $u_\varepsilon$  of (1) for laminate microstructure

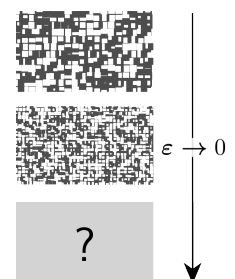
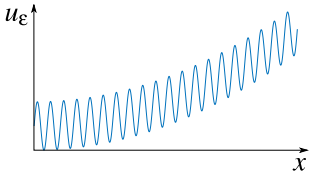
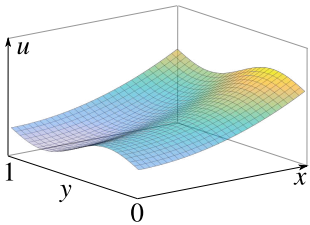


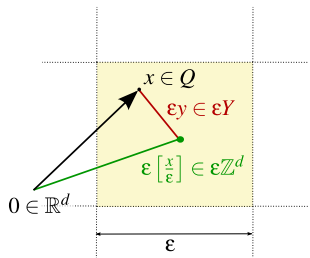
Fig. 3: Homogenization



**Fig. 4:** Rapidly oscillating one-scale function  $u_\varepsilon(x)$



**Fig. 5:** Smooth two-scale function  $u(x, y)$



**Fig. 6:** Two-scale decomposition

## Periodic versus stochastic homogenization

**Periodic coefficients.** Periodically distributed microstructures have been extensively studied in the literature. The periodic geometry allows us to turn a problem on the  $d$ -dimensional domain  $Q$  into a problem on the  $2d$ -dimensional space  $Q \times Y$ , where  $Y = [0, 1]^d$  denotes the so-called *reference cell*. In 1989, Nguetseng introduced the notion of *two-scale convergence* for periodic functions  $u_\varepsilon(x)$  as in Figure 4. As the period  $\varepsilon$  tends to 0, the limit function  $u(x, y)$  in Figure 5 depends on two scales  $x$  and  $y$ , where  $x \in Q$  describes the macroscopic behavior and  $y \in Y$  captures the microscopic fluctuations. In order to handle real heterogeneities, we employ the *periodic unfolding operator*  $\mathcal{T}_\varepsilon$  introduced by Jäger and Hornung as well as Cioranescu, Dambramian, and Griso. The operator  $\mathcal{T}_\varepsilon$  maps one-scale functions  $u(x)$  to two-scale functions  $(\mathcal{T}_\varepsilon u)(x, y)$  by decomposing any  $x = \tilde{x} + \varepsilon y$  into a macroscopic part  $\tilde{x} = \varepsilon[x/\varepsilon] \in \varepsilon\mathbb{Z}^d$  and a microscopic part  $y \in Y$ ; see Figure 6.

**Random coefficients.** At the end of the 1970s, Papanicolaou and Varadhan started to study problem (1) in case of random coefficients  $a_\varepsilon(x) = a_{\omega, \varepsilon}(x)$  (as in Figure 3), where  $\omega$  is a stochastic parameter. Stochastic homogenization problems are usually more complicated to handle than periodic ones, since the corresponding stochastic unfolding operator  $\mathcal{T}_{\omega, \varepsilon}$  becomes unbounded and non-coercive. However, Zhikov and Piatnitsky were able to generalize the concept of two-scale convergence to the stochastic case in 2006.

## Two-scale homogenization of nonlinear systems of parabolic equations

The theory of periodic homogenization has been widely studied and largely extended during the last five decades mainly in the context of linear problems. The application in the nonlinear context is more difficult and is less developed. The recent Ph.D. thesis [3] considered systems of evolution equations, meaning partial differential equations that depend on space and time, where nonlinear and noncompact coupling effects were taken into account. Here, the spatial dependency is strongly heterogeneous, which means that the coefficients of the equations are allowed to vary arbitrarily on the macroscopic scale and periodically on the microscopic scale; see Figure 7. Under these general assumptions on the data, it was possible to derive effective equations for two different classes of nonlinear evolution problems: namely, coupled systems of reaction-diffusion equations and Cahn–Hilliard equations describing phase separation. For Cahn–Hilliard equations, the homogenization limit was derived by exploiting their underlying gradient structure. Since this method was the subject of a highlight article in the WIAS Annual Research Report 2014, we do not discuss it further here.

Reaction-diffusion systems, however, do not admit a gradient structure in general, and, therefore, a new approach was developed, and its result is presented below. This approach has the great advantage that it made it possible to prove quantitative estimates for the difference between the original and the effective solution.

**Coupled systems of reaction-diffusion equations.** In a heterogeneous environment, we consider two different species  $X_1$  and  $X_2$  with densities  $u_\varepsilon$  and  $v_\varepsilon$  that react with each other and diffuse in the domain  $Q \subset \mathbb{R}^d$ . Whereas the characteristic diffusion scale of species  $X_1$  is proportional

to the macroscopic length scale, species  $X_2$  diffuses much slower: namely, of order of the microscopic length scale. In this model, the parameter  $\varepsilon$  does not only characterize the microstructure of the domain (Figure 7), but also the diffusion scale of  $X_2$ . The evolution of the densities  $u_\varepsilon(t, x)$  and  $v_\varepsilon(t, x)$  is given for  $t \geq 0$  and  $x \in Q$  via

$$\partial_t u_\varepsilon = \operatorname{div}(d_\varepsilon \nabla u_\varepsilon) + F_\varepsilon(u_\varepsilon, v_\varepsilon) \quad \text{and} \quad \partial_t v_\varepsilon = \operatorname{div}(\varepsilon^2 \kappa_\varepsilon \nabla v_\varepsilon) + G_\varepsilon(u_\varepsilon, v_\varepsilon). \quad (3)$$

The interaction of the two species is described via the nonlinear reaction terms  $F_\varepsilon$  and  $G_\varepsilon$ , and the diffusivity is determined by the positive tensors  $d_\varepsilon$  and  $\kappa_\varepsilon$ . When passing to the limit with  $v_\varepsilon$  as  $\varepsilon \rightarrow 0$ , standard methods in the theory of periodic homogenization fail due to the presence of slow diffusion and nonlinear reaction.

Using the method of two-scale convergence via the periodic unfolding operator  $\mathcal{T}_\varepsilon$  and defining moreover different folding operators, which map two-scale functions to one-scale functions, the two-scale homogenization limit for (3) was rigorously derived. In the limit, the density  $V(t, x, y)$  of species  $X_2$  depends on one additional spatial scale, namely  $y \in Y$ , whereas  $u(t, x)$  only depends on  $t$  and  $x$  as in the original model (3)

$$\begin{aligned} \partial_t u(t, x) &= \operatorname{div}(d_{\text{eff}}(x) \nabla u(t, x)) + \int_Y F(x, y, u(t, x), V(t, x, y)) dy, \\ \partial_t V(t, x, y) &= \operatorname{div}_y(\kappa(x, y) \nabla_y V(t, x, y)) + G(x, y, u(t, x), V(t, x, y)). \end{aligned}$$

The diffusion of  $X_1$  is determined by the effective tensor  $d_{\text{eff}}$  and the averaged reaction over  $Y$ . In contrast, species  $X_2$  does not diffuse on the macroscopic scale, but only on the unit cell  $Y$ . In other words,  $V$  is the solution of a reaction-diffusion equation on the two-scale space  $Q \times Y$ , where we attach to every point  $x \in Q$  one copy of  $Y$ ; see Figure 8. On the macroscopic level, i.e., with respect to  $(t, x)$ , one may interpret the equation for  $V$  as an ordinary differential equation.

**Quantitative estimates.** It was proved in [3] that not only the solutions  $u_\varepsilon$  and  $v_\varepsilon$  converge to the limits  $u$  and  $V$ , respectively, but also that their convergence rate can be controlled in terms of the parameter  $\varepsilon$ . By choosing initial conditions that match the microstructure, the errors between  $u_\varepsilon$  and  $u$ , respectively  $\mathcal{T}_\varepsilon v_\varepsilon$  and  $V$ , are of the order  $O(\varepsilon^{1/4})$ , whereas for general initial conditions the error is of order  $O(\varepsilon^{1/6})$ . The obtained error estimates are new even for linear and time-independent partial differential equations such as equation (1) with  $a_\varepsilon = \varepsilon^2 \kappa_\varepsilon$ . Moreover, it was possible to prove in the subsequent publication [4] that the convergence rate can be improved to  $O(\varepsilon^{1/2})$ .

## Homogenization of the discrete Laplace operator with random coefficients

Many analytical homogenization tools, such as two-scale convergence, were first developed for continuous problems. However, these techniques turned out to be relevant also to discrete problems from other fields. In this section, we study a discrete stochastic Laplace operator  $\mathcal{L}_\omega^\varepsilon = \operatorname{div}_d(\omega_\varepsilon \nabla_d)$  and show that the solution of the discrete Poisson equation converges to the solution of a continuous Poisson equation (2). Such operators appear as generators of Markov processes in random walk theory.

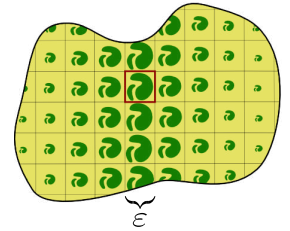


Fig. 7: Not-exactly-periodic microstructure

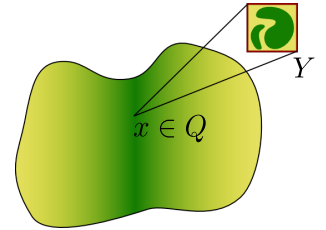


Fig. 8: Two-scale space

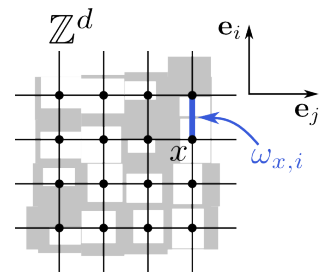
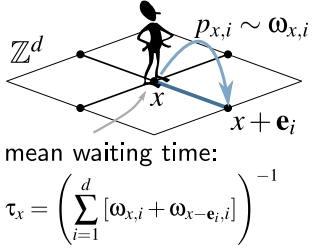


Fig. 9: Euclidean lattice  $\mathbb{Z}^d$  with edges between nearest neighbors. The edges carry a conductance  $\omega$





**Fig. 10:** Random walk among random conductances

**Random walk among random conductances.** Suppose that on the discrete Euclidean lattice  $\mathbb{Z}^d$  any two nearest neighbors  $x$  and  $x + z$  are connected by a random positive conductance  $\omega_{x,z}$ ; see Figure 9. On this grid, we place a *random walker* who behaves as follows (see Figure 10): When the random walker has arrived at a site  $x \in \mathbb{Z}^d$ , it waits for an exponentially distributed random time  $\tau_x$ . The smaller the surrounding conductances, the longer the random walker remains at the site  $x$ . Afterwards it jumps to one of the nearest neighbors of  $x$  with a probability that is proportional to the conductances on the respective edge.

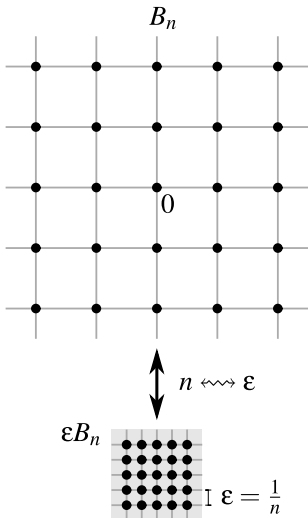
The movement of the random walker is described by the discrete Fokker–Planck equation

$$\partial_t p_t(x, \cdot) = \mathcal{L}_\omega p_t(x, \cdot) \quad \text{with } p_0(x, \cdot) = \delta_x,$$

where the operator  $\mathcal{L}_\omega$  acts on real-valued functions  $u \in \ell^2(\mathbb{Z}^d)$  via

$$(\mathcal{L}_\omega u)(x) := \sum_{z: |z|=1} [\omega_{x,z}(u(x+z) - u(x))] \quad \text{for } x \in \mathbb{Z}^d.$$

If we denote the discrete gradient by  $\nabla_d$  and the discrete backwards divergence by  $\text{div}_d$ , then the operator  $\mathcal{L}_\omega$  can be rewritten as  $\mathcal{L}_\omega = \text{div}_d(\omega \nabla_d)$ . Thus,  $\mathcal{L}_\omega$  is a discrete version of the divergence form operator in (1).



**Fig. 11:** The bounded domain  $B_n$  in  $n$  and  $\varepsilon = 1/n$  scalings

**Properties of the discrete Laplace operator in a bounded domain.** We are interested in the behavior of a random walker in a bounded domain  $B_n = \{x \in \mathbb{Z}^d : |x|_\infty < n\}$ , where  $n$  is large. Instead of studying  $n \rightarrow \infty$ , we rescale  $\mathbb{Z}^d$  by  $\varepsilon$  and let the lattice spacing  $\varepsilon = 1/n$  tend to zero; see Figure 11. The long-time behavior of the random walker in the box  $B_n$  is connected with the spectral problem

$$-\mathcal{L}_\omega^\varepsilon \psi_k^\varepsilon = \lambda_k^\varepsilon \psi_k^\varepsilon \quad \text{in } (-1, 1)^d \quad \text{with} \quad \psi_k^\varepsilon(x) = 0 \quad \text{for all } x \notin (-1, 1)^d,$$

where  $\mathcal{L}_\omega^\varepsilon u(x) = \varepsilon^{-2} \mathcal{L}_\omega u(\frac{x}{\varepsilon})$  is the rescaled Laplacian.

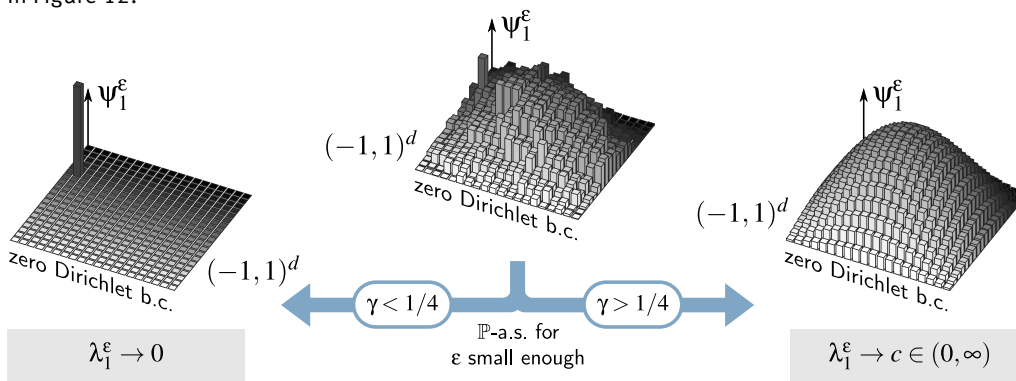
Our three main questions are the following (see [2]): (i) Given  $\omega$ , how do  $\lambda_k^\varepsilon$ ,  $\psi_k^\varepsilon$  behave when  $\varepsilon \rightarrow 0$ ? (ii) How does a solution  $u_\varepsilon$  to the Poisson equation  $-\mathcal{L}_\omega^\varepsilon u_\varepsilon = f_\varepsilon$  behave for small  $\varepsilon$ ? (iii) To what extent does the limit depend on the choice of the random environment  $\omega$ ? If we formulate the problem in the above  $\varepsilon$ -scaling, we can apply the framework of stochastic homogenization.

Based on earlier work, it was expected that  $u_\varepsilon \rightarrow u$ , where  $u$  solves a Poisson equation of the form  $-\text{div}(a_{\text{eff}} \nabla u) = f$  as in (2), and we could show that this holds true in a very broad range of conditions. To achieve this goal, we combined a generalized notion of the well-established stochastic two-scale convergence with the spectral convergence theory outlined in the monograph by Jikov, Kozlov, and Oleinik. In 2008, Faggionato already employed stochastic two-scale convergence to investigate the homogenization properties of the discrete random Laplacian with a spectral shift and in a less general setting. Further, Neukamm, Schäffner, and Schlömerkemper have recently proved homogenization in the sense of  $\Gamma$ -convergence.

In our ansatz [2], we assume moment conditions on the conductances that ensure the almost sure validity of a Poincaré inequality recently proved by Andres, Deuschel, and Slowik. In particular, we

can allow for percolation (i.e., some connections on the grid that have zero conductivity and are thus never crossed by the random walker) and long-range jumps as well. Here, very long jumps have to be sufficiently rare.

**Spectral asymptotics for independent and identically distributed conductances.** Let us consider the special case where the conductances on the edges are independent from each other but have the same distribution. Furthermore, we only consider nearest neighbors. Then the Dirichlet spectrum of  $\mathcal{L}_\omega^\varepsilon$  in the box  $(-1, 1)^d$  displays a dichotomy between two contrasting regimes depending on the value of  $\gamma = \sup\{q \geq 0: \mathbb{E}[\omega^{-q}] < \infty\}$ : Depending on whether  $\gamma < 1/4$  or  $\gamma > 1/4$  and as  $\varepsilon$  tends to zero, the principal Dirichlet eigenvector  $\psi_1^\varepsilon$  either almost surely concentrates increasingly on a single site (see [1]) or it almost surely converges to a cosine (see [2]) as depicted in Figure 12.



**Fig. 12:** Dichotomy between complete localization or homogenization of the principal Dirichlet eigenvector

## Conclusion and outlook

The highlight article demonstrates how one physical phenomenon, such as heat conduction in a heterogeneous environment, can be modeled with either periodic or stochastic microstructure. To derive an effective model, one requires techniques and methods from often quite distinct mathematical disciplines, namely, analysis and stochastics, also encouraging the interplay of these two.

In the near future, we plan to investigate interface and surface effects with periodic and stochastic microstructures in more detail.

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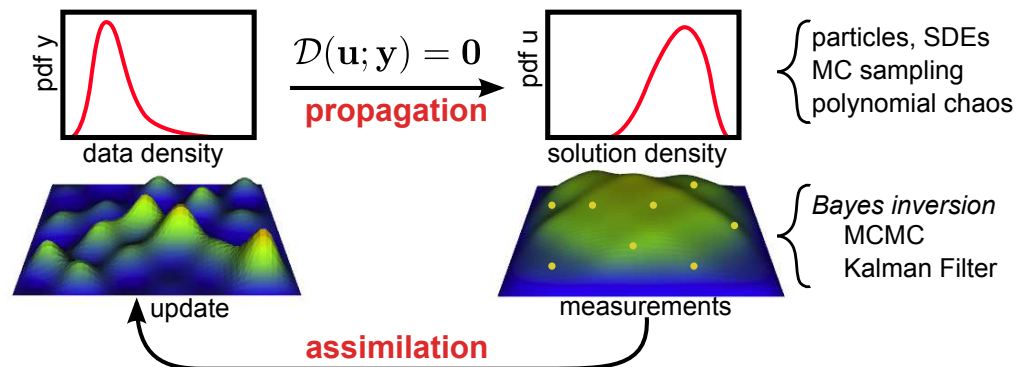
## 2.5 Uncertainty Quantification from Different Perspectives – Methodological Encounters and Inspirations

Christian Bayer and Martin Eigel

### Aspects of uncertainty quantification

Over the last decade, *uncertainty quantification* (UQ) has become a hugely popular research area across many mathematical and technical disciplines, ranging from applied mathematics to computer science and engineering. The topic subsumes methods and techniques for the examination of propagation and quantification of uncertainties in predictive modeling and simulation used in forward and inverse problems. The uncertainty can be described by means of probabilistic models<sup>1</sup>. A major distinction usually is made between *epistemic uncertainty*, resulting from incomplete knowledge, which in principle could be reduced (for instance, by better measurements), and *aleatoric uncertainty* inherent to the problem under consideration and which cannot be reduced.

**Fig. 1:** Illustration of the propagation of data uncertainty associated with random vector  $y$  by some model  $\mathcal{D}$  to the solution  $u$ . The inverse problem (data assimilation) is based on measurements of the solution (yellow dots) and a subsequent inference to update the assumed data probability density.



Uncertainties of various kinds play a central role in many real-world applications and in the simulation of physical phenomena, e.g., in structural mechanics, material science, fluid dynamics, geophysics, systems biology, and others. For carrying out numerical computations, an adequate modeling and description of uncertainty (or randomness or stochasticity) has to be devised depending on the problem and the numerical method of choice. It should be mentioned that there is no single optimal way to the description and treatment of uncertainty. Nevertheless, there are persuasive arguments to assume probability theory as a favourable vehicle for this task. In particular, the probabilistic or stochastic approach allows for the most detailed description and analysis, mathematically, and hence is chosen most often in practice. Such a description is usually accomplished by representing certain quantities in the examined models as *random variables*, *stochastic processes*, or *random fields*. In an abstract setting, we may consider some mathematical model  $A$  (e.g., the Navier–Stokes system or the Darcy equation (MP) stated below as model problem), which

<sup>1</sup> There are of course other approaches such as, e.g., interval analysis for worst-case scenarios, fuzzy set theory, and evidence theory, which are not in the scope of this overview.

establishes a relation between the space of actions  $F$  of the input (the real world, e.g., forces) onto the system and the space of outputs  $U$  (the reactions, e.g., pressure and velocity),

$$A : U \rightarrow F, \quad A : u \mapsto f,$$

where usually the action  $f \in F$  is known and the reaction  $u \in U$  has to be found by inversion. For instance, one solves the equation  $u = A^{-1}(f)$  in order to obtain the response  $u$  of the system. Here, it is “only” an application or computation. In the context of UQ, the action  $f$  as well as the operator  $A$  may be uncertain and hence depend on random variables  $y$ . One then is interested in the propagation of the uncertainty to the response  $u$  as pictured in Figure 1, where the model is denoted by  $\mathcal{D}(u; y) = A(u; y) - f(y)$ . The *inverse problem* seeks to determine the probability distribution of the data of some model by (iterated) measurements of some quantity of the system response  $u$  and subsequent updating of the data assumption.

While UQ has a long history, mainly in statistics or stochastics, in recent years many new influences have appeared that have broadened the applicability of such approaches, in particular from the areas of numerical analysis and computational (partial) differential equations (PDE). This development can be considered a natural as well as a beneficial connection of mathematical fields with related and partially common goals, which manifest in the joint aspiration to properly describe actual (observed) physical phenomena. It is the aim of this short review to elucidate a few of these aspects and, especially, to point out by example different views on the modeling and numerical treatment of problems with uncertain data. We want to show that the many mathematical and computational challenges still existing in this important field can probably benefit from the cooperation and coupling of different views and approaches to the problems. Due to the dependence on, typically, a very large number of random variables, UQ problems often are very high dimensional. Hence, the efficient treatment of high dimensionality is a central and recurring theme shared by the various mathematical perspectives on UQ.

Regarding two main directions from which such problems can be approached, namely stochastics and functional analysis, we accordingly identify two fundamentally different notions to obtain the solution in practice by employing

1. probabilistic methods, i.e., sampling techniques, which generate realizations or sampling paths of the uncertain data,
2. methods based on a functional representation of the randomness in appropriate (discrete) function spaces.

A prominent member of the class of sampling approaches is the classical Monte Carlo method known for its simplicity, robustness, and versatility, but also for its slow convergence. There is active research to alleviate this shortcoming, in particular, either by reducing the variance (Multilevel and Multi-index Monte Carlo) or by exploiting higher regularity with a more structured selection of sampling points (quasi-Monte Carlo, digital nets).

As an alternative to Monte Carlo sampling, (global) spectral methods employ an adequate discretization of the parameter space, typically by polynomials<sup>2</sup>. This approach has several important benefits, most notably: (a) One can obtain the optimal convergence rates with respect to the

<sup>2</sup>There are several alternative approaches to so-called *surrogate models* or *emulators*, e.g., Gaussian process models, neural nets, moving least squares, radial basis functions.

regularity of the solution. (b) The computed solution contains (approximately) all statistical information, e.g., regarding higher moments. (c) Adaptive error control based on some a posteriori error estimation is feasible. The price one has to pay with such sampling-free methods is the high computational complexity, which typically involves high-dimensional integration and the solution of high-dimensional coupled algebraic systems. Usually, the complexity grows exponentially with the number of stochastic dimensions, the well-known *curse of dimensionality*. However, modern compression techniques such as hierarchical tensor formats make these problems tractable again<sup>3</sup>.

In what follows, we provide illustrations of different approaches to UQ problems that can for instance all be employed to solve the frequently used Darcy equation with stochastic conductivity  $\kappa$  on some domain  $D$ ,

$$-\nabla \cdot (\kappa \nabla u) = f \quad \text{on } D, \quad u|_{\partial D} = g. \quad (\text{MP})$$

The stochastic fields  $\kappa(x, \omega)$  and  $u(x, \omega)$  depend on the physical position  $x \in D$  and some random event  $\omega$  in the set of events  $\Omega$ . In the first discussed sampling methods, a large number of realizations  $\omega$  is considered. Subsequently, functional representations are a second class of methods that discretize the entire stochastic space in some way without relying on specific samples. As a third approach, a novel method is presented that can be understood as a fusion of different concepts: namely, a particle path simulation combined with a global polynomial representation obtained by nonlinear regression.

A schematic overview of uncertainty propagation for forward and inverse problems is pictured in Figure 1.

### Sampling methods

Standard finite-dimensional sampling methods (as opposed to PDE methods) are highly relevant in many areas of applications. For example, many chemical and biological phenomena—but also problems from reliability, epidemiology, and many other areas—are modeled in terms of stochastic reaction networks (SRNs). In chemical terms, we consider  $d \geq 1$  chemical species interacting with each other. The state variable of the SRN is an integer-valued vector  $X(t) \in \mathbb{N}^d$  recording the number of individuals of each species present in the system at time  $t$ . The particles interact via  $J$  different reactions, which happen at random times with intensities depending on  $X(t)$ . (A particular reaction requiring individuals of species  $i$  and species  $j$  to interact might, for instance, have an intensity proportional to  $X^i(t) \cdot X^j(t)$ .) The exact intensities are usually derived from the *mass action principle* and are often of the form  $c_j g_j(X(t))$  for some known function  $g_j$  and some unknown parameters of proportionality  $c_j \geq 0$ ,  $j = 1, \dots, J$ .

The first step in a proper *uncertainty quantification* of such a system involves the estimation of the unknown parameters, given here by  $c_1, \dots, c_J$ . It is often reasonable to assume that the full vector  $X(t)$  can be observed in principle, but only for finitely many points in time, say  $t_0 = 0 < t_1 < \dots < t_n = T$ . At the same time, the dynamics of SRNs does not provide tractable expressions for the likelihood of  $(X(t_0), \dots, X(t_n))$  as opposed to the full (unobserved) trajectory  $(X(t))_{t \in [0, T]}$ . The celebrated *EM* (expectation-maximization) algorithm provides a remedy: The actually observed data

<sup>3</sup>Related techniques are POD (proper orthogonal decomposition), RBM (reduced basis methods), GEIM (generalized empirical interpolation).

are *augmented by artificial data*, simulated conditional on the observed data and an initial guess of the unknown parameters  $c_j$  (the  $E$  step). Then, the likelihood is maximized in the parameters (the  $M$  step), and the maximizer is used as initial guess for the next iteration of the EM algorithm.

The task of simulating a trajectory conditioned on the starting and terminal values—as required in the  $E$  step—is generally considered to be very difficult, especially in higher dimensions. The prevalent approach is probably to use a variant of the shooting method. In its most primitive form, this means to send out independent, random paths at the left endpoint value  $X(t_i)$  and only keep those that end up close to the right endpoint value  $X(t_{i+1})$ . The higher the dimension, the more unlikely it is to even get approximate hits. Despite a substantial literature introducing many variations of this method, the fundamental problem remains. We have added a new alternative sampling scheme (developed in [1]), where independent random paths are sent out from both the left and the right endpoints, forward and backward in time, respectively. All the pairs of such trajectories are connected that end up reasonably close to each other at a given intermediate point  $t^* \in (t_i, t_{i+1})$ . In some regimes (depending on the dimension  $d$  and the smoothness of the problem), the resulting *FREM* (forward-reverse EM, see [2]) algorithm allows us to avoid the curse of dimensionality. In Figure 2, we show the forward-reverse simulation for an application concerning the wear of Diesel engines, the actual estimation is shown in Figure 3.

For model problem (MP), a Monte Carlo method can easily be employed by sampling realizations of the data, computation of the pathwise solutions, and subsequent determination of statistics.

## Spectral methods

An alternative to sampling methods is to strive for functional representations of problem data and solutions. To this aim, a parametrization of the stochastic fields in a countable (independent) sequence of random variables  $y(\omega) = (y_1(\omega), y_2(\omega), \dots)$  is introduced. The image of  $y$  is the parameter domain  $\Gamma \subset \mathbb{R}^\infty$ . In the case of the model (MP),  $\kappa(x, y)$  and  $u(x, y)$  now depend on the random vector  $y$  instead of a random event  $\omega$ . A common choice for such a representation of stochastic fields with bounded variance is the Karhunen–Loève expansion. For a stochastic field  $\kappa$ , this yields

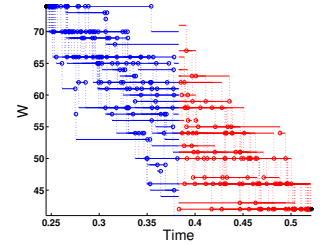
$$\kappa(x, y) = E[\kappa(x, \cdot)] + \sum_{m=1}^{\infty} a_m(x) y_m(y)$$

with Gaussian random variables  $y_m$ . One then is interested in the solution map  $y \mapsto u \in \mathcal{V}$  with solution space  $\mathcal{V} := \mathcal{X} \otimes \mathcal{Y}$  defined as tensor product of a physical space  $\mathcal{X}$  and a stochastic space  $\mathcal{Y}$ <sup>4</sup>. The solution admits a separated representation

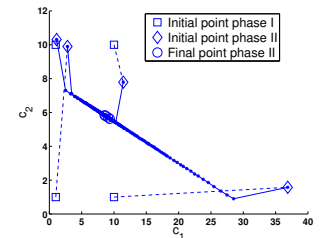
$$u(x, y) = \sum_{\mu \in \mathcal{F}} \alpha_\mu(x) P_\mu(y)$$

with coefficients  $\alpha_\mu$  and the set of compact multi-indices  $\mathcal{F}$ . If the basis  $\{P_\mu\}$  of  $\mathcal{Y}$  consists of orthogonal polynomials with respect to the joint probability measure of the data parameters  $y$ , it is called (generalized) *polynomial chaos* (gPC).

<sup>4</sup>For the model problem in  $(\Omega, \mathcal{B}, P)$ ,  $\mathcal{X} = H_0^1(D)$  and  $\mathcal{Y} = L_P^2(\Omega)$ .

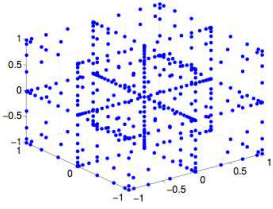


**Fig. 2:** The forward-reverse algorithm in one dimension. Blue paths are simulated forward in time, red paths are simulated backward in time. We consider all pairs that (almost) meet in the middle.

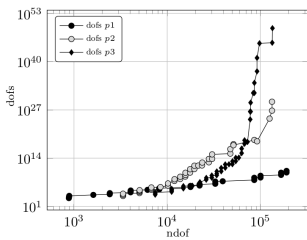


**Fig. 3:** The full algorithm for a two-dimensional example. A deterministic heuristic transformation is applied first (phase I), then we run the FREM algorithm.

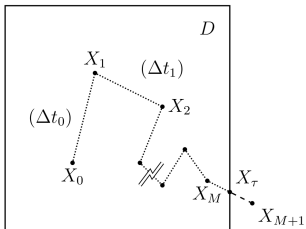




**Fig. 4:** Sparse grid illustration on a three-dimensional parameter space



**Fig. 5:** Uncompressed problem size of Galerkin polynomial chaos discretization (vertical axis) and compressed tensor degrees of freedom (horizontal axis)



**Fig. 6:** Simulation of the sample path of the stochastic process  $X_t$  in domain  $D$

A large variety of methods was developed to compute a finite-dimensional approximation of  $u$ . Since the number of random variables of the data determines the dimension of the stochastic space, the problems usually become very high dimensional, and the complexity grows exponentially with the dimension of  $y$ . Hence, the discretization of the spaces  $\mathcal{X}$  (often by finite elements) and  $\mathcal{Y}$  has to be carried out meticulously.

A popular approach is the use of some interpolation in  $\mathcal{Y}$ , which is then called *stochastic collocation* (SC). Instead of taking a full tensor set of collocation points, a common complexity reduction is achieved by the use of sparse grids as depicted in Figure 4. Thus, already dozens of dimensions become feasible, supposed that the solution exhibits sufficient mixed regularity. An *orthogonal projection* in the sense of a Galerkin method is much more involved but possible with some recent developments in model reduction approaches. Most notably, Galerkin methods immediately allow for a residual-based a posteriori error estimation, which was introduced in [4]. The proposed adaptive algorithm is provably convergent and considers physical as well as stochastic refinements in order to reliably control the overall error. A combination with modern low-rank approximations, such as hierarchical tensor formats, pushes the boundary further and allows the treatment of stochastic discretizations with *hundreds of dimensions* and  $10^{50} - 10^{100}$  (uncompressed) degrees of freedom; see [5]. Figure 5 illustrates the exponential growth of the uncompressed discretization with respect to parameter dimensions for the model problem (MP).

## Relating stochastic and random PDEs

Path sampling methods can also be used to solve random PDEs, thereby in a way combining parts of the last two sections of this review; see [3]. To fix ideas, consider again the stereotypical Darcy model (MP) with coefficient fields  $f$ ,  $g$ ,  $\kappa$  assumed to be random. In the deterministic case, it is very well understood that  $u(x)$  is obtained (as average) by following a particle  $X_t$  started at  $x \in D$  until the first time  $\tau$  that it hits the boundary. The same is true in the random case, except that now we have to condition on the random coefficients. More precisely,

$$u(x) = E \left[ g(X_\tau) + \int_0^\tau f(X_t) dt \middle| X_0 = x, f, g, \kappa \right],$$

for a trajectory  $X$  driven by an independent Brownian motion  $B$  via the *stochastic differential equation*

$$dX_t = \nabla \kappa(X_t) dt + \sqrt{2\kappa(X_t)} dB_t.$$

A schematic simulation of such a process is depicted in Figure 6.

Suppose that the actual quantity of interest is the function  $x \mapsto E[u(x)]$  on  $D$  or—more realistically—a linear map thereof. Then, we can easily avoid an expensive double simulation and apply regression (in the space variable  $x$ ) to obtain (an approximation of) the full solution  $E[u]$ . Indeed, denoting  $g(X_\tau) + \int_0^\tau f(X_t) dt$  with  $X_0 = x \in D$  by  $\Phi^x$ , we generate an i.i.d. sample  $\Phi_t^{x_i}$  from  $\Phi$  with starting value  $x_i$  sampled from the uniform distribution on  $U$ . Given a set of basis functions

$\psi_1, \dots, \psi_K$ , we then solve the least squares problem

$$\hat{\gamma} := \arg \min_{\gamma \in \mathcal{R}^K} \frac{1}{N} \sum_{i=1}^N \left( \Phi_i^{x_i} - \sum_{k=1}^K \gamma_k \psi_k(x_i) \right)^2.$$

The corresponding approximation  $\hat{u}(x) := \sum_{k=1}^K \hat{\gamma}_k \psi_k(x)$  converges to  $u$  in appropriate function spaces when  $N, K \rightarrow \infty$ .

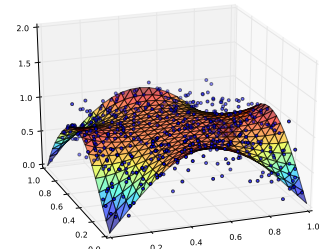
Notice that the regression (visualized in Figure 7) takes care of both the random samples from the Brownian motion and the randomness of the coefficients at the same time, i.e., there is no need for (expensive) nested simulations. We also remark that many variants and improvements of the above simple regression scheme are possible.

## Conclusion

In a way, uncertainty quantification is on the one hand a field with a rich and long tradition in the statistical sciences, on the other hand, it is a rather new discipline in the context of PDEs and numerical analysis. Without any doubt, research in this area has gained great popularity for many compelling reasons, and many new fascinating results in different directions have been discovered in recent years. It becomes apparent that the connection of stochastics, PDEs, and numerics provides a remarkable research area in which scientists of different disciplines strive to combine their perspectives, experience, and techniques in order to push the boundaries of structural understanding, analytical results, and real-world applications. Moreover, with research efforts in UQ mutually affecting related scientific areas, in particular, high-dimensional approximation and big data, machine (deep) learning, model reduction, and compressive sensing, it has great potential to stay a fascinating and practically relevant research area in applied mathematics.

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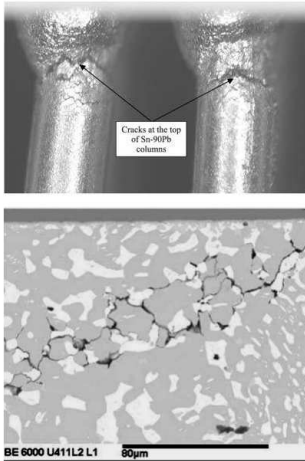
**Fig. 7:** Visualization of the regression procedure. The regression on the points gives the smooth surface solving the (random) PDE.

## 2.6 Modeling, Analysis, and Simulation of Damage Processes

Christian Heinemann and Markus Radszuweit

Fracture is a very common phenomenon that has a great impact on our daily life. Our personal safety and the functionality of devices that we permanently use depend on the structural integrity of modern materials (see Figure 1). Therefore, understanding the mechanisms of crack initiation and propagation has been an ongoing field of research for more than hundred years. While standardized stress tests have been the common tools for experimentalists, computer simulations gained increasing importance in the last decades. However, if one intends to develop and analyze mathematical models and suitable numerical methods, one has to face a number of difficulties. A variety of different approaches was designed, each having its own particular advantages and drawbacks. They all involve the key concept of fracture introduced by Griffith, namely that a crack will propagate if it is energetically more favorable to create interfaces than to resist elastic stresses. A promising concept for situations with complicated crack patterns is the phase field approach, where it is unnecessary to keep track of newly created surfaces. Within this framework, a regularized version of a sharp-interface model has been considered that introduces a damage field  $z$  with values inside the interval  $[0, 1]$ . The interval bounds represent the completely disintegrated state ( $z = 0$ ) and the intact state ( $z = 1$ ), respectively. A generic (quasi-static) model that approximates the sharp-interface fracture model was proposed in [1] and uses the free energy

$$\mathcal{F}[\mathbf{u}, z] = \int_{\Omega} \left( (\eta + g(z)) w_{\text{el}}(\mathcal{E}(\mathbf{u})) + \frac{G}{2\ell} (1 - z)^2 + \frac{G\ell}{2} |\nabla z|^2 \right) d\mathbf{x}. \quad (1)$$



**Fig. 1:** Top: broken Sn-Pb solder joints; bottom: tin- and lead-rich domains were made visible (images taken from [2])

Here,  $\Omega$  denotes the domain of the material in its initial configuration. The elastic energy density  $w_{\text{el}}$  depends on the displacement field  $\mathbf{u}$  via the linear strain  $\mathcal{E} = \mathcal{E}(\mathbf{u}) := \frac{1}{2}(\nabla \mathbf{u} + \nabla^t \mathbf{u})$ . The vector field  $\mathbf{u} = \mathbf{u}(x)$  specifies the displacements of the material points from the initial position  $x \in \Omega$  to their current position. Furthermore,  $G$  is called *fracture toughness*. The degradation function  $g$  is monotonous with  $g(0) = 0$  and  $g'(z) > 0$  for  $z \in (0, 1)$ . The free energy in (1) involves two small regularization parameters: the residual stiffness ratio  $\eta$  and the crack-interface width  $\ell$ .

However, this model is not capable to explain the behavior of many modern materials since it does not take inhomogeneity and anisotropy into account. Important examples, relevant to engineers, are grains in steels and alloys as well as inclusions in concrete. The resulting inhomogeneities of elastic properties and in thermal expansion coefficients yield local stress concentrations at sites where damage may initiate. For that reason the model should be augmented in order to take varying chemicals  $c$  and temperature distributions  $\theta$  into account. In our approach, we assume a binary mixture that can be described by a single order parameter  $c$ . A convenient choice is to define  $c = +1$  as pure “phase one” and  $c = -1$  as pure “phase two”. We intend to address the following issues in this survey:

- Deriving a thermodynamically consistent phase field model for damage processes coupled to heat conduction and the dynamics of a chemical phase field;
- Solving the resulting system of partial differential equations and inclusions;
- Implementing a numerical scheme that enables us to perform simulations of the model.

## Modeling

The total free energy depending on all functions  $\mathbf{u}$ ,  $z$ ,  $c$ , and  $\theta$  are chosen to (approximately) match the properties of binary metallic mixtures, in particular solder alloys. Evolution equations are obtained by a variational approach that requires a dissipative pseudo-potential besides the free energy. We extend the free energy from fracture mechanics given by (1) to our problem. The generic form of a free energy describing a binary mixture that can undergo spinodal decomposition is a double-well potential of the order parameter  $c$ . Since our model incorporates temperature effects, we consider the well-established Landau potential (see  $\varphi_{\text{ch}}$  below). It targets phase transition processes below a certain critical temperature  $\theta_c$ . The thermal contribution is chosen such that it yields a constant specific heat capacity  $c_V = -\theta \partial_\theta^2 \varphi_{\text{th}}$  with respect to the temperature ( $\partial_\theta$  is the partial derivative with respect to  $\theta$ ). In our model, we assume that the total free energy is

$$\begin{aligned} \mathcal{F}[\mathbf{u}, z, c, \theta] &= \int_{\Omega} f(\mathcal{E}(\mathbf{u}), z, \nabla z, c, \nabla c, \theta) \, d\mathbf{x} \\ &= \int_{\Omega} \left( \varphi_{\text{el}}(\mathcal{E}(\mathbf{u}), z, c, \theta) + \varphi_{\text{dam}}(z) + \varphi_{\text{ch}}(c, \theta) + \varphi_{\text{th}}(c, \theta) + \frac{G\ell}{2} |\nabla z|^2 + \frac{k}{2} |\nabla c|^2 \right) d\mathbf{x} \end{aligned} \quad (2)$$

with the contributions (we omit the  $x$ -dependence of all occurring functions)

$$\begin{aligned} \varphi_{\text{el}}(\mathcal{E}, z, c, \theta) &= \frac{1}{2} (\eta + g(z)) \mathcal{E}' : \mathbb{C}(c) : \mathcal{E}', \quad \varphi_{\text{dam}}(z) = \frac{G}{2\ell} (1-z)^2 + \mathcal{I}_{[0,1]}(z), \\ \varphi_{\text{ch}}(c, \theta) &= V_0 \left( \frac{1}{4} c^4 - \frac{1}{2} \frac{\theta_c - \theta}{\theta_c} c^2 \right), \quad \varphi_{\text{th}}(c, \theta) = -c_p(c) \theta \log(\theta). \end{aligned}$$

The symbol  $:$  denotes the double dot product between tensors (note that  $\mathbb{C}(c)$  is a fourth-order stiffness tensor) and  $\mathcal{I}_I(\cdot)$ , the indicator function that is zero in the interval  $I$  and infinite elsewhere. To include the effects of thermal expansion and lattice mismatch, we used the shifted linear strain

$$\mathcal{E}'(\mathbf{u}, c, \theta) = \mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)(\theta - \theta_0(c))\mathbf{1}.$$

The dynamic behavior is described by a dissipative pseudo-potential given in terms of

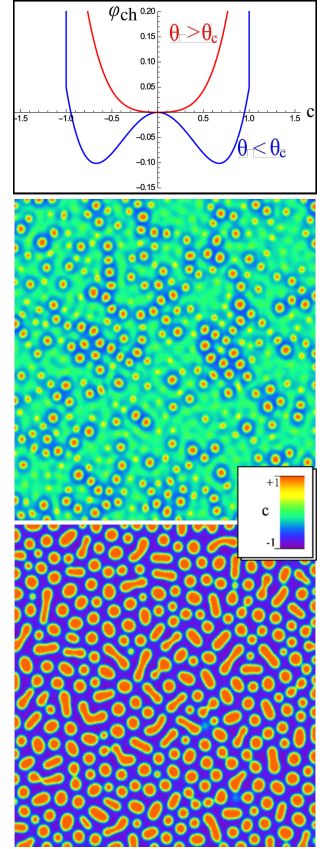
$$\mathcal{R}[\mathbf{u}_t, z_t, c_t] = \int_{\Omega} \left( \psi_{\text{el}}(\mathcal{E}(\mathbf{u}_t)) + \psi_{\text{dam}}(z_t) + \psi_{\text{ch}}(c_t) \right) d\mathbf{x}$$

with the density functions

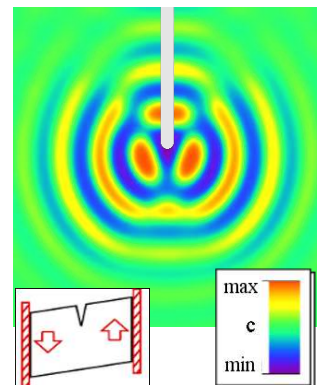
$$\psi_{\text{el}}(\mathcal{E}(\mathbf{u}_t)) = \frac{1}{2} \mathcal{E}(\mathbf{u}_t) : \mathbb{V} : \mathcal{E}(\mathbf{u}_t), \quad \psi_{\text{dam}}(z_t) = -\alpha z_t + \frac{1}{2} \beta |z_t|^2 + \mathcal{I}_{(-\infty, 0]}(z_t), \quad \psi_{\text{ch}}(c_t) = \frac{\eta_c}{2} |c_t|^2,$$

where the symbol  $\mathbf{u}_t$  denotes the time derivative of  $\mathbf{u}$  (similarly for  $z_t$  and  $c_t$ ). The dissipative damage potential  $\psi_{\text{dam}}$  indicates whether the damage propagation is rate dependent ( $\beta \neq 0$ ) or rate independent ( $\beta = 0$ ). An important feature is that we exclude “healing effects” in the material by incorporating the indicator function  $\mathcal{I}_{(-\infty, 0]}(z_t)$  in  $\psi_{\text{dam}}$  in order to force that  $z_t \leq 0$ . The rank four tensor  $\mathbb{V}$  denotes the (possibly anisotropic) viscosity tensor, and  $\eta_c$  is a regularization parameter as well. The dynamic behavior for the fields  $\mathbf{u}$  and  $z$  can be deduced by balance laws and expressed via variational derivatives (denoted by  $\delta \dots / \delta \dots$ ) as

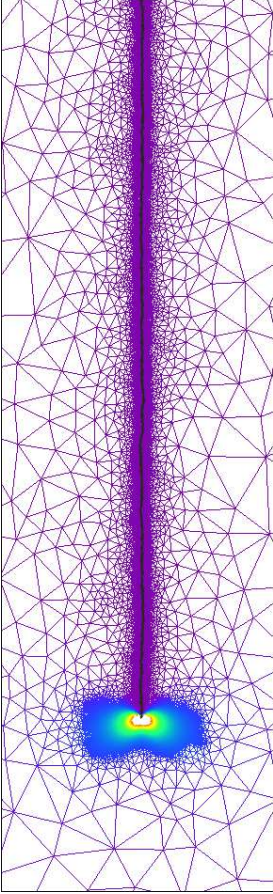
$$\frac{\delta \mathcal{F}}{\delta \mathbf{u}} + \frac{\delta \mathcal{R}}{\delta \mathbf{u}_t} = \mathbf{f}, \quad \frac{\delta \mathcal{F}}{\delta z} + \frac{\delta \mathcal{R}}{\delta z_t} \ni 0 \quad (3)$$



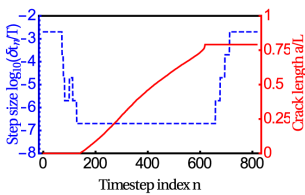
**Fig. 2:** Simulation of spinodal decomposition with double-well potential for  $\theta < \theta_c$



**Fig. 3:** Instability in the Cahn–Larché system for a shear load on a notch geometry



**Fig. 4:** Adaptive mesh color-coded by the elastic energy density around a crack (in black)



**Fig. 5:** Example of time-step adaptivity within a simulation where a crack occurs

with external forces  $\mathbf{f}$ . The first relation is referred to as the balance of forces, and the second equation is the evolution law for the damage process. These relations yield the system

$$-\nabla \cdot ((\eta + g(z))\mathcal{E}' : \mathbb{C}(c) + \nabla : \mathcal{E}(\mathbf{u}_t)) = \mathbf{f}, \quad (4)$$

$$-G\ell\Delta z + \frac{1}{2}g'(z)\mathcal{E}' : \mathbb{C}(c) : \mathcal{E}' + \frac{G}{\ell}(z - 1) + \partial\mathcal{I}_{[0,1]}(z) + \partial\mathcal{I}_{(-\infty,0]}(z_t) \ni 0, \quad (5)$$

where  $\partial\mathcal{I}_{[0,1]}(z)$  denotes the set of all subgradients of  $\mathcal{I}_{[0,1]}$  at  $z$  (analogously for  $\partial\mathcal{I}_{(-\infty,0]}(z_t)$ ). The order parameter  $c$  takes a special position since its mass is conserved and fulfills the following Cahn–Hilliard-type equation for phase separation

$$c_t = \nabla \cdot (m(c, z)\nabla\mu) \quad \text{with} \quad \mu = \frac{\delta\mathcal{F}}{\delta c} + \frac{\delta\mathcal{R}}{\delta c_t}. \quad (6)$$

The field  $\mu$  is the well-known chemical potential and  $m(\cdot, \cdot)$ , the corresponding chemical mobility. The coupling of the interface dynamics to elastic deformations that (3) yields is an extension of the Cahn–Larché system.

Finally, the equation for heat transport is deduced by using the laws of thermodynamics. By taking into account the definition of the entropy density  $s = -\partial_\theta f$  ( $f$  is the density function in (2)), the relation to the inner energy density  $e = f + \theta s$ , and the demand for the first and second law of thermodynamics, which we locally express by

$$\partial_t e + \nabla \cdot \mathbf{j}_e = 0, \quad (7)$$

$$\partial_t s + \nabla \cdot \mathbf{j}_s = \partial_t s_{\text{irr}} \geq 0, \quad (8)$$

give us the heat transport equation

$$c_p\theta_t + \nabla \cdot (\kappa(\theta)\nabla\theta) + \theta(-\partial_\theta\boldsymbol{\sigma} : \mathcal{E}(\mathbf{u}_t) - \partial_\theta v c_t - \partial_\theta\gamma z_t) = m(c, \theta)|\nabla\mu|^2 + \eta_c|c_t|^2 - \alpha z_t + \beta|z_t|^2 + \mathcal{E}(\mathbf{u}_t) : \mathbf{V} : \mathcal{E}(\mathbf{u}_t) \quad (9)$$

with the abbreviations  $\boldsymbol{\sigma} = \partial_\mathcal{E} f$ ,  $v = \partial_c f$ , and  $\gamma = \partial_z f$ .

A further assumption that we have used from near-to-equilibrium thermodynamics is *Fourier's law*, which states that  $\mathbf{j}_{\text{th}} = -\kappa(\theta)\nabla\theta$  holds for the heat flux. Because (7) and (8) are fulfilled, our system is referred to as *thermodynamically consistent*.

## Analysis

One important task in a rigorous mathematical treatment of the system (4)–(6), (9) is to prove its solvability, i.e. the existence of solutions for the unknowns  $\mathbf{u}$ ,  $z$ ,  $c$ , and  $\theta$ . This endeavor requires assumptions on the coefficient functions and certain simplifications in order to circumvent severe mathematical difficulties. In particular, under the assumption that the terms  $-\partial_\theta\boldsymbol{\sigma}$ ,  $-\partial_\theta v$ , and  $-\partial_\theta\gamma$  in (9) are close to constant values, we obtain the following heat transport equation

$$\theta_t + \nabla \cdot (\kappa(\theta)\nabla\theta) + \theta(\nabla \cdot \mathbf{u}_t + c_t + z_t) = m(c, \theta)|\nabla\mu|^2 + |c_t|^2 - z_t + |z_t|^2 + \mathcal{E}(\mathbf{u}_t) : \mathbf{V} : \mathcal{E}(\mathbf{u}_t). \quad (10)$$



Here, (physical) constants are assumed to be equal to 1, for simplicity. Under further assumptions, the damage evolution law is regarded in the simplified form as

$$z_t - \Delta_p(z) + \frac{1}{2}g'(z)(\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)) : \mathbb{C}(c) : (\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)) - \theta + \phi'_{\text{dam}}(z) + \partial\mathcal{I}_{[0,1]}(z) + \partial\mathcal{I}_{(-\infty,0]}(z_t) \ni 0, \quad (11)$$

whereas the Cahn–Hilliard system is considered as

$$c_t = \nabla \cdot (m(c, z)\nabla\mu) \quad \text{with} \quad (12)$$

$$\mu = -\Delta_p(c) + \frac{1}{2}\partial_c((\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)) : \mathbb{C}(c) : (\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c))) - \theta + \partial_c\phi_{\text{ch}}(c, \theta_{\text{fix}}) + c_t,$$

and the force balance equation is taken as in (4), incorporating the acceleration term  $\mathbf{u}_{tt}$ . The term  $\Delta_p(z)$  denotes the  $p$ -Laplacian  $\nabla \cdot (|\nabla z|^{p-2}\nabla z)$  with  $p > 3$  and serves as a mathematical regularization. The only known existence result for such a strongly coupled system has been recently established in the collaborative paper [3].

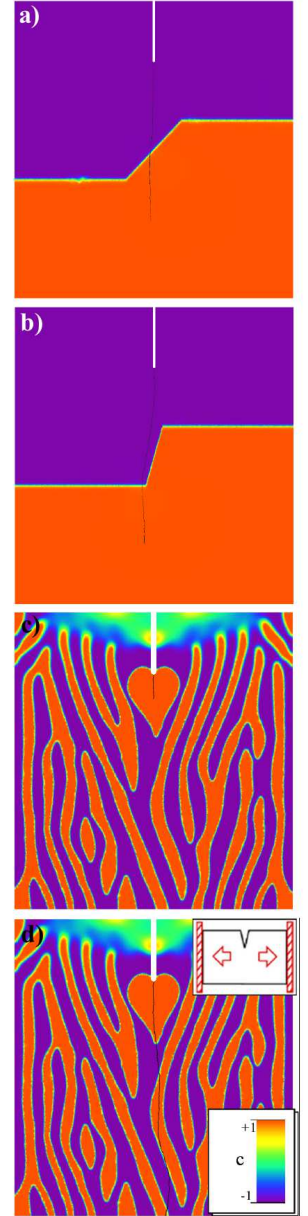
The first step to prove an existence result is to determine a suitable notion of solution. We remark that the damage law in (11) and the heat transport equation in (10) still feature plenty of mathematical challenges that require novel weak formulations. More precisely, we are faced with the following difficulties:

- Two multi-valued and unbounded operators  $\partial\mathcal{I}_{[0,1]}(z)$  and  $\partial\mathcal{I}_{(-\infty,0]}(z_t)$  in (11);
- The highly nonlinear coupling terms  $\frac{1}{2}g'(z)(\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)) : \mathbb{C}(c) : (\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c))$  in (11) and  $\frac{1}{2}\partial_c((\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)) : \mathbb{C}(c) : (\mathcal{E}(\mathbf{u}) - \alpha_{\text{th}}(c)))$  in (12);
- A right-hand side in (10) with low integrability (only  $L^1$ ).

A formulation that enables us to handle these complications simultaneously was used in [3] and originates from energetic principles for rate-dependent systems. For instance, one obtains that

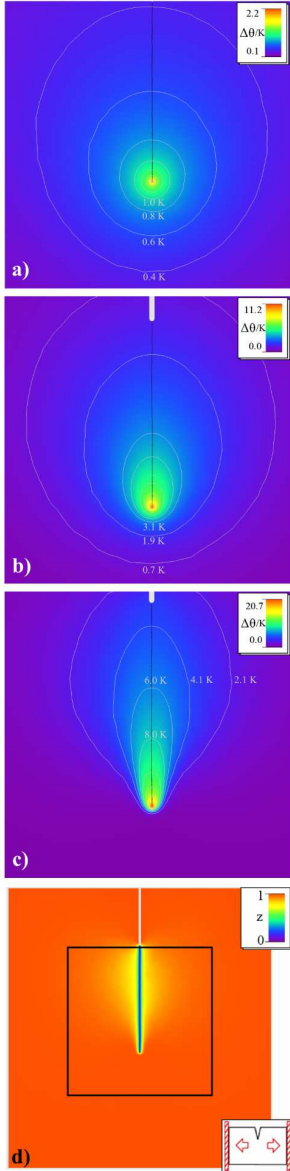
- Eq. (10) can be restated as an energy dissipation inequality together with an entropy inequality—a notion called *entropic formulation* and first used in the context of damage models in [4];
- Eq. (11) can be reformulated as an energy dissipation inequality together with a variational inequality—a notion developed in the Young Scientists' Group of WIAS and used, e.g., in [5].

Once an appropriate notion and solution space for the unknowns are fixed, one has to prove solvability. The considered proof strategy in [3] uses several nested approximation and time discretization methods that can also serve as a starting point for numerical investigations (see below). In order to set up a time discretization scheme, we regard an equidistant partition of the time interval  $[0, T]$  with nodes  $t_0, t_1, \dots, t_N$  such that  $t_0 = 0$  and  $t_N = T$ . A time discrete version of (4),(12),(10),(11) can be established with semi-implicit terms, such that the discrete energy dissipation inequality is fulfilled. Moreover, the subdifferentials  $\partial\mathcal{I}_{[0,1]}(z) + \partial\mathcal{I}_{(-\infty,0]}(z_t)$  in the damage law in (11) translate to a purely obstacle-type subdifferential  $\partial\mathcal{I}_{[0,z^{n-1}]}(z^n)$  in the time discrete setting. Existence of solutions of the resulting discrete system can be achieved by modern results from monotone operator inclusions.



**Fig. 6:** Influence of material interfaces on the crack morphology: In a) and b), an artificial static interface is given. c) and d) show snapshots for different times with interface dynamics. The degree of interaction is determined by the elastic moduli and the inclination angle of the crack.





**Fig. 7:** Temperature field in the region near the advancing crack tip. While the damage dissipation is left constant, the heat conductivity is decreased from a) to c). d) shows the corresponding damage phase field.

In further steps, a priori estimates of the time discrete solutions that are independent of the time-step size  $T/N$  were established. To this end, sophisticated estimation techniques, such as Boccardo–Gallouet-type and enhanced regularity estimates for elliptic operators, are applied. The a priori estimates provide a suitable control of the discrete solutions in order to pass to the limit in the time-step size where one finally obtains solutions of the desired time-continuous system.

## Simulations

Phase field models for fracture are particularly well suited for complex crack patterns. The system of PDEs given by (3), (6), and (10) is highly nonlinear and nonconvex. Furthermore, the presence of inequality constraints expressed by the subdifferentials renders the dynamics nonsmooth. In the following, we interpolate certain material properties  $p(c)$ , such as material stiffness or diffusion mobility between the pure material phases, by the formula

$$p(c) = \frac{1}{2}((1+c)p_{+1} + (1-c)p_{-1}). \quad (13)$$

To avoid unphysical values, the range of the order parameter  $c$  has to be limited. Therefore, we add an indicator function to the chemical free-energy density:  $\varphi_{\text{ch}}(c) \rightarrow \varphi_{\text{ch}}(c) + \mathcal{I}_{[-1,1]}(c)$ .

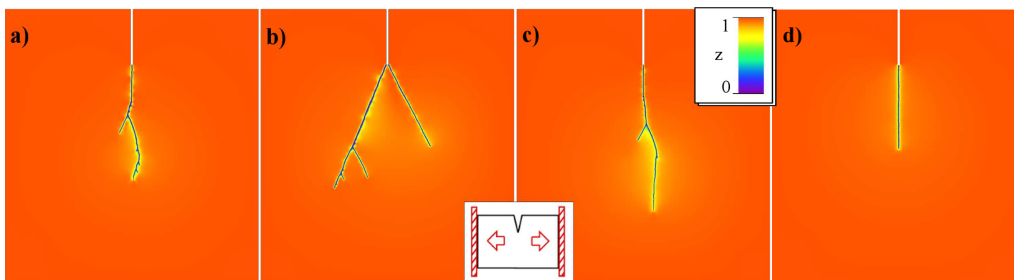
We implemented a finite element software that allows us to compute discrete solutions to the fully coupled set of equations presented in the previous section. Due to the numerical complexity, the computations are limited to two spatial dimensions. Within this scope, we are able to observe thermally-induced cracking, crack deflection at material interfaces, and heat generation at the advancing crack tip.

**Adaptivity.** The evolution of fracture is a truly multiscale phenomenon, both in space and time. The initiation of cracks on the micro-level is a complicated process, which involves, among other mechanisms, crystal plasticity and grain boundaries. The growth of these micro-cracks takes place on a much larger timescale than macro-cracks. They appear when micro-cracks nucleate to a certain critical level, and their growth rate may immediately rise up to the speed of sound of a specimen. Therefore, material models for brittle fracture separate these timescales and assume a quasi-static and rate-independent evolution as in [1]. In order to avoid difficulties in this approach, related to non-uniqueness (required by the implementation of, for instance, back-tracking schemes), we rather focus on a rate-dependent evolution and use an adaptive discretization.

We dynamically generate triangular meshes that are strongly refined only in the relevant regions: at the cracks themselves, regions of critical stress, and at the interfaces (see Figure 4). The time step is refined according to an energy balance check. As it can be seen in Figure 5 the time step is changed over several orders of magnitude while the crack propagates.

**Numerical experiments.** Examples of numerical experiments are presented in the following. Figure 6 shows the effect of inhomogeneities in material stiffness on the morphology of an advancing crack. In a) and b), an artificial static domain boundary with a different inclination angle with respect to a notch is given. Cracks are repelled by the stiff phase (here shown in orange), but the inclination angle also determines whether they will cross the interface barrier. Simulation results

that include coupling effects to the chemical interface dynamics are shown in c) and d) of Figure 6. In Figure 7, the heat distribution of an advancing crack is presented for different heat conductivities. The temperature rise at the tip depends on the ratio of dissipative heat generation and heat transport away from that region. Results for the fully coupled model can be seen in Figure 8. The mismatch of thermal expansion of the two phases during cooling, while the specimen is mechanically fixed at the boundaries, generates internal stresses. The regime of partial damage that we interpret as the presence of micro-cracks precedes a rapid growth of model-resolved macro-cracks. Our code is capable of simulating anisotropic linear elastic constitutive laws. Figure 9 displays the effect of different classes of two-dimensional symmetries on the crack path under mode-I load in a homogeneous material. While branching is suppressed by the stretch-compression anisotropy in a quasi-static setting, it can be regained by the extension to anisotropic constitutive laws. However, when chemical interface dynamics is considered, an extension of our model by an orientational dynamics for the crystal lattice becomes necessary. This issue is beyond the current scope and motivates future investigations.

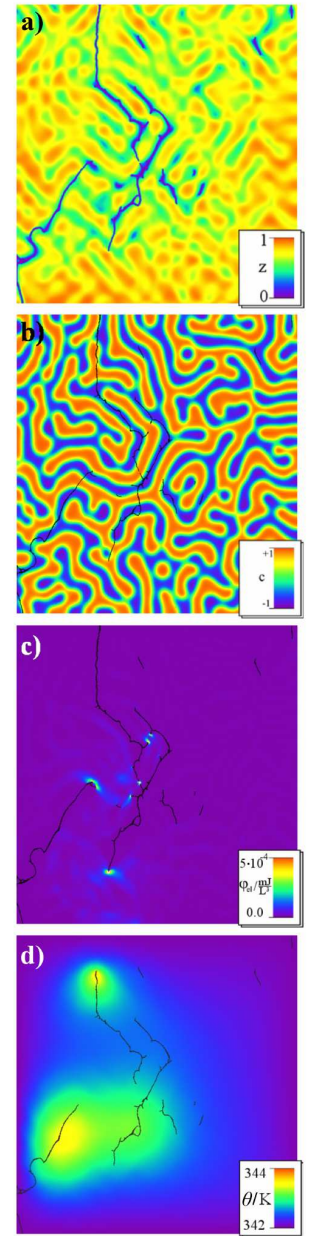


**Fig. 9:** Effect of different symmetries on the crack morphology: a) and b) show different orthotropic materials. In c), the material has square symmetry, and in d), the completely isotropic case is included for comparison.

## Conclusions and outlook

In this article, we presented a thermodynamically consistent phase field model for damage that is coupled to an evolution of spinodal decomposition and heat transport. A brief description of how to prove solvability of the resulting system was given. The concept of entropic formulation—the use of an entropy and an energy-dissipation inequality—plays a key role in the proof. Results from various numerical simulations were shown, providing insight into diverse phenomena like crack deflection at interfaces, heat dissipation at the crack tip, and failure due to mismatch of the thermal expansion coefficients. Furthermore, we identified elastic anisotropy as a mechanism for crack branching.

The cross-couplings of the different material properties and the high nonlinearity make this model mathematically hard to handle, but they are necessary to model failure in real-life materials like alloys, for instance. Additional modifications are required to achieve this goal: A constitutive law that includes ductility, an order parameter for the crystal-lattice orientation, and weaker adhesion at the domain interfaces are reasonable extensions. However, these are challenging to incorporate, both analytically and numerically. As a near-term advancement of our model, we consider an anisotropic damage-interface energy.

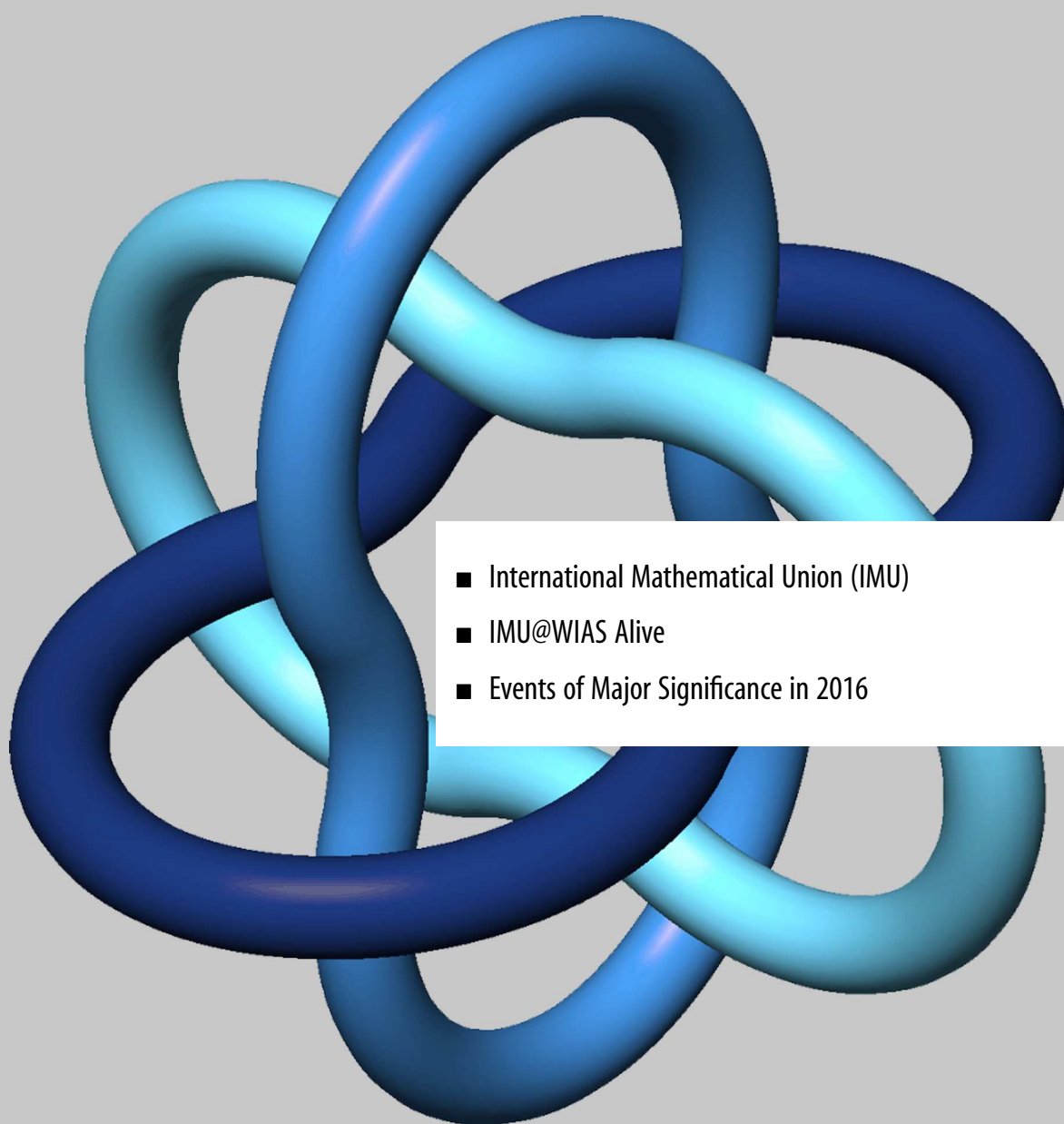


**Fig. 8:** Thermally-induced crack nucleation: The specimen is held at a certain temperature, such that phase separation takes place. Then it is cooled down rapidly, while the displacements at the boundaries are fixed.

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# 3 IMU@WIAS



- International Mathematical Union (IMU)
- IMU@WIAS Alive
- Events of Major Significance in 2016

### 3.1 International Mathematical Union (IMU)

*Sylvia Markwardt*

After moving around the world depending on where the IMU Secretary in office had his home institution, the Secretariat of the International Mathematical Union (IMU) has been permanently based in Berlin, Germany, at the Weierstrass Institute since January 2011. 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) as well as mainly technical assistance for the Committee on Electronic Information and Communication (CEIC) and the Committee for Women in Mathematics (CWM). The IMU Secretariat also hosts the IMU Archive.

A Memorandum of Understanding and a Cooperation Agreement provide the legal basis of the relationship of IMU and WIAS.



**Fig. 1:** The team

Staff members (Figure 1):

Alexander Mielke, *Head of the Secretariat and IMU Treasurer*. A. Mielke is a professor at Humboldt-Universität zu Berlin, Deputy Director of WIAS and head of Research Group 1 at WIAS. In his function as the head of the secretariat he is responsible for the IMU Secretariat as a separate unit within WIAS. He was appointed as IMU Treasurer by the IMU Executive Committee and 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, which is done in close cooperation with the IMU Secretary. She communicates with the IMU member countries, drafts written materials, writes minutes and reports, and supervises the IMU Web site. Her tasks include the steering and control of the secretariat's business operations and IMU finances, and monitoring the 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.

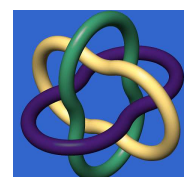
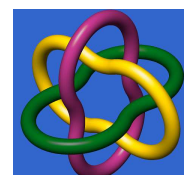
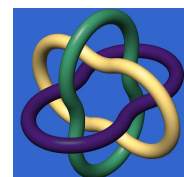
Birgit Seeliger, *IMU Archivist*. B. Seeliger is responsible for the IMU Archive and in charge of developing a strategy for preserving and making accessible paper documents, photos, pictures, and IMU artifacts and supporting IMU's decision process concerning the electronic archiving of IMU's steadily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

Ramona Keuchel, *Project Assistant*. R. Keuchel's task is to support the administrative work of the IMU Secretariat, in particular, to assist in the organization and wrap-up of the International Congress of Mathematicians in 2018 and the initialization of new CDC programs. (She is not in the Secretariat's group photo.)

Helge Holden (he is not in the group photo) is the IMU Secretary. He holds a professorship at the Norwegian University of Science and Technology, Trondheim, and at the Center of Mathematics for Applications, University of Oslo, Norway. Helge Holden is in contact with the IMU Secretariat regularly via electronic communication and visits the office about once a month.

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





### 3.2 IMU@WIAS Alive

At the end of this year, the IMU Secretariat will have been hosted for six years by the Weierstrass Institute. Six years full of activity, exciting events, new business, ...

Up to 2010, the legal domicile of the Union had been moving around the world depending on where the IMU Secretary in office had his home institution. The General Assembly (GA) 2010 decided to install a permanent secretariat and that the Weierstrass Institute in Berlin is the host institution of this permanent secretariat.

To have its headquarters (and legal domicile) permanently based at one place was a completely new situation.

Five people working together in one place on IMU administration was a novelty. Almost all office people were unexperienced with respect to IMU business. Everyone had to orient himself or herself and grasp his/her responsibilities. The bottom line is that this was a quick and very successful process to which WIAS made a major contribution. Support was received in terms of IT infrastructure, finance, legal advice, any other business, and, not least, the generous grant awarded by the German Federal Ministry of Education and Research (BMBF) and the State of Berlin.

The IMU Secretariat was represented at the WIAS executive meetings, thus regular exchange between the Secretariat and WIAS was secured. Periodical team meetings of the Secretariat staff effected internal exchange.



**Fig. 2:** Welcome to the IMU Secretariat

Over the years, the volume of the work to be done in the office has increased substantially. In order to cope with the work load, four student assistants were temporarily hired; recently, a project assistant reinforced the team.

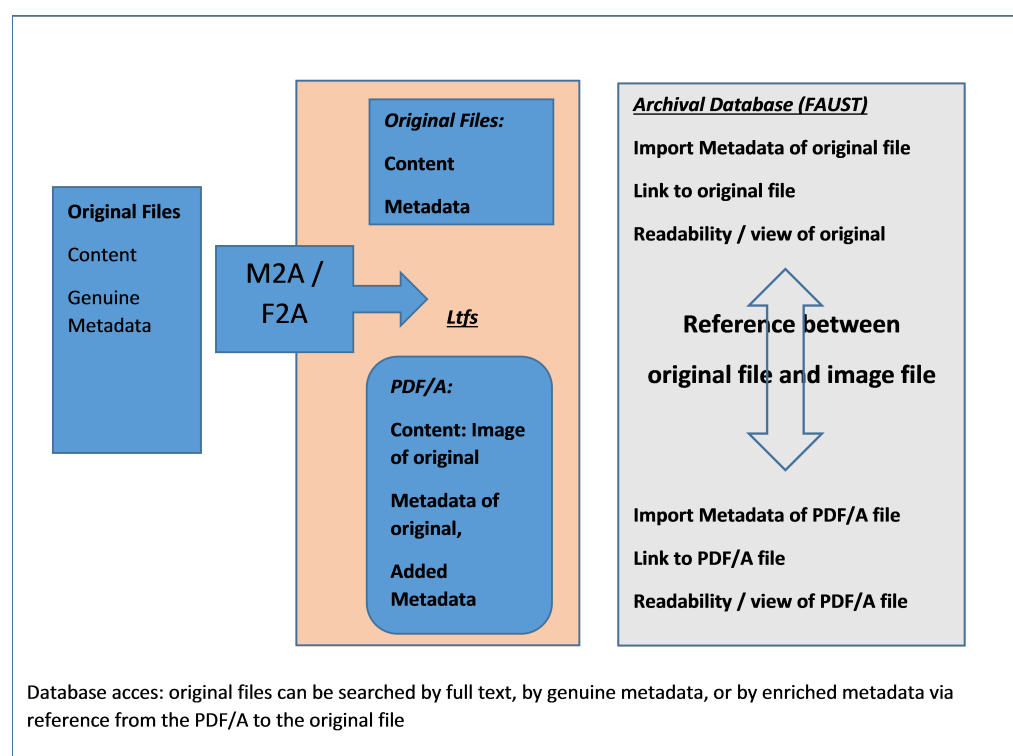
To list all the tasks, activities, responsibilities individually would go beyond the scope of this chapter. The Secretariat is very proud that it is well accepted and its work is appreciated. The Office Committee, which was appointed to evaluate the IMU Secretariat, reported to the IMU General

Assembly 2014: “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.” The GA 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.”

A landmark in the process of establishing the permanent secretariat was the setup of the IMU Archive. A particular archive room has been provided and professionally equipped in order to receive the archival material stored so far at the University of Helsinki. The Archive inauguration was attended by Olli Lehto (Finland), former IMU Secretary who had made outstanding contributions to the IMU chronicles.

A major challenge of these days is the archiving of electronic documents and data management. The IMU Archivist and the WIAS IT closely cooperate and interact on these issues, creative solutions and developments are being implemented, to the advantage both of IMU and WIAS. It should be mentioned that the IMU server is hosted by WIAS, and the IMU benefits from its infrastructure.



**Fig. 3:** This is a glimpse of how archival work and data storage function. For details contact the IMU Archivist Birgit Seeliger or the IMU Technician Gerhard Telschow

The Secretariat supports IMU's commissions and committees:

- IMU Executive Committee (EC)
- International Commission on Mathematical Instruction (ICMI)
- Commission for Developing Countries (CDC)
- Commission on the History of Mathematics (ICHM)
- Committee on Electronic Information and Communication (CEIC)
- Committee for Women in Mathematics (CWM)

This includes, among other things,

- Assistance with the implementation of decisions
- Administration of membership issues
- Administration and support of meetings, conferences, special events
- Handling of grant programs
- Developing and maintaining of Web pages, online application forms
- Instruction and support to committees who maintain their Web pages on their own
- Social media activities

A number of annual meetings of IMU committees and commissions were held in the office. The director of WIAS regularly joined these meetings, he welcomed the participants and had personal conversations with them.

Other meetings took place, for instance, individual members of the committees and commissions visited the Secretariat in order to discuss particular issues. The curators of the IMU Archive and the ICMI Archive typically paid visits to the office. Individual visitors being linked to IMU in some way or other or being generally interested in IMU dropped by. Sometimes, individual visitors at WIAS or groups of workshop participants showed interest in the work of the IMU Secretariat and stopped by for a short guided tour. Altogether, more than 30 IMU events were hosted, more than 25 individual visits were paid.

**ICMI and CDC since the inception of the IMU Secretariat at WIAS in 2011.** Having been asked if and how ICMI and CDC have benefited from the IMU Secretariat at WIAS, two officers have a clear answer. It is thanks to WIAS's support to the IMU Secretariat that these IMU commissions have been able to work without any difficulties, foster and even extend their range of activities. They could use the technical infrastructure and manpower of the IMU Secretariat and, thus, they profited, on a very high level, from the resources provided by WIAS. WIAS guarantees that everything is running smoothly and the IMU office members can focus on their tasks for the international mathematical community.

Bill Barton (New Zealand), active supporter of ICMI for many years and the 2010–2012 ICMI President, well knows the “before and after”. B. Barton spoke very enthusiastically about the new setup. He found it essential for ICMI to have, thanks to the Secretariat, an administrator who takes care of all the administrative details and plays an active role in many ICMI activities. The IMU Secretariat has become sort of a center and a constant for the commission, “... and all this was achieved at no extra cost on the ICMI budget.”



**Fig. 4:** Impressions from the ICMI General Assembly and ICME-13. Photos: ICMI/Thomas Panzau

Barton said that “expectations were more than fulfilled . . . If we did not have the Secretariat I do not think that we would have been able to be so outward looking, and hence, contributing significantly to mathematics education development worldwide.”

Ragni Piene (Norway) has long experience in service for the IMU and CDC. She was a member of the IMU Executive Committee 2003–2010 and a member of CDC 2011–2014. She could observe how CDC took advantage from the permanent office at WIAS.

R. Piene said: “Since the CDC activities have expanded over the past years, due to an increased budget, the existence of administrative support has become even more essential.” And she confirmed as follows: “As an example, the Abel Visiting Scholar Program, though a small program consisting in travel and subsistence funds for one month each for three early career mathematicians (per year) from developing countries, would not be feasible without the support from the IMU office. Indeed, once the selection committee has made its choice, the office takes over, including all necessary communication with the grantees, the reimbursements, help with tickets and other issues when necessary, and, not least, the reporting and the maintenance of the program’s Web pages. Similar procedures apply to the other grant programs. Thus, the existence of the office makes it possible for even relatively small donations to the CDC/IMU to have quite some impact.”

### 3.3 Events of Major Significance in 2016

#### Grants

**IMU was granted the IMU-Simons African Fellowship Program.** IMU's application to the Simons Foundation for support for mathematicians from Africa was successful. The Simons Foundation approved funding for a program under which grants are awarded to African mathematicians to be used for collaborative research. The amount of \$50,000 per year will be paid for a five-year period to the IMU. The Simons Foundation, based in New York City and founded in 1994, seeks to advance mathematics and the basic sciences. The IMU-Simons African Fellowship Program is administered by IMU's Commission for Developing Countries. All administrative duties for this program are coordinated and managed by the IMU Secretariat, more information can be found at <http://www.mathunion.org/cdc/grants/imu-simons-african-fellowship-program/>.

#### Meetings



**CDC meeting.** The newly appointed Secretary for Policy of the Commission for Developing Countries, O. Gil Medrano, met CDC President W. Ogana and IMU Secretary H. Holden in the IMU Secretariat in Berlin on January 14–15, 2016. O. Gil was introduced to her office responsibilities and made acquainted with the staff and the fields of action of the Secretariat.

**ICMI Executive Committee meeting.** The Executive Committee of the International Commission on Mathematical Instruction met in the IMU Secretariat in Berlin from July 22–23, 2016.



#### Events

**IMU President and IMU Secretary met new WIAS Director.** IMU President S. Mori and IMU Secretary H. Holden came to Berlin on January 13, 2016, in order to meet the new Director of WIAS M. Hintermüller in the IMU Secretariat. The WIAS and IMU leaders presented their institutions and discussed topics of mutual interest such as joint activities of WIAS and IMU, long-term perspectives, and continued hosting of the IMU Secretariat at WIAS (Figure 5).

**Visit of the Leibniz Association President M. Kleiner at the IMU Secretariat.** On February 18, 2016, the Leibniz Association President visited WIAS and used this opportunity to go to see the premises of the IMU Secretariat in order to learn about the activities and services provided there for the international scientific community (Figure 5).



**Fig. 5:** Left: Meeting of WIAS and IMU leaders. Right: Leibniz Association President Matthias Kleiner visiting the IMU Secretariat

**Random selection for the IMU Nominating Committee 2018.** The Nominating Committee is one of the most important IMU committees, its task is to present slates of nominations to the IMU Adhering Organizations prior to a meeting of the IMU General Assembly. According to the rules for appointing the Nominating Committee, three members of the committee have to be chosen at random from nominations submitted by the Adhering Organizations. On September 8, 2016, a random draw, arranged like a lottery, took place in the Secretariat. The event was videotaped and can be watched at [http://www.mathunion.org/fileadmin/IMU/Publications/CircularLetters/2015-2016/Nominating\\_committee\\_IMU.mp4](http://www.mathunion.org/fileadmin/IMU/Publications/CircularLetters/2015-2016/Nominating_committee_IMU.mp4) (Figure 6).

**Heidelberg Laureate Forum.** The fourth Heidelberg Laureate Forum (HLF) took place from September 18–23, 2016, 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 IMU, who is a partner of the HLF, nominated two members of the HLF Scientific Committee. Among the participating laureates at the HLF 2016 who had been awardees of the Fields Medal (FM) or the Nevanlinna Prize (NP) were: Sir Michael Francis Atiyah (FM), Gerd Faltings (FM), Heisuke Hironaka (FM), Shigefumi Mori (FM), Ngô Bảo Châu (FM), Robert Endre Tarjan (NP), Vladimir Voevodsky (FM), and Sir Andrew Wiles, who has been recipient of a Silver Plaque of the IMU.

#### Participation of IMU Secretariat members in international events.

- IMU Executive Committee meeting, Kyoto, Japan (S. Markwardt, A. Mielke)
- ICMI meeting, Rehovot, Israel (L. Koch)
- 7th European Congress of Mathematicians (7ECM), Berlin, Germany (R. Keuchel, S. Markwardt, A. Mielke, B. Seeliger, G. Telschow)
- ICMI General Assembly, Hamburg, Germany (R. Keuchel, L. Koch, S. Markwardt)
- International Congress on Mathematical Education (ICME-13), Hamburg, Germany (R. Keuchel, L. Koch, S. Markwardt, A. Orlowsky, B. Seeliger, G. Telschow)
- Heidelberg Laureate Forum, Heidelberg, Germany (S. Markwardt)



**Fig. 6:** Three members of the IMU Nominating Committee 2018 were drawn at random



### List of guests at the IMU Secretariat

Date	Guests	Event
Jan 14 – 15	Olga Gil Medrano, Spain; Wandera Ogana, Kenya	CDC meeting
Jan 15	Björn Engquist, Sweden/USA; Aline Bonami, France; Martin Bridson, UK; Gerhard Huisken, Germany; Elon Lindenstrauss, Israel/USA; Stefan Müller, Germany; Stefan Nemirovski, Russia; Rahul Pandharipande, Switzerland; János Pintz, Hungary; Idun Reiten, Norway; Tomáš Roubíček, Czech Republic	EMS Prize Committee
Feb 18	Matthias Kleiner, Germany; Caroline A. Lodemann, Germany	Individual visit
Feb 24	John Ball, UK	Individual visit
Feb 25 – Mar 3	Bernard Hodgson, Canada	ICMI Archive
July 19	Bill Barton, New Zealand; Shreemayee Bora, India; Sunsook Noh, Republic of Korea; Marie-Françoise Ouedraogo, Burkina Faso; Marie-Françoise Roy, France; Caroline Series, UK; John Toland, UK; Karen Vogtmann, USA	CWM
July 19	Beatrice Pelloni, UK; Marie-Françoise Roy, France; Caroline Series, UK; Elisabetta Strickland, Italy	EMS Comm. for Women in Mathematics
July 22–23	Abraham Arcavi, Israel; Ferdinando Arzarello, Italy; Yuriko Yamamoto Baldin, Brazil; Bill Barton, New Zealand; Alicia Dickenstein, Argentina; Jean-Luc Dorier, Switzerland; Zahra Gooya, Iran; Helge Holden, Norway; Roger Howe, USA; Shigefumi Mori, Japan; Cheryl E. Praeger, Australia; Angel Ruiz, Costa Rica; Catherine P. Vistro-Yu, Philippines	ICMI EC
Sep 8	M. Grötschel, Germany; C. Ohst, Germany	IMU Nominating Committee
Oct 4	Jill Adler, South Africa	ICMI
Oct 19 – 20	Abraham Arcavi, Israel	ICMI
Nov 30	Birgit Rehse, Germany; Irina Schwab, Germany; Kristina Starkloff, Germany	Berlin Scientific Archives working group

# 4 Research Groups' Essentials

- RG 1 *Partial Differential Equations*
- RG 2 *Laser Dynamics*
- RG 3 *Numerical Mathematics and Scientific Computing*
- RG 4 *Nonlinear Optimization and Inverse Problems*
- RG 5 *Interacting Random Systems*
- RG 6 *Stochastic Algorithms and Nonparametric Statistics*
- RG 7 *Thermodyn. Modeling and Analysis of Phase Transitions*
- RG 8 *Nonsmooth Variational Problems and Operator Equations*
- YSG *Modeling of Damage Processes*
- ERC 1 *EPSILON*
- ERC 2 *EntroPhase*

## 4.1 Research Group 1 “Partial Differential Equations”

The mathematical focus of this research group is the analytical understanding of partial differential equations and their usage for the 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 Hamiltonian systems, gradient flows, or consistently 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

The qualitative study of partial differential equations provides a deeper understanding of the underlying processes and is decisive for the construction of efficient numerical algorithms. In cooperation with other research groups, corresponding software tools are under development that will enable parameter studies or the optimization of technological devices.

### Semiconductors

The mathematical modeling of semiconductor devices is one of the central topics in RG 1, which is supported by researchers in the following projects with third-party funding. The investigations on “Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters” are done jointly with RG 2 *Laser Dynamics* and the Zuse Institute Berlin and are embedded as subproject B4 in the physical Collaborative Research Center 787 *Semiconductor Nanophotonics: Materials, Models, Devices*. We refer to the related Scientific Highlights article “New Approaches to Numerical Simulation of Current Flow in Semiconductor Devices” on page 20.

The topics “Mathematical modeling, analysis, and optimization of strained germanium microbridges” and “Electrothermal modeling of large-area organic light-emitting diodes” are run as MATHEON subprojects D-OT1 and D-SE2, respectively, and are funded by the Einstein Center for Mathematics Berlin (ECMath). The first one is a joint project with the Humboldt-Universität zu Berlin, while the second one is a close cooperation with the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP, TU Dresden).

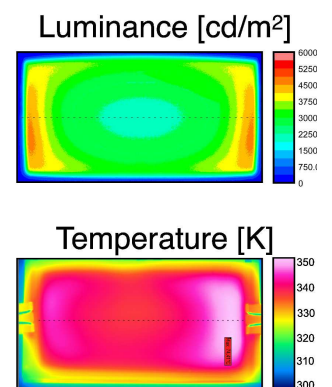
**Variational modeling of open quantum systems.** Open quantum systems appear in many areas of applications such as quantum information theory and quantum optoelectronics. The relevant quantum system is not isolated, but it interacts with an environment and can exchange information and energy, which is crucial for the functionality of quantum-dot lasers or single-photon emitters.

Typically, such a quantum dynamics is modeled through a Lindblad equation of the form  $\dot{\rho} = \frac{i}{\hbar} [\rho, H] + \mathcal{L}(\rho)$ , where the dissipative part  $\mathcal{L}(\rho)$  models the interaction with the environment and has the special structure of complete positivity. In the recent work [4], it was shown that all finite-dimensional Lindblad generators  $\mathcal{L}$  that satisfy a suitable detailed-balance condition with respect to the thermal equilibrium state can be written as a gradient system with respect to the relative entropy. This work, which was done in the ERC project “Analysis of Multiscale Systems Driven by Functionals” (AnaMultiScale), generalizes gradient structures from classical probability theory to the non-commutative setting for density matrices providing a quantum analog to the well-known Wasserstein gradient structure for Fokker–Planck equations and, thus, opens the door to a thermodynamically consistent coupling of quantum systems to macroscopic systems such as spin drift-diffusion models for spintronics or the Maxwell-Bloch system in nonlinear optics.

**Electrothermal modeling of large-area OLEDs.** The MATHEON subproject D-SE2 continues the successful cooperation with the IAPP (TU Dresden) on novel organic lighting concepts. Organic semiconductor devices show a strong temperature dependence, which in connection with self-heating leads to unpleasant spatial inhomogeneities in the luminance of large-area lighting panels, see Figure 1. To understand the origin of these inhomogeneities, we modeled the current and heat flow and the resulting self-heating on a phenomenological level. The model consists of a system of partial differential equations (PDE) of thermistor type for the electrostatic potential and the temperature. One of the main features of the system is that the equation for the current flow is of  $p(x)$ -Laplace type, where the variable exponent  $p(x)$  takes the non-Ohmic behavior of the several organic layers into account. The temperature dependence of the electrical conductivity, arising from the temperature-activated hopping transport of charge carriers in organic materials, is modeled by an Arrhenius law.

First analytic results concerning existence and properties of solutions to the  $p(x)$ -Laplace thermistor system were extended successfully using different approaches: In [1], a constructive method based on a regularization method and Galerkin approximation is established. This technique works in arbitrary spatial dimensions and for general, possibly discontinuous, and measurable exponents  $p(x)$  satisfying  $1 < \text{ess inf}_x p(x) \leq \text{ess sup}_x p(x) < \infty$ . In this setting, the temperature is an entropy solution to the corresponding heat equation with Robin boundary conditions. Moreover, in two spatial dimensions, more regular solutions can be obtained for certain geometric configurations with piecewise constant  $p(x) \geq 2$ . Higher integrability of the gradient of the electrostatic potential was obtained, which ensures that the Joule heating in the energy equation is good enough to allow for higher regularity of the temperature.

**Semiconductor device optimization.** Studies of semiconductor device optimization via optimal control methods have been the subject of a number of previous works; see, e.g., Hinze & Pinnau (2002). In recent years, there has been an increase in research on optoelectronic devices, e.g., aimed at on-chip integration of lasers in order to increase communication bandwidths for computing and telecommunication applications. Recently, it has been demonstrated that germanium can be used as an optically active medium; however, advanced engineering techniques such as high doping or application of large mechanical strain are necessary to improve optical properties of laser cavities. In [5], a new model of an edge-emitting laser based on strained germanium microstrips was investigated using analysis, numerics, and optimization. The optimal control of the

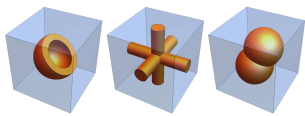


**Fig. 1:** Inhomogeneous luminance and temperature distributions in large-area lighting panel measured by IAPP

carrier transport in the optoelectronic device with respect to the doping profile was done by a cost functional that is based on the modal net gain. Then, a numerical discretization is established, for which optimized solutions for different regularizations and with vanishing weights were studied. This general topic is joint work with the Materials Research Department of the Leibniz-Institut für innovative Mikroelektronik (IHP) in Frankfurt/Oder.

### Modeling of materials

This area deals with the mathematical modeling and the analysis of solids and fluids and includes chemical reactions, diffusion and phase separation processes, phase transformations, plasticity, damage, and delamination as well as processes in biological tissues. The research is carried out jointly with the ERC Group 2 *Entropy Formulation of Evolutionary Phase Transitions*, the Young Scientists' Group *Modeling of Damage Processes*, and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*.



**Fig. 2:** Possible periodic microstructures in a unit cell

**Corrector estimates for PDEs in periodic media.** Nonlinear reaction-diffusion systems that combine different diffusion length scales with cross-coupling effects were studied in the subproject “Pattern formation in systems with multiple scales” within the Collaborative Research Center SFB 910 *Control of Self-Organizing Nonlinear Systems*. The equations of interest were posed in heterogeneous domains with periodic microstructures such as perforations or inclusions; see Figure 2. Based on previous results for linear elliptic equations, it was possible to give quantitative estimates for the modeling error when replacing the microscopic reaction-diffusion system by the corresponding homogenized system. We refer to the Scientific Highlights article “Effective Modeling of Multiscale Phenomena” on page 35 for further details.

**Analysis of improved Nernst–Planck–Poisson systems.** In collaboration with the WIAS research groups RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* and RG 3 *Numerical Mathematics and Scientific Computing*, a breakthrough result was achieved concerning the analysis of an improved Nernst–Planck–Poisson (NPP) system for the ion transport through liquid electrolytes. NPP models were developed at WIAS over the last five years and have applications ranging from energy technology to life science. In such contexts, the NPP system is coupled to the Navier–Stokes equations for the barycentric velocity of the mixture and for the pressure. The analytical investigations were conducted in close collaboration with the modeling team of RG 7. In [2], new a priori estimates were developed that allow us to deal with the NPP–Navier–Stokes system in the compressible, isothermal regime, thus proving the existence of global-in-time weak solutions for the full problem. The result also includes the analytical treatment of bulk and surface chemical reactions with generalized constitutive equations for the reaction rates.

**Applications of regularity results in mathematical biology.** The so-called *Keller–Segel model*, established in the early 1970s, is one fundamental model to describe the interaction of cells with their environment and has attracted much attention from the scientific community. The full system consists of four strongly coupled, nonlinear parabolic equations, the well-posedness of which could not be proved up to now. Using deep abstract results on quasilinear parabolic equations of Herbert Amann (Zürich) in combination with recently obtained elliptic and parabolic regularity results, it could be proved that the full Keller–Segel model is well-posed even on every two-dimensional Lipschitz domain and also on fairly general three-dimensional domains. Moreover, in

a cooperation with Hannes Meinlschmidt (Darmstadt) and Dirk Horstmann (Köln), it was shown that the full Keller–Segel model possesses a unique local-in-time solution.

### Abstract methods for PDEs

**Entropy transport problems.** The deep connection between optimal transport problems and scalar diffusion problems has been under intensive research in the last decades. One of the essential connecting factors is the interpretation of the Kantorovich–Wasserstein distance in a Riemannian sense, i.e., it is induced by a symmetric and positive semidefinite differential operator, also called *Onsager operator*, whose inverse is an infinite-dimensional version of a Riemannian tensor. Starting from this important observation, we introduced generalizations of the Onsager operator that can be associated with certain PDEs of reaction-diffusion type via gradient flow formulations. In particular, the energy-drift-diffusion systems used in the modeling of charge and energy flow in semiconductor devices were shown to have this beneficial structure.

However, a central question is related to the analytic and geometric properties of the distance that is induced by the Onsager operator that defines the gradient structure. In [6], several useful characterizations of such a distance were established for the case of a scalar reaction-diffusion equation that model the spreading and growth of biological tissue. It is called *Hellinger–Kantorovich distance* and is defined on the space of all finite nonnegative measures. The most interesting characterization gives rise to so-called *entropy transport problems* that consist of a classical transport part describing the effective cost of moving some mass, and an entropy part penalizing the deviation of the initial and final transported mass distributions from the initial and the final given mass distributions. A recently started collaboration with RG 6 *Stochastic Algorithms and Nonparametric Statistics* considers applications of the entropy transport method in biomedicine, such as automated tumor detection via magnetic resonance imaging (MRI) data.

**Advances in parabolic regularity theory.** Based on the progress concerning elliptic and parabolic equations in recent years, it is now possible to attack new applications involving strong nonlinearities on complex geometries for heterostructures. Within the long-term cooperation with A.F.M. (Tom) ter Elst (Auckland), the classical isomorphism

$$\frac{\partial}{\partial t} + A(\cdot) : W_0^{1,p}((0, T); V^*) \cap L^p((0, T); V) \rightarrow L^p((0, T); V^*), \quad (1)$$

which is due to J.-L. Lions for  $p = 2$ , was extended to other integrability exponents  $p \neq 2$  and to constellations, where  $V$  and  $V^*$  are replaced by spaces that are “close” to  $V, V^*$  within a suitable interpolation scale. In consequence, this result implies the solvability of *quasilinear non-autonomous* parabolic equations even if the data of the problem are highly nonsmooth; see [3].

### Further highlights of 2016

**ERC Workshop “Modeling Materials and Fluids using Variational Methods”.** As the last major event of the two ERC projects *AnaMultiScale* (within RG 1) and *EntroPhase* (ERC 2), this one-week workshop took place from February 22 to 26 and gathered about 40 mostly international scientists working in variational analysis of materials and fluids with heterogeneous and multiscale structures.



**Joint Annual Meeting of Gesellschaft für Angewandte Mathematik und Mechanik (GAMM) and Deutsche Mathematiker-Vereinigung (DMV) (TU Braunschweig, March 7–11).** Karoline Disser and Caroline Kreisbeck (Regensburg) jointly organized the Young Researcher's Minisymposium "Multiscale Evolutionary Problems".

**ESI Program "Nonlinear Flows".** From May to July, the Erwin Schrödinger International Institute for Mathematics and Physics (ESI, Vienna) hosted this special program, which was organized by Eduard Feireisl (Prague), Ansgar Jüngel (Freiburg), Alexander Mielke (RG 1), Giuseppe Savaré (Pavia), and Ulisse Stefanelli (Vienna), and which included the two workshops "Entropy Methods, Dissipative Systems, and Applications" (June 13–17) and "Variational and Hamiltonian Structures: Models and Methods" (July 11–15).

**ECMI 2016: 19th European Conference on Mathematics for Industry (Santiago de Compostela, June 13–17).** Nella Rotundo and Dirk Peschka co-organized the minisymposium "Charge Transport in Semiconductors: Emerging and Established Mathematical Topics".

**Ph.D. thesis "Analysis for Dissipative Maxwell–Bloch-Type Models".** Florian Eichenauer (advisor: Alexander Mielke) successfully defended his thesis at the Humboldt-Universität zu Berlin on June 30.

**7ECM: 7th European Congress of Mathematics (TU Berlin, July 18–22).** The following researchers of our group contributed to the success of ECM: Alexander Mielke was a member of the Local Organizing and the Scientific Program Committees, Pierre-Etienne Druet organized the minisymposium (MS) "Analysis of Thermodynamically Consistent Models of Electrolytes in the Context of Battery Research", Nella Rotundo and Dirk Peschka co-organized the MS "Mathematical Methods for Semiconductors", and Marita Thomas co-organized the MS "Nonsmooth PDEs in the Modeling Damage, Delamination, and Fracture".

**"Zwischen Flüssigkristallen und Informationstheorie" (Between liquid crystals and information theory).** That was the title of a summer course for Berlin grammar school pupils that was co-organized by Markus Mittnenzweig.



**Fig. 3:** Vietnamese students with the organizers (center right)

**'Winter School on  $\Gamma$ -Convergence and Homogenization in Continuum Mechanics.** Marita Thomas, Chiara Zanini (Torino), Tran Thanh Tuan (Hanoi), and Pham Chi Vinh (Hanoi) organized this school, which took place at the Vietnam Institute of Advanced Study in Mathematics (Hanoi), October 31 to November 4.

**Research internship.** The French master student Paul Helly, Ecole Polytechnique Paris, was supervised by Sina Reichelt. He studied structure-preserving numerical algorithms for the one-dimensional Cahn–Hilliard equations.

**8th Workshop “Optimal Transport and Applications” (De Giorgi Center, Pisa, November 7–11).** The workshop was organized by Luigi Ambrosio (Pisa), Giuseppe Buttazzo (Pisa), Alexander Mielke, and Giuseppe Savaré (Pavia).

**German Equality Symposium.** Among 100 leading officers and junior managers from industry and science, Marita Thomas took part in this event on equal opportunities in the society, which was organized and headed by the Federal Chancellor Dr. Angela Merkel.

**Berlin Dresden Prague Würzburg Workshops.** This series is organized by Martin Kružík (Prague), Alexander Mielke, Stefan Neukamm (Dresden), and Anja Schlömerkemper (Würzburg) and is devoted to the mathematical analysis in materials science. Two one-day workshops took place at TU Dresden: “Homogenization and Related Topics” (June 22) and “Mathematics of Continuum Mechanics” (December 5).

**Honorary Medal of the Czech Mathematical Society.** Konrad Gröger, a honorary member of RG 1, was celebrated with a special colloquium on April 13, 2016, on the occasion of his 80th birthday. During this ceremony, he was awarded the *Honorary Medal of the Czech Mathematical Society* by his lifelong contribution to the cooperation between Czech and German mathematicians.



**Fig. 4:** Prof. Dr. Konrad Gröger (center) was awarded the Honorary Medal of the Czech Mathematical Society by Prof. Jiří Rákosník (left) and Prof. Pavel Krejčí (right)



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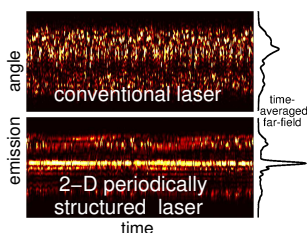
## 4.2 Research Group 2 "Laser Dynamics"

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 2016 within the Research Center MATHEON (subproject D-OT2 "Turbulence and extreme events in nonlinear optics"), the DFG Collaborative Research Center (SFB) 787, subprojects B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters" (jointly with research group RG 1 *Partial Differential Equations* and Zuse Institute Berlin (ZIB)), and B5 "Effective models, simulation and analysis of the dynamics in quantum-dot devices", the DFG individual grant "Ab-initio description of optical nonlinearities in femtosecond filaments", as well as the DFG Collaborative Research Center SFB 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*, subproject A3 "Activity patterns in delay-coupled systems" (jointly with S. Yanchuk, TU-Berlin). Furthermore, RG 2 established close collaboration with the industry in the framework of the BMBF funding measure "Efficient high-performance laser beam sources" (EffiLAS), as a subcontractor of the Ferdinand Braun Institute for High Frequency Technology (FBH) in the projects HotLas (Effiziente und brillante Breitstreifendiodenlaser mit hohen Leistungen für den Betrieb bei hohen Umgebungstemperaturen) and PLUS (Puls-Laser und Scanner für LiDAR-Anwendungen: Automotive, Consumer, Robotic), as a partner (together with the companies Monocrom from Spain, Femtika from Lithuania, and Raab-Photonic GmbH from Germany) in the EU framework EUROSTARS project E!10524 "High power composites of edge emitting semiconductor lasers" (HIP-Lasers), as well as in direct industry collaboration with the TRUMPF Laser GmbH.

### Dynamics of semiconductor lasers

The research in this field was focused on dynamical effects in various types of lasers, a selection of which will be described below, as well as on single-photon sources. A particular highlight was the Workshop "Nonlinear Dynamics in Semiconductor Lasers", organized by RG 2 in May 2016.



**Fig. 1:** Simulated evolution and time averages of the far-fields in conventional and periodically structured BA lasers, demonstrating narrowing of emission

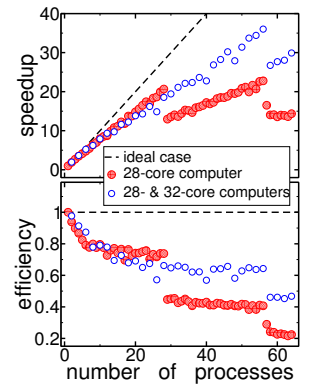
**High-power broad-area (BA) semiconductor lasers** are compact, efficient, and reliable light sources playing a crucial role in modern laser technologies. However, the emission characteristics of typical BA lasers are spoiled by many undesired effects. Thus, mathematical modeling, theoretical analysis, simulation, and optimization of devices or creation of novel laser design concepts are highly demanded in modern applications and became a focus of RG 2, see, e.g., Figure 1. In this context, RG 2 became a partner in the BMBF funding measure EffiLAS (projects HotLas and PLUS), the EUROSTARS project HIP-Lasers, and established a direct collaboration and a contract with the TRUMPF Laser GmbH. BA lasers and the related WIAS software *BALaser* of RG 2 play a central role in all these projects. *BALaser* uses parallel numerical algorithms for the integration of the

underlying nonlinear partial differential equations in time and two lateral spatial dimensions and is executed on multicore computers at WIAS. The exploitation of multicore computers allows a substantial speedup of the calculations, see Figure 2, which is desired due to the large size of the problems and the long CPU time required. The incorporation of new physical effects, needed by project partners, into the underlying mathematical model makes *BALaser* subject to permanent extensions and modifications. These modifications concern the inclusion of heating and carrier transport effects in the vertical direction (HotLas project), the modeling of nonlinear two-photon absorption effects in high-power BA lasers under strong pulsed operation (PLUS project), or the incorporation of models for specially designed photonic-crystal-type filters, as well as novel feedback and beam-combining schemes for arrays of individual lasers (EUROSTARS HIP-Lasers project). The modeling, implementation, and simulation of residual optical feedback and quasi-static heating effects were supported by contracting with the TRUMPF Laser GmbH.

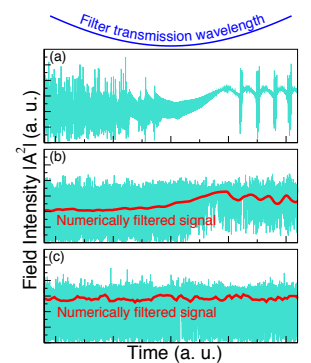
**Mode-locked semiconductor lasers** are compact and efficient sources of short optical pulses and high-quality optical frequency combs. Hybrid mode-locking is commonly applied to suppress pulse timing jitter in these lasers. However, recent experiments demonstrated that alternatively coherent optical injection can be more efficient to improve the output characteristics of passively mode-locked (PML) lasers, which was proven also from the theoretical side using the delay-differential equation (DDE) semiconductor laser model [1]. Within the framework of subproject B5 of SFB 787, analytical estimates of the locking range were obtained on the base of asymptotic techniques, and the dependence of the locking regions on model parameters was revealed. These results allow, in particular, the optimization of the output radiation of monolithic PML semiconductor lasers.

**Frequency swept lasers** operating in a Fourier domain mode-locking (FDML) regime are efficient sources of light used in optical coherence tomography. Within the framework of SFB 787, a mathematical model of FDML frequency swept lasers was developed that takes into account the chromatic dispersion of a long fiber delay line incorporated into the laser. This model is based on a set of DDEs with a distributed delay term. It was successfully applied to investigate the emergence of modulation instability leading to turbulent behavior that is observed experimentally in FDML lasers operating in the anomalous dispersion regime. The research group demonstrated numerically that their new DDE model exhibits a rich spectrum of dynamical behaviors (see Figure 3), which were in agreement with measurements, and obtained an analytical criterion for the modulation instability in the long delay time limit. Apart from FDML lasers, the proposed approach can be applied to study the effect of chromatic dispersion on the dynamical characteristics of mode-locked and other types of multimode lasers.

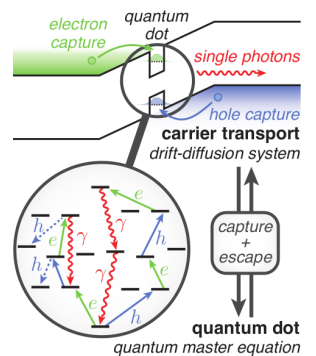
**Single-photon sources** (SPSs) based on single semiconductor quantum dots (QDs) are key components for many applications in secure data transmission (quantum communication networks) and for optical quantum computing. A mathematical model for the description of electrically driven SPSs constitutes a quantum-classical coupling problem: It requires the self-consistent embedding of an open quantum system (describing the microscopic QD physics using quantum master equations in Lindblad form) into a spatially resolved carrier transport model; see Figure 4. Such a *hybrid model* was developed in a joint effort with the research group RG 1 “Partial Differential Equations”. Moreover, SPSs are typically operated under extreme conditions (ultra-low temperatures),



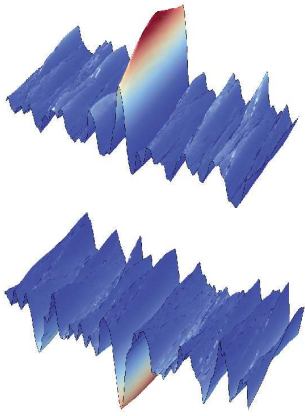
**Fig. 2:** Speedup and efficiency of multi-process simulations of a test problem on multicore computers



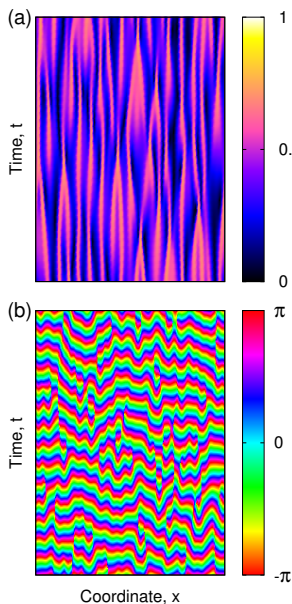
**Fig. 3:** Simulated output intensity of a FDML laser. Normal (a) and anomalous dispersion case, (b) and (c).



**Fig. 4:** Simulation scheme for single-photon sources



**Fig. 5:** Oceanic rogue wave (top) and rogue hole (bottom) obtained in the limit of a linear interference model [4]



**Fig. 6:** Amplitude and phase of a turbulent solution in a system of coupled oscillators

which lead to strong degeneration effects in the electron-hole plasma and impose exceptional challenges to the implementation of robust numerical algorithms; see the Scientific Highlights article on page 20. In a collaboration within SFB 787, the numerical simulations have already yielded significant contributions towards the enhancement of particular devices developed at the Technische Universität Berlin [2].

### Pulses in nonlinear optical media

RG 2 has a strong focus on the mathematical modeling and analysis of nonlinear wave equations that describe the propagation of ultrashort pulses with large spectral bandwidth. Within this frame, in the MATHEON subproject D-OT2, an adiabatic perturbation theory for solitons was recently developed, which enables an analytic description of all-optical switching processes in nonlinear optical fibers. For details we refer to the Scientific Highlights article on page 25.

In particular, the nonlinear Schrödinger equation (NLSE) is a well-studied integrable equation for pulse propagation, which is of fundamental importance for fiber telecommunications. It belongs to an infinite hierarchy of integrable equations, the solutions of which can be constructed in analytical form by means of the inverse scattering transform; see [3]. Analytical solutions of the higher-order equations can be classified as classical solitons, breathers, and rogue waves, being of fundamental importance for the study of rogue wave formation in systems governed by pulse propagation equations, which are significantly more complex than the NLSE.

The research on extreme nonlinear optics was focused on rogue wave formation and extreme wave statistics. Interestingly, rogue waves in optical systems bear close analogies to oceanic rogue waves, but unlike their optical counterparts, oceanic rogue waves seem to be explicable in the limit of a linear interference model [4]; see Figure 5.

### Theory of dynamical systems

The research in the field of dynamical systems is aiming to provide the mathematical background for the applied research on semiconductor lasers and optical fibers. This includes research on DDEs and on high-dimensional dynamical phenomena in large coupled oscillator systems. DDEs are an important class of models for optoelectronic systems, where the delay typically arises from the propagation of optical signals at finite speed inside a cavity. It can give rise to a wealth of dynamical phenomena, in particular, related to the formation and control of localized structures.

In the field of large coupled systems, the research on the emergence of collective dynamics was successfully continued. An outstanding result was the discovery of turbulent states (see Figure 6) in the Ott–Antonsen equation for the continuum limit of a one-dimensional array of oscillators with nonlocal coupling [5]. It was shown that the phase lag parameter in the interaction function can induce a Benjamin–Feir-type instability of the partially coherent plane waves. The emerging collective chaos appears as an intermediate stage between complete incoherence and stable partially coherent plane waves and is organized in a codimension-two bifurcation.

Destabilization mechanisms of localized solutions induced in spatially extended systems by delayed feedback were investigated by means of numerical simulations and asymptotic analysis [6]. Using a model of a wide-aperture laser with a saturable absorber and delayed optical feedback, the



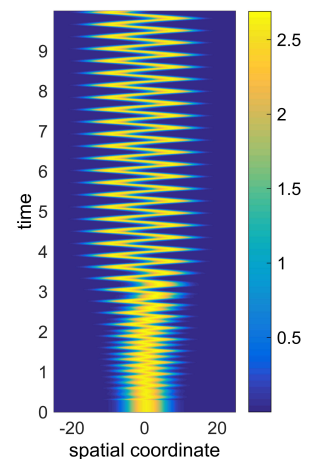
research group demonstrated that at sufficiently large delay times this system can exhibit metastability leading to a coexistence of multiple stable laser cavity solitons. In addition to the drift and phase instabilities, cavity solitons demonstrate a delay-induced modulational instability associated with the translational neutral mode. The combination of drift and modulational instabilities can produce a zigzagging motion, see Figure 7, which is either periodic, with the period close to the delay time, or chaotic, with low-frequency fluctuations in the direction of the soliton motion. The delay-induced modulational instability of localized solutions is generic and can arise in various spatially extended models of nonlinear optics including the well-known cubic-quintic complex Ginzburg–Landau equation.

The effect of delayed optical feedback on the spatiotemporal dynamics of the Lugiato–Lefever model was analyzed. By performing a linear stability analysis of the spatially homogeneous solution, the influence of the feedback rate and phase on the Turing, Andronov–Hopf, and traveling-wave instability regions was investigated. A clustering behavior of cavity solitons as a function of the feedback rate was revealed. It was shown that at certain parameters the feedback can induce a drift bifurcation of a stationary cavity soliton as well as an Andronov–Hopf bifurcation of a drifting soliton. Above a certain threshold in the feedback rate, the system enters a region of spatiotemporal chaos.

A further highlight was the WIAS Workshop “Dynamics of Delay Equations, Theory and Applications” organized together with Jan Sieber (Exeter) and Serhiy Yanchuk (TU Berlin) giving a broad range of recent results on delay equations and their applications in various fields of science, including neuroscience, optoelectronics, as well as biological or mechanical systems.

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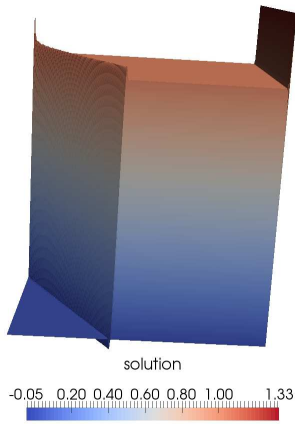
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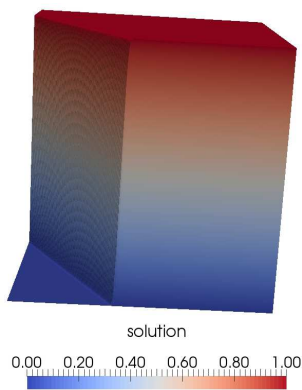
**Fig. 7:** Zigzagging solitons appearing above the drift and modulational instability thresholds



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



**Fig. 1:** Typical numerical solution obtained with the SUPG method. There are non-negligible spurious oscillations in a vicinity of the interior and the boundary layer (the analytical solution possesses values in  $[0, 1]$ )



**Fig. 2:** Numerical solution obtained with an algebraic stabilization

RG 3 studies the development of numerical methods, their numerical analysis, and it works on implementing software for the numerical solution of partial differential equations and differential-algebraic systems. Many of the research topics were inspired by problems from applications. A selection of research topics of the group will briefly be described below. Further topics include semiconductor device simulation (in collaboration with RG 1 *Partial Differential Equations* and RG 2 *Laser Dynamics*), the simulation of gas turbines (in collaboration with RG 6 *Stochastic Algorithms and Nonparametric Statistics*), of problems from hemodynamics, of population balance systems (in collaboration with RG 5 *Interacting Random Systems*), the development of algorithms for mesh generation, reduced-order modeling, and the simulation and control of two-phase flows modeling ladle stirring (in collaboration with RG 4 *Nonlinear Optimization and Inverse Problems*).

#### Analysis of algebraic stabilizations for convection-diffusion equations

In the practically relevant case of dominant convection, a stabilization is required for the discretization of convection-diffusion equations. Classical approaches, like the streamline upwind Petrov–Galerkin (SUPG) method, augment the Galerkin finite element discretization with additional terms. The convergence analysis of such methods is well understood, often even for higher-order finite elements. However, the computed numerical solutions usually show non-negligible spurious oscillations in a vicinity of layers; see Figure 1. This feature prevents the use of classical schemes in many applications. In competitive studies of stabilized finite element methods, it was found that algebraic stabilizations performed well in many aspects. In particular, solutions with physically correct values were computed and only a moderate smearing of layers was observed; compare Figure 2.

The construction of algebraic stabilizations starts with the algebraic system of equations obtained with the Galerkin finite element method

$$\mathbb{A}U = G, \quad \mathbb{A} \in \mathbb{R}^{N \times N}. \quad (1)$$

Then, a matrix  $\mathbb{D}$  is defined by

$$d_{ij} = d_{ji} = -\max\{a_{ij}, 0, a_{ji}\}, \quad i \neq j, \quad d_{ii} = -\sum_{i \neq j} d_{ij},$$

such that (1) can be written in the form

$$(\mathbb{A} + \mathbb{D})U = G + \mathbb{D}U.$$

The new term on the right-hand side can be decomposed in so-called *fluxes*

$$(\mathbb{D}U)_i = \sum_{j \neq i} f_{ij} = \sum_{j \neq i} d_{ij} (u_j - u_i).$$

Now, the ansatz for an algebraic stabilization is

$$((\mathbb{A} + \mathbb{D})U)_i = G_i + \sum_j \beta_{ij} f_{ij}, \quad i = 1, \dots, M, \quad (2)$$

with the limiters  $\beta_{ij} \in [0, 1]$ ,  $\beta_{ij} = \beta_{ji}$ , where  $M$  is the number of non-Dirichlet values. The limiters should be close to 1 in smooth regions of the solution, thus leading to the original discretization, and they should be chosen such that there are no spurious oscillations at layers. Consequently, the limiters depend on the solution, and (2) is a nonlinear discretization.

A numerical analysis of algebraic stabilizations for convection-diffusion equations was started in [1], and then the first fundamental results were presented in [2]. In this paper, it was proved that (2) with the popular Zalesak limiter has a solution and that the linearized problems occurring in a fixed-point iteration possess a unique solution. In addition, the satisfaction of the discrete maximum principle on Delaunay meshes was proved. The most important contribution of [2] is the presentation of the first finite element convergence analysis for an algebraic stabilization. For continuous piecewise linear finite elements, an error estimate was derived. Surprisingly, the error bound provides in the convection-dominated regime only the order of error reduction of 0.5 and in the diffusion-dominated regime no convergence at all. Numerical studies showed that this bound is sharp within the assumptions of the analysis. Using the Zalesak limiter, the optimal order of convergence as it is reported in the literature, e.g., second order for the error in  $L^2(\Omega)$ , could be seen only on special grids.

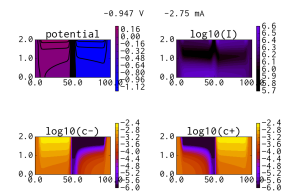
Altogether, [2] presents the first approach for performing a finite element error analysis of algebraic stabilizations. Some drawbacks of currently used algebraic stabilizations became apparent from the analytical and numerical results. Improving these methods is a scientific goal in the future.

### Charge, transport, and reactions in electrochemical systems and semiconductors

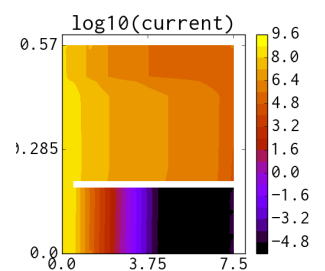
Continuum-level models of electrochemical systems and semiconductor devices include the drift of charged particles (ions, electrons, holes) in the electric field, the diffusion due to gradients of the chemical potential together with terms describing heterogeneous or homogeneous reactions. The densities of the charged particles influence the electric field via the Poisson equation for the electrostatic potential. In cooperation with RG 1 *Partial Differential Equations*, RG 2 *Laser Dynamics*, and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, the investigations of novel numerical methods based on the Scharfetter–Gummel upwind finite volume method taking into account finite particle volumes, solvation effects, and the contribution of the solvent (in the case of electrolytic systems [6], Figure 3) and different variants and approximations of Fermi statistics (in the case of semiconductors [5]), respectively, were continued.

Together with RG 1 and RG 2, considerable effort was devoted to the development of a prototype of the semiconductor device simulation tool box *DDFERMI* based on the *PDELIB* toolbox for the solution of partial differential equations; see Figure 4.

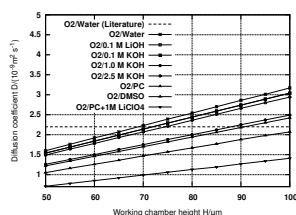
Contributing to the WIAS subproject of the interdisciplinary research network “Perspectives for Rechargeable Magnesium–Air Batteries” funded by the German Ministry of Education and Research



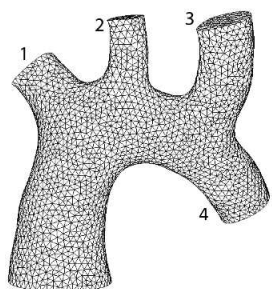
**Fig. 3:** Electrolytic diode in reverse bias



**Fig. 4:** Current density in a single photon source

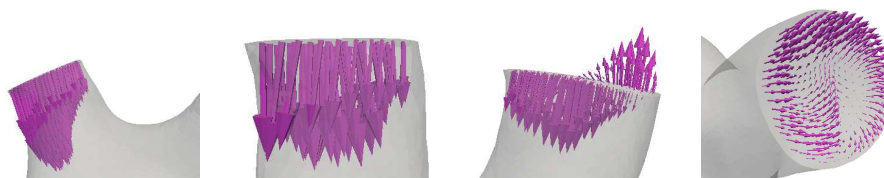


**Fig. 5:** Oxygen diffusion coefficients in different solvents, depending on the height of the working chamber of the flow cell



**Fig. 6:** A computational mesh of the ascending aorta, with four open boundaries

**Fig. 7:** Stabilized simulation of blood flow in the ascending aorta: snapshots of the velocity profile at the different open boundaries



as a part of the research initiative “Energiespeicher”, novel, efficient pressure-robust methods for the numerical solution of the incompressible Navier–Stokes equations were combined with up-wind finite volume methods in order to simulate organic electrolyte flow and solute transport in a thin-layer flow cell to perform differential electrochemical mass spectroscopy. Comparing measured and simulated values, an inverse modeling strategy allowed to obtain realistic values for oxygen diffusion coefficients in organic electrolytes [7]; see also Figure 5.

### Modeling and simulation of physiological flows

Numerical simulations of physiological flows provide a better understanding of medical data, characterize pathological conditions, and estimate non-invasively quantities that are difficult to access (such as three-dimensional fields and blood vessel properties). In this field, the research at the Weierstrass Institute focuses on different aspects of modeling and simulations, aiming at improving the robustness of computational methods and their accuracy with respect to available data.

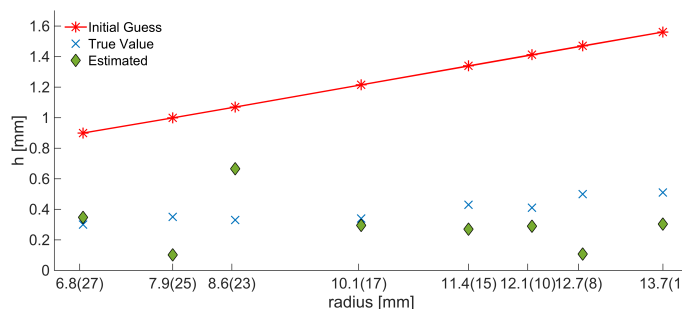
A first topic concerns the prescription of conditions at *open boundaries*, i.e., the boundaries where the velocity is not prescribed. The need to set proper open boundary conditions becomes very relevant when the computational domain is obtained by truncating the geometry in order to focus on a region of interest (see, e.g., Figure 6), in particular, when full three-dimensional data are not available (as in the case of blood flow modeling).

It is well known that numerical simulations with natural conditions (an approximation of the fluid stress tensor) suffer from unphysical instabilities in the presence of *backflow*, i.e., when the flow re-enters the domain from an open boundary. In [3], a new method for addressing backflow instabilities was developed. This method, which is based on penalizing the residual of a linearized problem on the open boundary, was shown to be able to handle large backflow regimes in blood flow (Figure 7) and airflow simulations, outperforming recent methods. Moreover, a workshop within the 7th European Congress of Mathematics (ECM, held in Berlin, July 18–22, 2016) was organized on this topic, and a collaborative benchmark article gathering several experts in the field is in preparation.

A second research topic focuses on the importance of model parameterization in clinical contexts. To this purpose, so-called *data assimilation* methods aim at optimizing the model parameters starting from a set of available measurements on the real system.

Among different available methods, in [4] the performance of the reduced-order unscented Kalman filter was assessed in the context of one-dimensional blood flow models. In particular, starting from experimental flow and pressure measurements available for an *in vitro* model of the human

arterial network (Figure 9), the potential of the filter in terms of efficiency and accuracy was investigated, aiming at the estimation, among others, of mechanical properties of the aorta (Figure 8).

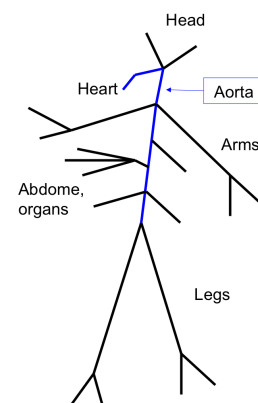


**Fig. 8:** Results of the estimation of aorta thickness (eight parameters) using eight experimental flow measurements. The graphs compare initial guesses of the parameters (red stars), estimated values (green diamonds), and target (reference) values (blue crosses).

The result highlights the difficulties of using real data for the solution of inverse problem, as well as providing useful information on the potential of identifiability analysis.

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**Fig. 9:** For the data assimilation study, a one-dimensional model made of 37 segments was considered. The segments modeling the aorta are depicted in blue.

## 4.4 Research Group 4 “Nonlinear Optimization and Inverse Problems”

Research Group 4 investigates optimization and inverse problems occurring in current engineering and economic applications. A specific focus of research in optimization and optimal control is the investigation of special structures resulting from the presence of uncertain and nonsmooth data. Research in inverse problems is centered around the reconstruction of geometries and surfaces with complex or stochastic components from the scattering of acoustic, electromagnetic, or elastic waves. Together with RG 3 *Numerical Mathematics and Scientific Computing* and RG 6 *Stochastic Algorithms and Nonparametric Statistics*, we investigate direct and inverse problems for partial differential equations (PDEs) with uncertain coefficients.



**Fig. 1:** Group picture during MIMESIS kick-off meeting, June 2016

This year's work was marked by three international events co-organized by our group and hosted at WIAS. In May, we organized the joint WIAS-PGMO Workshop “Nonsmooth and Stochastic Optimization with Applications to Energy Management”, co-financed by the Fondation Mathématique Jacques Hadamard.

In June, the second kick-off meeting of the Marie Skłodowska-Curie EID Project “MIMESIS” took place at WIAS, after finishing the recruitment phase with hiring eight students from France, India, Iran, Italy, and Spain. Last but not least, in September we organized a very successful summer school on “Uncertainty Quantification” in collaboration with the GAMM Activity Group on Uncertainty Quantification, TU München, and TU Berlin with 50 participants from 11 countries, which was fully booked already four weeks after its announcement.

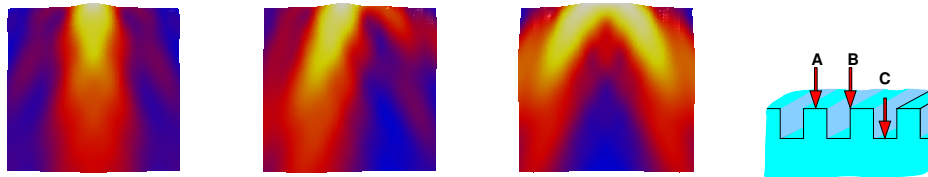
In the following, selected scientific achievements of RG 4 in 2016 are detailed.

### Inverse problems

For the difficult analysis of inverse scattering problems many new results were obtained. In the case of acoustic scattering from a bounded penetrable obstacle imbedded in an isotropic homogeneous medium, it was shown that an obstacle with a circular conic point or with an edge point has always a non-trivial scattered far field [4]. Looking at the singularity behavior of solutions, local and global uniqueness results for the inverse problem of recovering the shape of a penetrable scatterer from a single incoming wave could be established. Further results [1] were derived for the cloaking of nearly elastic obstacles, using the concept of scattering coefficients.

Another research topic in scattering was to apply field-tracing methods for diffraction gratings and to study the mathematical properties of Fourier series based methods for the simulation of such optical devices. The electromagnetic simulation of the scattering of general time-harmonic electromagnetic fields by periodic structures is based on the approximation of the incidence field by plane waves, the numerical solution of the corresponding diffraction problems, and the superposition of the plane wave solutions obtained. A new adaptive algorithm was developed and implemented in 2014–15 that allows the computation of diffracted fields up to a prescribed accuracy.

The realization is based on an integral method solver for conical diffraction and an adaptive cubature method for two-dimensional integrals. To enhance the efficiency of the algorithm, an alternative adaptive approach and different modifications were implemented and tested. In particular, the diffraction of extremely focused beams is important for scatterometric applications; see Figure 2.



**Fig. 2:** Diffraction pattern of a lamellar grating illuminated by an extremely focused Gaussian beam. Focus center A, B, and C (A is the left figure).

Most of the Fourier series based methods for the simulation of diffraction gratings were developed in the engineering community, but a mathematical foundation is still lacking. In cooperation with Lifeng Li (Beijing), special discretization matrices were studied, appearing in rigorous coupled-wave analysis (RCWA) formulations of transverse magnetic (TM) diffraction with materials of negative refraction index. The matrices are closely connected to so-called *finite section matrices* of sums of Toeplitz and Hankel operators with piecewise continuous symbols. With the study of the invertibility of those operators, a first step was taken towards the theoretical foundation of the RCWA and other Fourier methods.

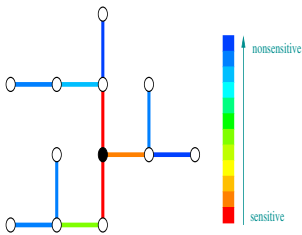
In the Central Innovation Programme (ZIM) of the Federal Ministry of Economics and Technology for small and medium-sized enterprises, RG 4 has a project with cooperation partners from the Leibniz-Institut für innovative Mikroelektronik (IHP Frankfurt/Oder) and an industrial partner, LayTec (Berlin). Here, the task is the in-situ scatterometric measurement and control of periodic and biperiodic surface structures during the manufacturing process of etching. This scattering measurement requires the determination of the reflectivities depending on the wavelength and the solution of an inverse reconstruction of the geometry from the reflectivity spectrum by a numerical algorithm.

For this aim, a simulation tool based on the scattering matrix algorithm was developed, which is a variant of the RCWA. It is based on a vertical decomposition of the geometry (slicing) and on the ordinary differential equation (ODE) integration of Maxwell's equations, discretized by Fourier mode expansions in horizontal direction. To apply this RCWA in scatterometry, several geometry models were set up to simulate periodic surface structures during etching. The RCWA was extended to the computation of the derivatives with respect to the geometry parameters. Using these derivatives, a gradient-based search algorithm for the geometry reconstruction (indirect measurement) could be employed. Moreover, the derivatives collected in Jacobi matrices enabled a sensitivity analysis for the indirect measurement and a first estimate for the measurement uncertainty. Finally, a fast in-situ simulation of the spectra was implemented using a sparse grid interpolation.

### Optimization and optimal control

Shape optimization algorithms easily become numerically unstable when the optimal shape is not close to the initial shape. We investigated a newly developed method which exploits a relation to





**Fig. 3:** Robustness sensitivity for uncertain friction coefficients in a stationary gas network

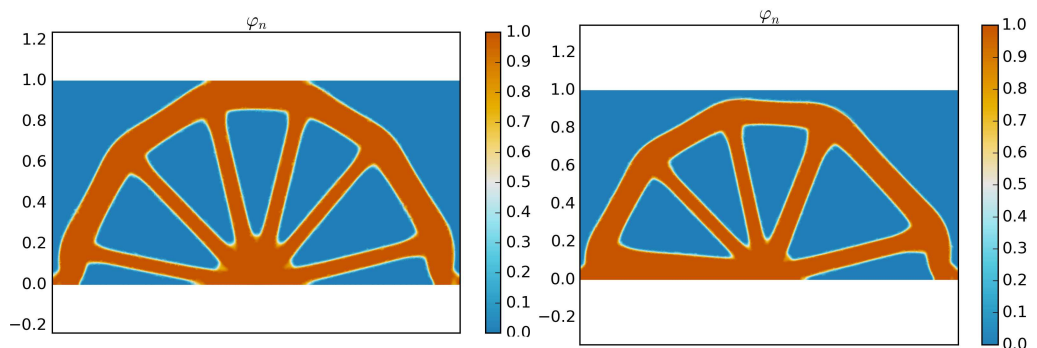
reproducing kernels and allows for initial shapes far away from the goal [3].

A major research topic of our group is stochastic and nonsmooth optimization. An essential part of the work was devoted to the subproject “Nonlinear probabilistic constraints in gas transportation problems” within the DFG Transregio (TRR) 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks*. In an associated Ph.D. project, a class of optimization problems with joint probabilistic/robust constraints was introduced and applied to uncertain demands/friction coefficients in a stationary gas network with one entry (black) under a probabilistic constraint for satisfying random demands at exits (white); see Figure 3.

In another problem of stochastic optimization, the efficiency of quasi-Monte Carlo algorithms in two-stage stochastic programs was addressed [5]. The analysis of (sub-) gradient formulae for probability functions, initiated in 2015, could be substantially advanced and led to a prolongation by another year of a research project within the Gaspard Monge Program for Optimization and Operations Research funded by the Jacques Hadamard Mathematical Foundation. At the same time, progress in the algorithmic treatment of probabilistic constraints under Gaussian distribution was made towards nonlinear models and the preparation of a corresponding software tool. In nonsmooth optimization, a major achievement consisted in the derivation of necessary optimality conditions for the control of sweeping processes, which are differential inclusions with the right-hand side given by the negative normal cone to a controlled moving polyhedron [2].

Within the ECMath project C-SE13, we investigated chance constraints in PDE-constrained optimization. In a first step, we generalized some of the well-known semi-continuity and convexity properties in a finite-dimensional setting to a setting of control problems subject to uniform state chance constraints. In collaboration with Reinhold Schneider (Berlin), a novel method for risk-aware topology optimization under uncertainties was developed. Based on a phase-field approach for the distribution of material, stochastic models of the material properties (random imperfections) and the load (random directions) were employed with a constrained minimization formulation. In order to take into account probabilistic influences, the conditional value at risk (CVaR) was incorporated as a risk measure. This approach ensures that the optimal topology is found for a chosen quantile of all possible parameters. The high-dimensional parametric problems were solved by functional tensor reconstructions and Monte Carlo sampling; see Figure 4.

**Fig. 4:** Optimized bridge structure with respect to mean value of random perturbations (left) and risk-averse topology with respect to 0.7-quantile in CVaR optimization emphasizing critical rare events (right). Load is applied at the bottom center in random directions.



The lognormal case for random PDEs is still considered a challenge for practical applications since the diffusion coefficient is unbounded and the algebraic coupling structure of the stochastic sys-

tem becomes very complicated. As a continuation of previous results on adaptive methods for random PDEs with affine coefficients, research on adaptive stochastic finite element method (FEM) for this case was carried out for a sparse adaptive log-transformed problem and a discretization in the tensor train format, which resembles an optimal reduced basis construction.

RG 4 coordinates the European Industrial Doctorate (EID) project “MIMESIS – Mathematics and Materials Science for Steel Production and Manufacturing”. In this interdisciplinary and intersectorial project, training courses play an important role. One highlight was the course on “Finite element simulation for multifield problems”, for which all eight MIMESIS students spent three months at WIAS. From November 2016, all students attended a three-months training course on “Physical metallurgy of metals and steels” at the University of Oulu in Finland.

Besides the overall project coordination, RG 4 is responsible for three Ph.D. projects related to high-frequency induction welding, single- and multi-frequency induction hardening of helical and bevel gears, and inductive pre- and post-heating for the thermal cutting of steel plates. The Ph.D. projects will extend results obtained within the Federal Ministry of Education and Research joint research project “MeFreSim: Modeling, simulation and optimization of multifrequency induction hardening as part of modern manufacturing technology” [6] (duration 2010–2013). A fourth project on optimal control of ladle stirring is jointly supervised with RG 3 *Numerical Mathematics and Scientific Computing*. In all projects, the models consist of coupled, nonlinear systems of partial differential equations. Depending on the application, the equations involve the heat equation, Navier–Stokes, and/or Maxwell equations to compute the magnetic field as the source of the inductive heating, the equations of elasticity to account for structural deformations as the consequence of thermal expansion and phase transition phenomena in steel, and a system of ODEs to describe the evolution of different phases in steel.

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## 4.5 Research Group 5 "Interacting Random Systems"

In 2016, RG 5 continued its research in a large number of research programs that were running as a result of its fundraising successes in earlier years. These were on various topics like interacting particle systems, concentration properties of spectra of random operators, biological evolution models, and in particular on *Probabilistic Methods for Mobile Ad-hoc Networks* in the *Leibniz Group* LG 4 that carries this name. Additionally, we also contributed to the success of the application for a new DFG Research Unit on *Rough Paths and Stochastic Partial Differential Equations*, which commenced in the spring and which made it possible that another member joined us in October.

The research spectrum of RG 5 is complemented by some particular topics like a large-deviations approach to physically interesting models for the polaron, connections between large-deviation analysis of large interacting stochastic particle systems and gradient flows, and branching-process descriptions of certain important equations like the (time-dependent) Schrödinger equation. The group members produced a number of research results with a large impact, as is documented by the list of WIAS preprints. A particular highlight were contributions by younger group members, for example the joint work of our Ph.D. student Franziska Flegel with young members of the Research Group RG 1 *Partial Differential Equations* (see the Scientific Highlights article on page 35), her co-organization of the WIAS Analysis-Stochastics seminar, and an international research prize (the Itô Prize of the Bernoulli Society) that our new postdoc Adrián González Casanova Soberón, received for a joint paper<sup>1</sup> written during his Ph.D. time, prior to joining RG 5.

In 2016, some members of the group were active finishing books, like the extended survey on *The Parabolic Anderson Model* authored by the head of group, Wolfgang König, which appeared with Birkhäuser, or a monograph on *Cellular Network Analysis and Design using Stochastic Geometry*, co-authored by Paul Keeler and soon appearing with Cambridge University Press, and the group head's companion publication as editor, *Mathematics and Society*, for the 7th *European Congress of Mathematicians*, which took place in Summer 2016 at the Technische Universität Berlin. The latter book is meant to help improve the understanding of the general public of the impact of mathematics on the society.

Two important workshops were (co-)organized by RG 5: In August, the 75th birthday of one of the most influential probabilists of our time (S.R.S. Varadhan, Courant Institute New York) was celebrated with a one-week conference that featured a large number of distinguished speakers and attracted people from all over the world, and in November, the first workshop of the Leibniz Group LG 4 took place at WIAS and brought together researchers from stochastics and from telecommunications.

Also in teaching, Wolfgang König, supported by some group members, supervised a very large quantity of bachelor's and master's theses at the Technische Universität Berlin on various subjects in the scientific spectrum of his research group. This was not without success: One of the most gifted graduates started a Ph.D. thesis supervised by the head of the group and with a stipend of the Berlin Mathematical School.

A closer description of some of the group's achievements in 2016 follows on the next pages.

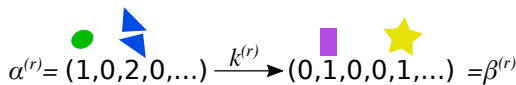
<sup>1</sup>A. GONZÁLEZ CASANOVA SOBERÓN, N. KURT, A. WAKOLBINGER, L. YUAN, *An individual-based model for the Lenski experiment, and the deceleration of the relative fitness*, Stochastic Process. Appl., **126**:8 (2016), pp. 2211–2252.

## Large deviations of reaction systems

Large deviation principles (LDPs) are a very powerful tool in the analysis of microscopically interacting particle systems where extensive microscopic randomness combines to produce larger-scale structures. In [4] (joint work with the Research Group RG 1 *Partial Differential Equations*; see their Scientific Highlights article in the Annual Research Report of WIAS of 2013, pp. 33–38), generalized gradient structures for the limiting behavior of infinite reacting particle systems were derived from an LDP for the underlying microscopic model.

During 2016, intensive work was carried out to rigorously establish the LDP, whose existence was assumed in [4], in particular, to include the case of coagulation (infinitely many possible particle sizes and reactions) and to clarify the role of reversibility. A list of species  $\mathcal{Y}$  is considered, in Figure 1 depicted as colored shapes, to emphasize the flexible, abstract nature of the approach. An appropriate choice of its contents covers many applications, including chemical species, polymer lengths, raindrop diameters, and soot particle aggregate structures.

Reactions, indexed by  $r$ , are defined by a list of reactant species  $\alpha^{(r)}$  converted into a list of product species  $\beta^{(r)}$  and the rate  $k^{(r)}$  at which they do this. Finding expressions for these rates is often a major obstacle in real-world problems.



**Fig. 2:** Reaction  $r$  converts one green ellipse and two blue triangles into a purple rectangle and a yellow star with a mean of  $k^{(r)}$  reactions per unit time and volume

A preliminary result says that, for well-mixed volumes  $V$ , the sequence of concentration vectors  $c^{(V)}(t)$ , defined as the number of copies of each element of  $\mathcal{Y}$  divided by  $V$ , converges in the limit of large  $V$  with probability 1. The limit  $\bar{c}(t)$  has the time derivative  $\sum_r k^{(r)}(\bar{c}(t))(\beta^{(r)} - \alpha^{(r)})$ . The LDP in broad terms shows that for large  $V$

$$\mathbb{P}(c^{(V)} \approx c) \sim \exp\left(-V \int L(c(t), \dot{c}(t)) dt\right),$$

where  $L$  is the minimum entropy of the possible fluxes through each reaction channel consistent with the evolution of the concentrations given by  $c(t)$ . These results are presented in [5] and represent progress towards two distinct goals:

- Estimating the mixing properties of simulations in order to efficiently use time averaging to reduce computational costs.
- Analyzing versions of these reaction systems that additionally have spatial structure, typically with more than one characteristic length scale.

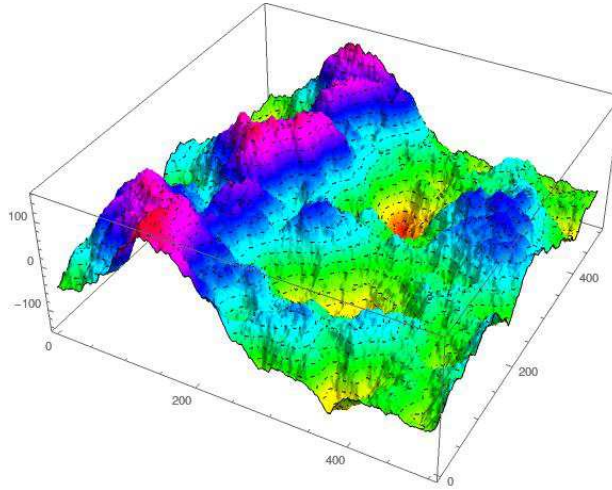
## The membrane model

Water changes its state (solid, liquid, and gas) depending on temperature. At the transitions, more than one phase can coexist in space. They are usually separated by fairly sharp hypersurfaces called *interfaces*. These objects are macroscopic in the sense that they are ordered arrangements

$$\mathcal{Y} = \{\bullet, \blacksquare, \blacktriangleleft, \blacktriangleright, \star, \dots\}$$

**Fig. 1:** Abstract, potentially infinite, list of species

of atoms or molecules on a microscopic scale. It is a principal goal of statistical mechanics to understand such macroscopic phenomena from the microscopic viewpoint of atoms or molecules.



**Fig. 3:** A sample of the membrane model

To study hypersurfaces separating two different states of matter, one typically views them as Gaussian random variables sampled for each point of a  $d$ -dimensional large grid (see Figure 3). The *membrane model* or *bilaplacian model* is the interface sampled from a centered Gaussian distribution whose covariance matrix is the discrete bilaplacian  $\Delta^{-2}$ , the inverse of the iteration (second power) of the discrete Laplace operator.

The membrane model has been introduced in physics and biology to model natural interfaces tending to have constant curvature. Mathematically, it has proved to be very interesting: It indeed shares many common features with other, apparently, unrelated models. This similarity appears strongly as the mesh size of the grid becomes finer; for example, if the dimension  $d$  is large enough, the largest peaks of these models have the same limiting behavior.

Another common feature of the class of the bilaplacian model is that, when the interface is “forced” to be zero at several points of the grid (a procedure called *pinning*), then the underlying random heights become almost independent: The covariance between two points in the new pinned model has an exponential decay in the distance, as was shown in [2], [3].

### Concentration of mass flows through random potential

The parabolic Anderson model (PAM) concerns the solution to the Cauchy problem

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

where  $\Delta$  is the discrete Laplace operator and  $\zeta = (\zeta(x))_{x \in \mathbb{Z}^d}$  is a field of independent and identically distributed random variables. The operator  $\Delta + \zeta$  is known as the *Anderson operator*. For an application of the problem (1) in the context of population dynamics, we refer to the Scientific Highlights article 2.5 “Population growth on random fitness landscapes” in the WIAS Annual Research

Report 2014 on pages 40–43.

A key characteristic of the solutions to (1) is *intermittency*, which may be loosely described as the development, at large times, of relatively small regions in space, called *intermittent islands*, where most of the total mass  $\sum_x u(x, t)$  is contained. In collaboration with Marek Biskup (UCLA), the group considers in [1] the positive solution to (1) with localized initial datum  $u(x, 0) = \mathbf{1}_0$ . As reported in the WIAS Annual Research Report 2014, we show that, as  $t \rightarrow \infty$ , most of the mass of the solution is concentrated with large probability in a single island with bounded diameter. We identify the scaling limit of the center of the island and obtain ageing properties for both the center and the solution itself. The potentials that we consider are in some sense *critical*, meaning that the solution exhibits a non-trivial structure around the concentration center. In particular, the mass cannot be compressed into a single point, which is the behavior previously obtained in the literature for potentials with heavier tails and is known as *complete localization*.

An interesting effect arises in the related *Bouchaud–Anderson model*, where the Laplacian in (1) is replaced with the generator of a Bouchaud trap model, defined in terms of an additional field of independent and identically distributed random variables  $(\sigma(x))_{x \in \mathbb{Z}^d}$  of positive random variables (called *traps*), independent of  $\xi$ . This approach adds random diffusivity to the medium. Together with Stephen Muirhead (Oxford), Richard Pymar (UCL), and Nadia Sidorova (UCL), the group recently showed that, for  $\xi$  critical as in [1] and as soon as  $\sigma(0)$  is unbounded from above, the solution exhibits complete localization, in sharp contrast to the behavior of the PAM. This phenomenon is related to the *fit and stable* hypothesis of population dynamics, according to which a population with space-dependent reproduction rates given by a *fitness landscape* (the field  $\xi$ ) and migration rates given by a *trapping landscape* (the field  $\sigma$ ) should concentrate on regions that are both fit (i.e., have optimal potential) and stable (i.e., have deep traps). A manuscript is in preparation.

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## 4.6 Research Group 6 “Stochastic Algorithms and Nonparametric Statistics”

The Research Group 6 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.

RG 6 has a leading position in the above-mentioned fields with important mathematical contributions and the development of statistical software.

Members of the research group participated in the DFG Collaborative Research Center SFB 649 *Economic Risk*, DFG Research Unit FOR 1735 *Structural Inference in Statistics: Adaptation and Efficiency*, DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, and DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*.

Group members were also involved in several industrial contracts and cooperations, such as a project with GE Technology (jointly with RG 3 *Numerical Mathematics and Scientific Computing*) on “Process simulation for industrial gas turbines”, a collaboration with Deloitte, and other projects.

Scientific highlights achieved by the research group in 2016 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. The research includes, e. g., methods for dimension reduction, change-point detection, regularization and estimation in inverse problems, multiple testing, model selection, feature identification, and adaptive smoothing in various applications.

#### Highlights 2016:

The highlight of 2016 was the publication of the papers [1] and [2].

Research within this subarea covered both theoretical and applied statistical problems.

In [1], a new bootstrap-based approach to parameter tuning in model selection was offered. The method allows to build fully data-driven efficient procedures for the model selection in realistic situations when no prior information about the noise distribution is available.

In paper [2], we demonstrated that ignoring the deviation from Gaussianity caused by a low signal-to-noise ratio (SNR) leads to a severe bias in the estimated characteristics in diffusion magnetic resonance imaging (MRI). Our approach to correct for these shortcomings is based on a new proposal for the estimation of the noise level in MRI images that employs structural adaptive smoothing.

Finite sample results were established in paper [3] on the properties of the quasi-maximum likelihood regularized estimator. The explicit error term of approximation was given via the so-called *effective dimension* of the problem.

In cooperation with the Max Planck Institute for Human Cognitive and Brain Sciences Leipzig, the group investigates a new method (multi-parameter mapping) for in-vivo diagnostics that relates series of MR images obtained with different imaging contrasts and imaging parameters. The method is designed to obtain invariant, with respect to scanner properties, characterizations of brain tissue by a set of three to four parameters. These techniques aim for resolutions far below 1 mm and are again prone for low SNR.

A novel method of adaptive clustering developed in RG 6 was presented in a plenary talk at the 2016 Interdisciplinary School and Conference of the Kharkevich Institute for Information Transmission Problems in Repino (Russia).

### Stochastic modeling, optimization, and algorithms

This project area focuses on the solution of challenging mathematical problems in the field of optimization, stochastic optimal control, and stochastic and rough differential equations. These problems are particularly motivated by applications in the finance and energy industries. One central theme is the rigorous mathematical analysis of innovative methods and algorithms based on fundamental stochastic principles. These methods provide effective solutions to optimal control and decision problems for real-world high-dimensional problems appearing in the energy markets, for instance. Another focus of the project area is on 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 is active in the highly emerging field of rough path analysis and regularity structures, which led, in particular, in the past year to the approval of the DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*.

#### Highlights 2016:

- ERC Consolidator Grant on geometric aspects in pathwise stochastic analysis for Peter K. Friz.
- Outstanding publication:  
CHRISTIAN BAYER, PETER K. FRIZ, SEBASTIAN RIEDEL, JOHN G.M. SCHOENMAKERS, *From rough path estimates to multilevel Monte Carlo*, SIAM J. Numer. Anal., **54** (2016), pp. 1449–1483.
- Successfully finished collaboration project with Deloitte & Touche on multi-curve LIBOR modeling, calibration, and pricing of related products. The main WIAS researcher on this project, Fabian Dickmann, was headhunted by Deloitte after the finalization.
- Offer to Christian Bayer to become an associated professor (equivalent to German W2 professorship) at the Royal Institute of Technology (KTH), Stockholm (Sweden).
- Successful Ph.D. defense by Martin Redmann (*magna cum laude*) at the Universität Magdeburg.
- Start of the DFG Research Unit FOR 2402 for 2016–2019, spokesmen Peter K. Friz and Wilhelm Stannat (TU Berlin), principal investigators in subproject P3: Christian Bayer and John G.M. Schoenmakers.

2016 was a remarkable year in that the new DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics* with two subprojects located at WIAS (RG 5 *Interacting Random Systems*, RG 6) started, followed by an ERC project (Consolidator Grant) on geometric aspects in pathwise stochastic analysis.

The collaboration with RG 4 *Nonlinear Optimization and Inverse Problems* on stochastic differential equation-based regression methods for partial differential equations with random coefficients was continued. Details are exposed in the Scientific Highlights article by Christian Bayer and Martin Eigel on page 40 in this report. In particular, the method was extended to allow for adaptive sampling of the underlying stochastic processes, thereby improving the computational efficiency of the method. Currently, regressions methods for *rough stochastic partial differential equations* are in development in the context of the Research Unit FOR 2402.

The research on rough stochastic volatility models (driven by fractional Brownian motions with Hurst index  $H \ll 1/2$ ) was continued, this year with special focus on the development of asymptotic and numerical methods. In particular, asymptotic formulas for option prices in the moderately-out-of-the-money regime were considered, based on novel large deviation techniques. Moreover, interesting connections with Hairer's theory of re-normalization were applied in the context of the simulation of rough stochastic volatility models, allowing for Wong–Zakai-type approximations.

A new method for computing prices of basket option was developed (WIAS Preprint no. 2280). The method is based on a two-stage procedure. First, the payoff function was smoothed using inherent smoothing properties of the model instead of an artificial outside mollification. Hence, the smoothing is unbiased, i.e., the actual price is not affected by the smoothing. As we now had a (high-dimensional) numerical integration problem with a smooth integrand, standard techniques from numerical analysis could be employed. In this project, the adaptive sparse grid method was specifically chosen. It was observed that the method typically leads to drastic improvements in the computational cost as compared to standard Monte Carlo or quasi-Monte Carlo methods.

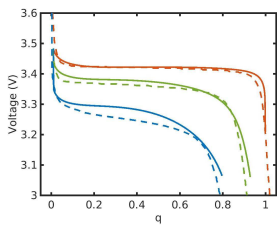
Nonlinear Markov processes or McKean–Vlasov, which are related to nonlinear Fokker–Planck equations, are stochastic processes whose transition functions may depend on the current distribution of the process. Such processes naturally arise in a wide range of applications, including financial mathematics, population dynamics, and neuroscience. In a collaboration with Denis Belomestny (Universität Duisburg-Essen), a novel projection-based particle method for the solution of these processes was developed. This approach is based on a projection-type estimation of the marginal density of the solution in each time step. As such, the method leads in many situations to a significant reduction of numerical complexity compared to the usual kernel-based density estimation in McKean–Vlasov-type algorithms. A detailed convergence analysis was carried out, and several applications will be considered.

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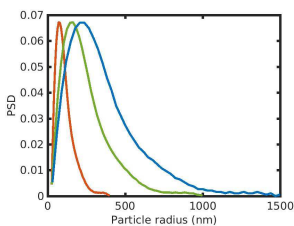
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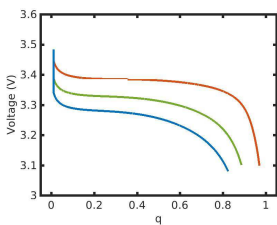
## 4.7 Research Group 7 "Thermodynamic Modeling and Analysis of Phase Transitions"



**Fig. 1:** Comparison between simulation (solid) and experiment (dashed) for voltage-capacity plot for 20 minutes (blue), 1 hour (green), 25 hours (red)



**Fig. 2:** Storage particle size distributions



**Fig. 3:** Impact of size distributions on voltage during discharge, see Figure 2

Research Group 7 works on the thermodynamically consistent modeling, analysis, and simulation of processes in materials. The application fields of the group are focused on

- Mathematical models of electrochemical processes in the context of lithium-ion batteries
- Mathematical models of nano-structured materials within photovoltaic applications and for complex liquids
- Hysteresis of electromagnetic-mechanical components and of biological systems

From a mathematical point of view, the resulting models are typically represented by free boundary problems for systems of nonlinear partial differential equations. In addition, systems of stochastic ordinary differential equations are investigated in the context of battery research. A further research area is the treatment of diffuse interfaces and boundary layers by the methods of asymptotic analysis.

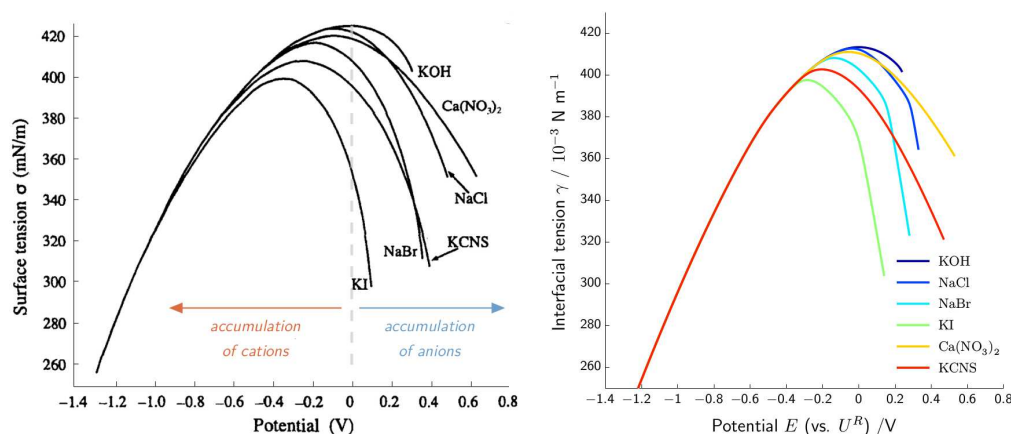
### Mathematical models of electrochemical processes in the context of lithium-ion batteries

**A new stochastic model for lithium iron phosphate (LFP) electrodes.** With support from the Research Center MATHEON funded by the Einstein Center for Mathematics Berlin, a new thermodynamically consistent model for many-particle electrodes in lithium-ion batteries based on a system of stochastic differential equations (SDE) was developed and studied in cooperation with scientists from RG 3 *Numerical Mathematics and Scientific Computing* and RG 6 *Stochastic Algorithms and Nonparametric Statistics* [1]. The SDE model allows to study the behavior of a many-particle electrode for different charging rates and different particle size distributions in the full physically relevant parameter range. Furthermore, the model enables to simulate the phase transition within the particle ensemble for phase separating materials like  $\text{LiFePO}_4$ .

The comparison between experiment and simulation yields very good results, i.e., the typically observed capacity-voltage curves for different charging regimes were reproduced by the simulations using only two phenomenological parameters; see Figure 1. We were able to show that the main rate-limiting process within the electrode is the lithium intercalation into the electrode material. Further, the experimental observation that small particles prefer to undergo the phase transition before larger particles for electrodes with a high electrical conductivity was confirmed by the SDE model. The ability of the model to capture the particle sizes of the electrode is particularly important in regard to optimizing the structural features of the electrodes. Figure 3 shows the impact of the particle size distribution, see Figure 2, on the battery voltage of an LFP electrode under the same charging rate.

**Analysis of an improved Nernst–Planck–Poisson–Navier–Stokes system.** In addition, a new model for electrolytes was developed in our research group, which tackles several problems of classical Nernst–Planck–Poisson systems for electrolytes. In this context and in cooperation with Pierre-Étienne Druet (RG 1), existence results for a model for mixtures of electrically charged fluids were also derived.

**Electrocapillarity.** Charging an electrochemical interface by applying a potential results in a change of the observed interfacial tension. This phenomenon is described by the well known Lippmann equation. Recently, this equation was recovered from the new electrolyte model based on combined volume and surface thermodynamics. The derivation of the Lippmann equation was then extended to include rather general electrochemical surface reactions. For a liquid metal–electrolyte interface a current-charge relation was established that is the basis for an experimental confirmation. Similar to the differential capacity, electrocapillarity curves show a characteristic fingerprint of a metal–electrolyte interface. While the cathodic branch of the curves is always the same due to the lack of cation adsorption, the anodic branches differ because of adsorption and surface reactions. By a systematic study of the different phenomena that are included in our model, we were able to identify the relevant parameters for a qualitative and quantitative reproduction of experimentally measured electrocapillarity curves.



**Fig. 4:** Left: measured electrocapillarity according to Grahame [Chem. Rev., 41(3):441–501, 1947]; right: their reproduction by numerical simulation based on the new electrolyte model

**Butler–Volmer equations for electrochemical interfaces.** One central ingredient for modeling electrochemically active interfaces, i.e., where some net charge is transferred from an electrolyte phase to an electrode, is the Butler–Volmer equation. It describes the relation between a current passing an interface and the so-called *over-potential*, the deviation from the potential where this current vanishes. Even though frequently used, there are some discrepancies regarding the actual functional relationship of the thermodynamic quantities entering this equation.

RG7 has solved this problem in the last year via a rigorous modeling of the transfer reactions based on coupled volume-surface thermodynamics [2]. The boundary conditions obtained [3] allow to model various kinds of interface reactions, e.g., intercalation reactions occurring in lithium batteries, electro-catalytic reactions of fuel cells, redox shuttle reactions, and many more. The actual improvement is a systematic incorporation of the respective material functions, i.e., chemical potentials, of the reactive constituents. First numerical studies showed a remarkable improvement of the resulting current-voltage relation, especially with respect to the model parameters entering the relation. Further, it turned out that the definition of the over-potential actually requires an asymptotic limit of a thin double layer, a requirement that is, for example, violated in small pores of porous materials.

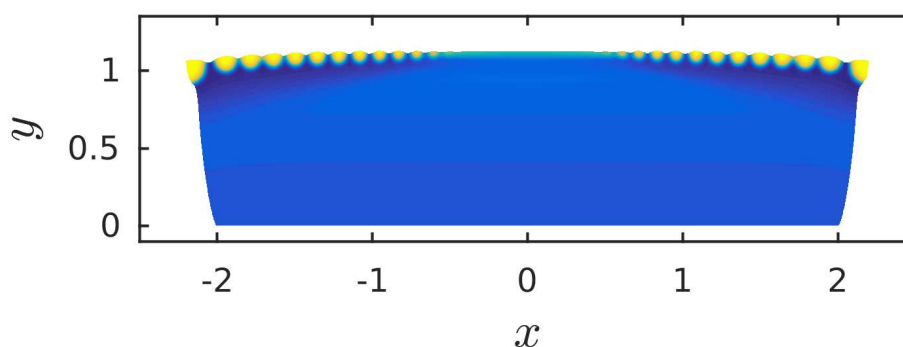
This relation is a core feature of the ongoing research on the modeling of electrochemical systems, providing a model-based understanding of experimental data such as cyclic voltammetry.



### Mathematical models of nanostructured materials within photovoltaic applications and for complex liquids

**Phase transitions of thin-film electrodes when lithiated.** The research, funded by the MATHEON subproject C-SE4, used a Larché–Cahn approach together with a simplified geometry to allow a comprehensive study of parameter regimes during lithium intercalation in high-capacity silicon; see [5]. For the phase field model coupled to elasticity, a corresponding sharp-interface limit between lithiated and non-lithiated phases was derived, including complex nonlinear boundary conditions. The resulting free boundary problem is similar to the Mullins–Sekerka problem, but it also includes elasticity. Interestingly, it turned out that the form of the boundary conditions is essentially preserved in the sharp-interface limit. Numerical simulations of the phase field model as well as a stability analysis established for the first time that lithiation of the layer induces an instability at the absorption boundary. This instability is akin to spinodal decomposition, but confined near the boundary, and is also affected by elasticity. A linear stability analysis performed for this phase field instability and for the corresponding sharp-interface instability in the receding interface show that both instabilities, albeit different, can be described in the same context, see Figure 5.

**Fig. 5:** *Instability in the concentration of lithium during the lithiation of a thin-layer electrode. When phase separation occurs, it creates first small pockets of lithiated material (in yellow) spaced with a characteristic wavelength that eventually coarsens and merges. Cross section of the electrode with the scaled position in the deformed configuration denoted by  $x$  and  $y$ .*



**Phase-field modeling for solid-state dewetting.** Solid-state dewetting is one of the important processes used for nanostructuring and functionalizing surfaces for a variety of technological applications, such as, for example, in thin-film solar cells and other optoelectronic devices. As a part of the doctoral thesis “Dewetting of thin solid films: Modeling, analysis and numerical simulation” by Marion Dziwnik (Technische Universität Berlin, March 2016, funded by the Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin), a phase field model for anisotropic solid-state dewetting on a substrate was correctly developed that recovers the physical mechanism of capillarity-driven surface diffusion. The resulting model is an anisotropic version of the Cahn–Hilliard equation with degenerate mobility and anisotropic boundary conditions at the solid substrate. For this free boundary problem existence of weak solutions was shown on a rectangular domain with homogeneous Neumann boundary conditions and under the additional assumption that the anisotropy is sufficiently weak. Extensions of this model can be found in [6].

**Liquid-liquid dewetting of polymer films.** This research topic was funded by the DFG Priority Program SPP 1506 “Transport Processes at Fluidic Interfaces”. For systems of dewetting polystyrene (PS) films from polymethyl methacrylate (PMMA) substrates, where both are Newtonian liquids

with comparable viscosities, the evolution of initially flat layers of different thicknesses was investigated. Numerical simulations of our coupled system of thin-film equations were compared to experimental results carried out at the Experimental Physics Lab of Ralf Seemann at the Universität des Saarlandes, where the evolution of the PS-air, the PMMA-air, and the PS-PMMA interfaces for long times using in situ atomic force microscopy (AFM) were measured. These measurements were in excellent agreement with our theoretical prediction from thin-film models describing the evolution of a multiphase system of viscous liquids that are purely driven by interfacial tensions. Based on these comparisons, we could settle the question on the dewetting rates of two-layer systems, see Figure 6, that was discussed controversially in the literature. In particular, our theoretical and numerical studies lead to the prediction of local flow fields and energy dissipation that otherwise would be inaccessible to experiments; see [7].

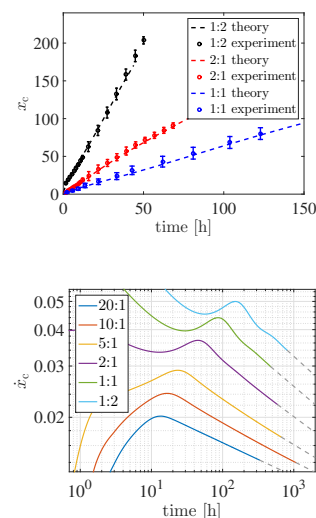
### Hysteresis, electromagnetic-mechanical components, and uncertainty quantification

The methods of uncertainty quantification were applied to hysteresis operators and to models for electro-magneto-mechanical components, including situations where the observable macroscopic state may be generated by many unobservable microscopic states; see [4].

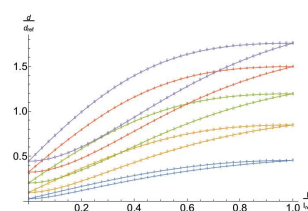
Moreover, using experimental data for Terfenol-D provided by Daniele Davino (Benevento, Italy), appropriate values for the parameters for a generalized Prandtl–Ishlinskii operator as in Sec. 5.1 of Davino–Krejčí–Visone (2013) were computed. For both parameters  $c_1 > 0$  and  $c_2 > 0$  in the weight function  $[0, \infty) \ni r \rightarrow c_1 e^{-rc_2}$  considered in the Prandtl–Ishlinskii operator, sets of approximation values were determined, allowing to compute the corresponding mean value and the standard deviation. In Fig. 7, hysteresis curves are shown that were derived by using for  $c_2$  the corresponding mean value and variations computed by adding/subtracting the standard deviation.

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**Fig. 6:** Above: dewetted distance  $x_c$  for aspect ratios 1:1 (240 nm : 240 nm), 2:1 (90 nm : 45 nm), 1:2 (45 nm : 90 nm) from experiment (circles with error) and simulation (dashed lines), suggesting constant dewetting rates  $\dot{x}_{c,1:1} = 4.4 \times 10^{-2}$  nm/s,  $\dot{x}_{c,2:1} = 3 \times 10^{-2}$  nm/s,  $\dot{x}_{c,1:2} = 5.2 \times 10^{-2}$  nm/s, where (below) longer simulations prove that rates  $\dot{x}_c$  decrease depending on the aspect ratio (gray dashed lines guide the eye)



**Fig. 7:** Hysteresis loops generated by considering the computed mean value for a parameter for Terfenol-D and its modifications by  $\pm 1$  and  $\pm 2$  times its standard deviation

## 4.8 Research Group 8 “Nonsmooth Variational Problems and Operator Equations”

The focus areas of this research group are the mathematical modeling and analysis of the resulting variational problems or operator equations, as well as the design, analysis, and computer-oriented realization of the pertinent solution algorithms. Particular fields of interest include

- nonsmooth models for energy functionals and/or state systems,
- quasi-variational inequality problems or nonsmooth coupled systems and their optimal (open loop) control,
- equilibrium problems and game-theoretic approaches.

Concerning applications, various processes in medicine, nature, engineering, and economy play a central role. Regarding WIAS's main application areas, the research group contributes to *Quantitative Biomedicine*, *Optimization and Control in Technology and Economy*, as well as aspects of *Materials Modelling*. In all instances, nonsmooth and set-valued analysis or geometry for the treatment of nonsmooth systems of partial differential equations (PDEs) or nonsmooth energies on infinite-dimensional spaces are advanced. In this way, compromising smoothing schemes, which are often responsible for wrong system predictions, are avoided.

With the arrival of the new director, RG 8 was initiated at the beginning of the year. Currently, it is still in a *statu nascendi* with several positions expected to be filled in 2017. Despite this status, the group has already contributed in several ways to the broad research agenda of WIAS.

### General relevance of the scientific topics considered by the RG

In many technological applications or economic models, nonsmooth structures are fundamental for a faithful mathematical description of the underlying real-world processes. For instance, in recent years nonsmooth energies based on generalizations of the well-known regularization by total variation have succeeded in medical image processing due to their edge-preserving properties<sup>2</sup>. Further, continuum mechanic descriptions of material conditions for the prevention of material interpenetration naturally lead to nonsmooth model structures. An interesting example of such a situation arises when studying the dynamic behavior of epi- and pericardium during a cycle of the human heart. Also, in optimal control of technical processes or pertinent game-theoretic approaches in case of multi-objective/multi-control situations, one typically needs to account for constraints on the common state of the underlying system. Generalized Nash equilibria provide the proper concept in such a context, thus leading to a nonsmooth and typically set-valued generalized PDE system characterizing such equilibria.

Motivated by the above, the mathematical approaches and techniques developed by RG 8 are aimed at furthering the understanding of mathematical models and the associated real-world applications by avoiding compromising smoothing techniques. In such a way and from a mathematical standpoint, important problem classes such as quasi-variational inequalities and their control

<sup>2</sup>A sharp variation in (image) intensity values is referred to as an “edge”.

are made accessible, and subsequently the analytical investigations help the advance of mesh-adaptive and mesh-independent numerical solvers.

This philosophy behind RG 8's research ansatz lead to a series of results in several application fields, successful project acquisitions, and cooperations with industry.

### Selected research results

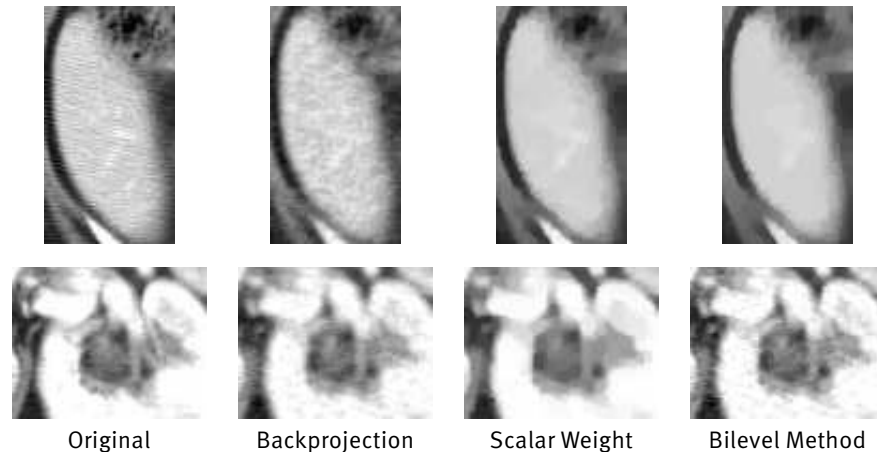
**Nonsmooth models for energy functionals and/or state systems.** Due to their excellent ability of preserving edges, nonsmooth filters represent a central element in mathematical image processing. In a DFG project entitled "Free boundaries and level set methods", a new generalized formulation of the renowned total variation regularization was introduced [3, 4]. The project is funded under the D-A-CH agreement between DFG and the Austrian Science Fund FWF for joint applications of the DFG with Austria and Switzerland. It participates in the Collaborative Research Center SFB F32 *Mathematical Optimization and Applications in Biomedical Sciences*, which is funded by the FWF as the lead agency. The new regularization functional incorporates a distributed weight function which allows for a varying filter effect depending on local image features (details vs. homogeneous regions). The filter weight is determined automatically through a novel bilevel optimization framework. In this context, the parameterized image reconstruction problem represents the lower level problem, and the upper level problem aims at fixing the filter weight properly. Inspired by an unsupervised learning approach and the statistics of extremes, a localized variance corridor for the image residual is considered and its violation provides a suitable choice for the upper level objective. Figure 1 depicts a corrupted image (left), the reconstruction obtained by the novel bilevel framework (middle), and the computed filter weight (right), where light color belongs to small positive weight values and intense color to higher values. A performance comparison (with respect to the peak signal-to-noise index and a structural similarity measure) proved that the new framework is superior to state-of-the-art single-level approaches with scalar regularization.



**Fig. 1:** Application of the bilevel approach to deblurring for the benchmark image "cameraman"

Figure 2 presents solutions to a problem of Fourier inpainting arising in parallel magnetic resonance imaging of a chest, where the original data (left) are restored by known methods utilizing backprojection or a scalar weight as well as the bilevel approach. The spatial distribution of the weight allows to handle local properties, i.e. homogeneous and detailed regions, properly. For more information we refer to [2]. The extension of this topic is one of the cornerstones of the subproject I02 "Advanced reconstruction for multiparametric and multimodality imaging" within

the proposed DFG Collaborative Research Center SFB 1255 *Multiscale Modelling of Cardiovascular Physiology and Pathophysiology*, whose evaluation is scheduled for January 2017.



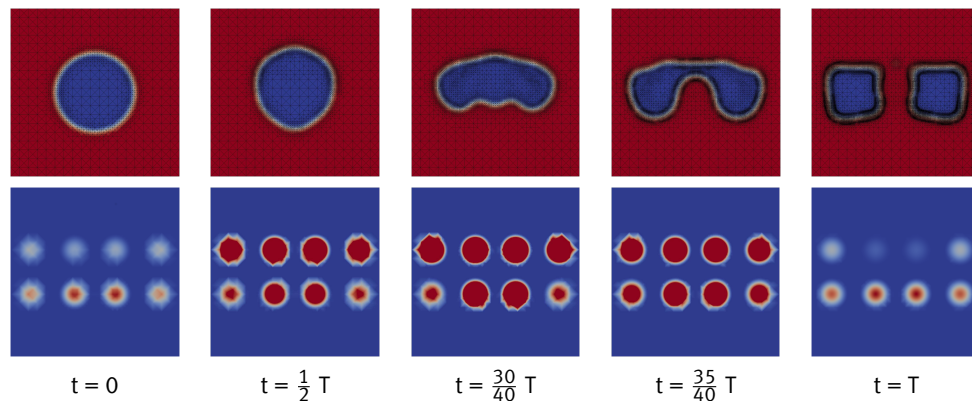
**Fig. 2:** Results obtained by different methods for Fourier inpainting for an image of a chest

In the case of Parseval frames, an algorithmic alternative was discussed in [1], where instead of the regularizing term, the data fidelity term was weighted and the algorithmic optimization was performed with a surrogate technique. A detailed study concerning analytical properties of the novel total variation generalization was presented in [3]. For example, it was shown that in contrast to classical regularization approaches employing total variation seminorms for problems with small contrast reduction compared to the scalar regularization parameter, new discontinuities may form in the reconstructed data.

Several other research activities of RG 8 benefit from the aforementioned bilevel optimization framework. For example, the method was successfully applied in image processing, where the kernel of an underlying convolution that models contrast reduction or blurring was identified. This result allowed for an extension of the local regularization by a blind deconvolution used in microscopy below resolution limits or imaging in the presence of unknown heterogeneous media.

**Nonsmooth coupled systems and their optimal control.** Within this area, RG 8 participated in the DFG Priority Program SPP 1506 *Transport Processes at Fluidic Interfaces* and contributed to MATHEON research activities within the Einstein Center for Mathematics Berlin. Motivated by mathematical problems arising in photovoltaics, lab-on-a-chip applications, or microfluidic devices, two configurations were studied: (I) Cahn–Hilliard–Navier–Stokes systems with nonsmooth homogeneous energy densities, providing models for multiphase fluids, and (II) Hele–Shaw systems, modeling electro-wetting on dielectric media. Concerning optimal control, the underlying physical processes are characterized by essentially degenerated sets of feasible state-control pairings, rendering the derivation of first- and second-order optimality conditions challenging. Here, RG 8 made crucial progress in establishing suitable stationarity systems and their numerical realization (see Figure 3 for time snapshots of an optimal state-control pairing in configuration (I), where the control enters as the right-hand side of the Navier–Stokes equation and acts through parameter functions with local support in disks centered at the corners of the desired terminal state. The

computations are based on an adaptive finite element method (AFEM)). In our activities within the newly established DFG Priority Program SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization*, these research efforts are a cornerstone for further developing analytical and numerical aspects such as strong stationarity conditions for related problems of optimal control and model predictive control, respectively.



**Fig. 3:** Numerical results using AFEM with Taylor-Hood finite elements for splitting up a ring-shaped region into two separate squares under gravity. Upper row: States. Lower row: Controls.

**Equilibrium problems and game-theoretic approaches.** Motivated by problems arising in modeling, simulation, and optimization in the context of natural gas transportation networks, generalized Nash-equilibrium problems were considered. Instead of applying scalarization techniques or Pareto optimization, this class of models bears a large potential in dynamical processes in the economic, engineering, and life sciences that are characterized by several individual objectives and corresponding control parameters. Examples for such problems comprise market models including transport processes or quorum-sensing behavior of bacteria. Existence of a solution and its characterization by conditions of Karush–Kuhn–Tucker type were established for linear elliptic and parabolic state systems subject to pointwise state- and individual control constraints. In addition, path-following techniques for an efficient numerical treatment of these problems were introduced. By participating in the DFG Priority Program SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* and the DFG Collaborative Research Center SFB/TRR 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks* as well as collaborating with RG 4 *Nonlinear Optimization and Inverse Problems*, RG 8 will intensify its activities in this area.

**Dense embedding of convex sets.** A typical result arising from applying Legendre–Fenchel dualization to nonsmooth variational problems is a minimization problem subject to convex constraints, as, for example, in the context of elasto-plasticity in [7] and in mathematical image processing in [2, 4]. Here, relating (pre-)dual to primal problems requires the dense embedding of dual constraints on smooth test functions into sets with the same constraint type but for functions in Lebesgue or Sobolev spaces. In other words, given a function space  $X$  and a dense subspace  $Y$ , does the identity  $\overline{K \cap Y^X} = K$  for certain convex  $K \subset X$  hold? In [6], this property was derived for pointwise constraints on the state or its gradient of an underlying system. Table 1 presents particular results for  $X = L^1(\Omega)$ , where  $\Omega \subset \mathbb{R}^N$  is a bounded Lipschitz domain, a function  $\alpha : \Omega \rightarrow (\varepsilon, \infty]$  to be specified,  $\varepsilon > 0$ , and the set  $K = K(X; \alpha) = \{\phi \in X \mid |\phi| \leq \alpha \text{ almost everywhere}\}$ .



**Table 1:** Dense intersection results for  $K(X; \alpha)$  in various settings for  $p < \infty$

$\alpha$	$Y$	$X$	density?
$C(\overline{\Omega})$	$C_c^\infty(\Omega)/\mathcal{D}(\overline{\Omega})$	$L^p, W_0^{1,p}, H_0(\text{div})/W^{1,p}$	yes
l.s.c./ $W^{1,p}$ -l.s.c.	$C_c^\infty(\Omega)$	$L^p/W_0^{1,p}$	yes
measurable	$C_c^\infty(\Omega)/\mathcal{D}(\overline{\Omega})$	$W_0^{1,p}/W^{1,p}, p > N$	yes
$W^{1,N}$	$C(\Omega)$	$L^p, p < \infty, W^{1,p}, p \leq N$	not in general

Similar density results are necessary for establishing convergence results of finite-element approximations, utilized in the numerical realization of the original problems. Summarizing, the theory developed by RG 8 is an entirely novel contribution to the literature and forms a basis for developing generalized Newton methods solving the dual problems and in the convergence analysis of discretized problems.

**Optimal control and inverse problems with hyperbolic partial differential equations.** RG 8 participates in the DFG Collaborative Research Center SFB/TRR 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks*. In the report period, discretization methods for scalar hyperbolic conservation laws were investigated that are consistent with adjoint methods of optimization in the sense that both the primal and adjoint discretization schemes converge to the physically relevant solutions in the function space setting. Such methods are crucial since shocks, a major characteristic of the underlying physics and also the associated partial differential equation models, typically prohibit the differentiability of control-to-state operators. Here, established consistency theory for total variation diminishing discretization methods was extended by higher-order time-stepping methods of Runge–Kutta type. In addition, parameter identification in gas networks was considered and first results for identifying the friction law in a damped wave equation were established.

### Further highlights in 2016



The DFG Priority Program SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* coordinated by Michael Hintermüller with WIAS as the associated coordinating institution was successfully implemented, and the kickoff meeting was held on October 27–28 at WIAS.

In collaboration with ERC 1 *Elliptic PDEs and Symmetry of Interfaces and Layers for Odd Nonlinearities*, the Workshop “Free Boundaries, Partial Differential Equations and Related Topics” was organized at WIAS on December 19–20.

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## 4.9 Young Scientists' Group "Modeling of Damage Processes"

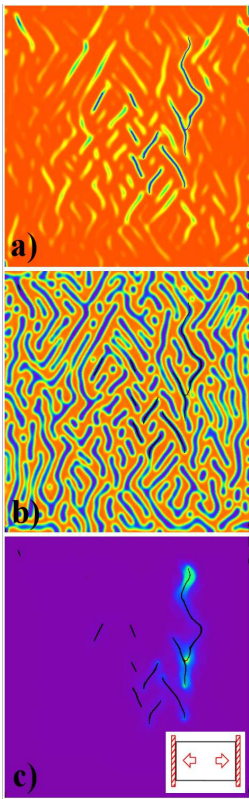
Within the competitive procedure of the Leibniz Association in the Pact for Research and Innovation, Dorothee Knees and Christiane Kraus successfully applied for a grant that provided the basis for the Young Scientists' Group. The group was formed at WIAS in 2009, working on the modeling, analysis, simulation, and optimization of damage processes until December 2016. Collaborations existed with the Research Groups RG 1 *Partial Differential Equations*, RG 4 *Nonlinear Optimization and Inverse Problems*, RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, and ERC 2 *Entropy Formulation of Evolutionary Phase Transitions* on the modeling, analysis, and optimization of multifunctional materials.

### Modeling, analysis, numerics, and optimization 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 worked on the modeling, analysis, numerics, and optimization of *phase separation* and *damage processes* including heat conduction in alloys with the intention to predict and optimize the strength and lifetime of materials for practical relevance. In addition, the group developed multi-scale damage models that reflect the evolution of microdefects in effective models on the macroscopic level in a mathematically justified way.

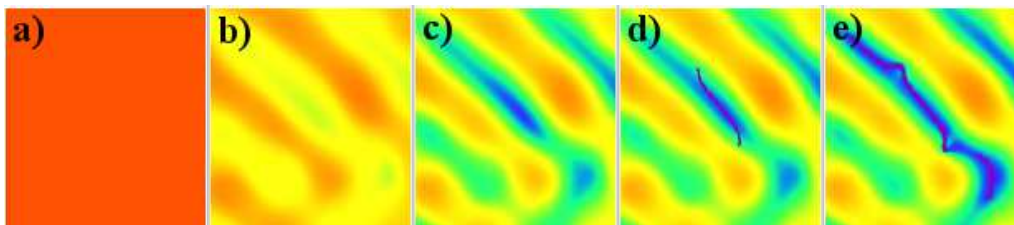
In general, the resulting models consist of strongly coupled, nonlinear, and nonsmooth time-dependent systems of partial differential equations (PDEs). The analytical investigation of these systems requires tools from the calculus of variations for nonlinear and nonsmooth evolution systems and from geometric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

Based on previous work in the group, a very complex system describing different physical phenomena was developed and investigated. In particular, the question of how material inhomogeneities promote the initiation of cracks and how these are affected by domain interfaces was considered. The model developed in the group may be considered as a "hybrid" ansatz between damage and fracture since it allows to describe both partial damage—interpreted as the presence of microcracks that are not resolved—and macroscopic cracks, which evolve from the first mentioned (Figures 2 a)-e)). The expansion of the model by temperature yields an additional coupling, namely mechanical stress by inhomogeneity of thermal expansion coefficients. Scenarios where a sufficient temperature change at the boundaries induced stress in the bulk and finally fracture were successfully simulated in the group. The dynamics included also the formation of domains by phase separation in a unified setting (Figure 1). This multi-scale evolution was handled in the group by a strongly adaptive scheme. In order to deal with realistic scales in the model, reasonable parameter values had to be estimated. With regard to possible applications to solder alloys, this estimation was done for lead and tin. In such a setting (e.g., cooling of solder joints after soldering process), the temperature may change by an order of 100 K. Therefore, an Arrhenius-like law for the temperature dependence of the mobility was included in the model. Furthermore, an additional mechanism for branching was described: While branching is suppressed for quasi-static models with stretch-compression anisotropy, the effect is retrieved when a strong anisotropy is present in the



**Fig. 1:** Snapshot of a simulation of the fully coupled model: a) damage field, b) material phase field, and c) temperature

elastic tensor (Figure 3). The above-mentioned aspects required continuous enhancement of the numerical code, such as, for instance, mesh refinement to maintain reasonable computation times; cf. [3].



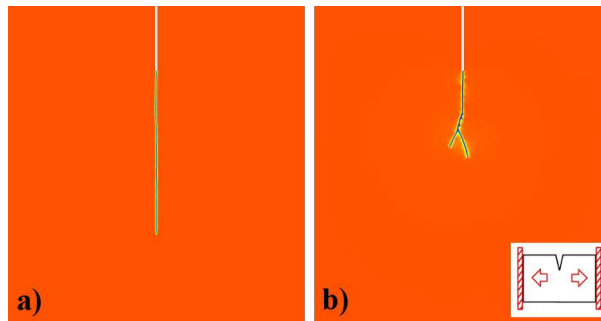
**Fig. 2:** Evolution of the two-phase material model with time under constant load. Plotted is the damage phase field  $z$ . Partial damage precedes fracture: a) initial state, b), c) partial damage, d), and e) cracks nucleate and propagate.

While material models for damage and crack propagation had been subject to many research efforts in the last decade, their associated inverse problems remained virtually unexplored, and optimality conditions seemed to be not achievable due to the usually non-unique solutions and highly non-smooth behavior of the model. Recently, in the Young Scientists' Group, a class of so-called *viscous damage models* was identified where stability results and existence of global-in-time strong solutions are available [1]. Based on this foundation, the group was able to derive a first-order optimality system to an optimal control problem for damage evolution in visco-elastic media. In the considered type of problems, the boundary forces act as the control variable, and the cost functional penalizes deviations of the damage function with respect to some prescribed profile. The damage function results from an evolution process modeled by a coupled PDE system. In order to facilitate numerical implementations in future, projects following the challenging paradigm "first optimize – then discretize", an adjoint state system was also established and solved in the class of very weak solutions. The existence proof of the adjoint system makes use of an approximation procedure with PDE problems solvable in the class of weak solutions, which are also suitable for finite element method (FEM) implementations.

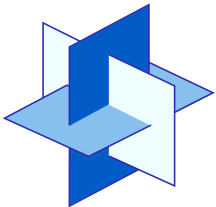
In a further related research project, optimal shapes for semi-discrete damage-elasticity systems where a (tracking-type) cost functional is aimed to be minimized were explored in the group together with one of the group's external collaborators. In a joint work [2], optimality conditions for these shapes were proven. The conditions are justified for a large class of shape optimization problems for semi-linear variational inequalities and extend the classical theory for linear variational inequalities established by Sokolowski and Zolesio. The group further enriched the classical theory by a concept that is referred to as "dynamic obstacles". In the classical setting, an obstacle is a fixed function that is associated to the region in which the problem should be solved. However, in the considered dynamical situation, the obstacle function can be simultaneously subject to another variational problem. Only due to these extensions, the group was able to apply the developed framework to a time-discrete damage-elasticity system, since the dynamic obstacle is given there by the damage profile from the previous time step and arises from a different variational inequality. In order to establish optimality conditions, the group developed sensitivity estimates in an abstract monotone operator setting where the operators are defined on polyhedral subsets of reflexive Banach spaces.

Starting from models studied in the Young Scientists' Group in recent years, a novel viscous, vector-valued Cahn–Hilliard reaction model (CHR) coupled to both elasticity and to rate-dependent dam-

age processes was proposed and analyzed. Since this novel model takes into account different chemical species, mechanical strains, and stresses as well as chemically active boundaries, it is well suited to describe multi-component systems with chemical reactions at the surfaces like, e.g., lithium-ion batteries. Mathematically, the description of the reactions at the surfaces is realized by a nonlinear Newton boundary condition for the chemical potential, which leads to challenging analytical and numerical tasks. The group proved that the proposed system has an underlying generalized gradient structure that incorporates the nonlinear boundary condition naturally. This additional structure of the CHR equations seemed not to be known before and is a breakthrough in the theory of the CHR system since it allows to transfer results known from the Cahn–Larché system to the CHR system. In particular, it was achieved to prove the existence of weak solutions for the whole nonlinearly coupled system using a variational approach combined with several sophisticated techniques from the field of convex analysis [4].



**Fig. 3:** Comparing fracture with isotropic and anisotropic elasticity: a) isotropic, b) orthotropic elastic tensor



## Projects

Third-party funding was secured within the Research Center MATHEON with the subproject C-SE 4 “Mathematical modeling, analysis and novel numerical concepts for anisotropic nanostructured materials”. In addition, the research group participates in the DFG Collaborative Research Center SFB 1114 *Scaling Cascades in Complex Systems* for the subproject “Effective models for interfaces with many scales”.

## References

- [1] M. H. FARSHBAF SHAKER, C. HEINEMANN, *Necessary conditions of first order for an optimal boundary control problem for viscous damage processes in 2D*, WIAS Preprint no. 2269, 2016.
- [2] C. HEINEMANN, K. STURM, *Shape optimisation for a class of semilinear variational inequalities with applications to damage models*, WIAS Preprint no. 2209, 2016.
- [3] C. KRAUS, M. RADSZUWEIT, *Modeling and simulation of non-isothermal rate-dependent damage processes in inhomogeneous materials using the phase-field approach*, WIAS Preprint no. 2299, 2016.
- [4] A. ROGGENSACK, C. KRAUS, *Existence of weak solutions for the Cahn–Hilliard reaction model including elastic effects and damage*, WIAS Preprint no. 2231, 2016.

## 4.10 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 postdocs Annalisa Massaccesi (until December 2013), Stefania Patrizi (until July 2015), Eleonora Cinti (from January 2015), Joaquim Serra (from January 2016 until August 2016), Matteo Cozzi (from January 2016 until July 2016), and Carina Geldhauser (from September 2016) were members of the group, and more partners visited the institute to establish scientific collaborations.

The investigations of ERC 1 were dedicated to the analysis of interfaces of layers that arise, e.g., in phase transitions and surface tension phenomena. The focus was on the geometry, structure, and regularity of the interfaces. Mathematically, elliptic variational problems were addressed, in particular, problems involving fractional Laplace operators.

In 2016, Enrico Valdinoci held several research courses and many invited seminars and talks (in Magdeburg, Gießen, Marseille, Mbour, Pisa, Perth, Leeds, Rome, Naples, Bari, New York, Toronto, Vancouver, Lecce, Będlewo, Potsdam, Melbourne, Trieste, Santiago, etc.).

In the context of the ERC project, he organized and sponsored several events, such as the *Otto-von-Guericke-School in Partial Differential Equations* in Magdeburg, the *Research Meeting on Non-Local Operators* in Cagliari, the *Workshop on Recent Trends in the Analysis of PDEs* in Pavia, and the workshop *Free Boundary, Partial Differential Equations and Related Topics* in Berlin.

Jointly with Eleonora Cinti, Matteo Cozzi, Stefania Patrizi, Joaquim Serra, 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, and nonlocal diffusion equations.

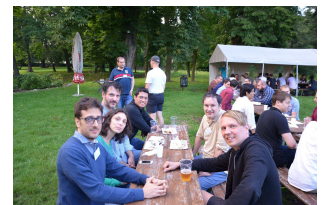
In particular, in [1], we proved that every function can be locally approximated by functions whose fractional Laplacian vanishes in a given region. This is a new feature with respect to the classical case, in which the rigidity of the harmonic functions prevents this type of approximation. Also, this result has important consequences, for instance, in mathematical biology, since it shows that populations with a nonlocal behavior can better plan their distribution in order to take advantage of the whole of the resource in a given strategic area, thus avoiding any unnecessary waste.

In [2], we proved that any nonlocal minimal surfaces whose prescribed datum outside a cylinder is a continuous graph is necessarily a continuous graph also inside the cylinder, though these two graphs do not necessarily match at the boundary. In this sense, the global graph may be discontinuous, which corresponds to a new stickiness phenomenon for nonlocal minimal surfaces.

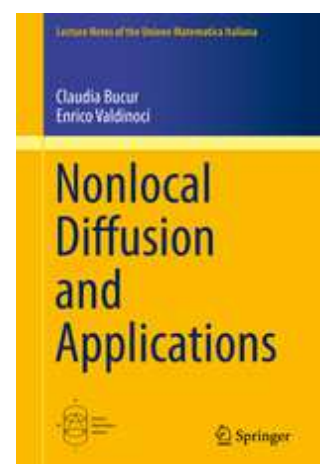
In [3], we studied an evolution equation whose solution represents the atom dislocation in a periodic crystal. The dislocation function has the tendency to concentrate at single points, which evolve in time according to the external stress and a singular, long range potential. We provided accurate estimates on the relaxation times of this system in view of the plastic deformation of the material.



**Fig. 1:** Lecturing in Będlewo



**Fig. 2:** Social dinner in Będlewo



**Fig. 3:** The monograph [6]



In [4], we studied a stationary partial differential equation of elliptic type that describes a model of phase coexistence, and we proved the one-dimensional symmetry of the solution from the geometric properties of the limit interface. These symmetry properties are important in the applications since they imply that the value of the state parameter only depends on the distance from the interface.

In [5], we obtained monotonicity results for the energy density, rigidity results for the solutions, and classification results for a class of partial differential equations. The setting comprises also degenerate and singular equations and anisotropic media.

The monograph [6] collects some recent results in the area of nonlocal equations, with applications to phase transitions, water waves, and crystal dislocations.

Enrico Valdinoci also acted as an advisor for the Ph.D. students Julien Brasseur, Claudia Bucur, Luca Lombardini, and Pietro Miraglio.

## References

- [1] S. DIPIERRO, O. SAVIN, E. VALDINOCI, *All functions are locally  $s$ -harmonic up to a small error*, to appear in: J. Eur. Math. Soc. (JEMS).
- [2] S. DIPIERRO, O. SAVIN, E. VALDINOCI, *Graph properties for nonlocal minimal surfaces*, Calc. Var. Partial Differ. Equ., **55**:4 (2016), pp. 86/1–86/25.
- [3] S. PATRIZI, E. VALDINOCI, *Relaxation times for atom dislocations in crystals*, Calc. Var. Partial Differ. Equ., **55**:3 (2016), pp. 71/1–71/44.
- [4] A. FARINA, E. VALDINOCI, *1D symmetry for semilinear PDEs from the limit interface of the solution*, Comm. Partial Differential Equations, **41**:4 (2016), pp. 665–682.
- [5] M. COZZI, MATTEO, A. FARINA, E. VALDINOCI, *Monotonicity formulae and classification results for singular, degenerate, anisotropic PDEs*, Adv. Math., **293** (2016), 343–381.
- [6] C. BUCUR, E. VALDINOCI, *Nonlocal Diffusion and Applications*. vol. 20 of Lecture Notes of the Unione Matematica Italiana, Springer International Publishing Switzerland, Cham, 2016, xii+155 pages.

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

The ERC-Starting Grant “EntroPhase — Formulation of Evolutionary Phase Transitions” has been funded by the European Union since April 2011 and lasts six years. The group members in January and February 2016 were Elisabetta Rocca (PI) and Riccardo Scala (postdoc).

The group leader, Elisabetta Rocca, accepted an offer of a professorship at the University of Pavia. So, starting from March 1, 2016, the ERC group continued its work in Italy.

In the first two months of 2016, the group mainly focused on the objective to find relevant mathematical results in order to get further insight into new models for biological phenomena and special materials and the corresponding evolution partial differential equation (PDE) systems, in particular:

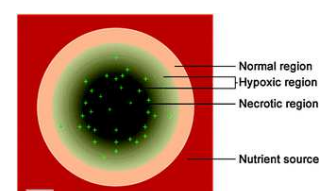
- Proving existence of weak solutions,
- Studying most refined properties of such solutions, like weak-strong uniqueness, the long-time behavior of solutions, the parameter reduction in finite time (sliding modes) and the associated control problems, as well as the sharp interface limits as some small physical parameter goes to zero.

These topics are important for applications to physically, biologically and engineering relevant problems like:

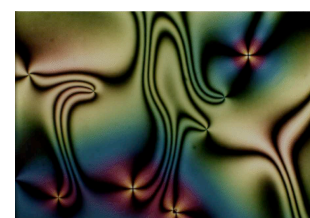
- Control problems related to
  - Nonlocal Cahn–Hilliard/Navier–Stokes systems (jointly with RG 7 *Thermodynamic Modelling and Analysis of Phase Transitions*; see [5]),
  - Tumor growth models (jointly with RG 7; see [3]),
  - Penrose–Fife and Caginalp-type models of phase transitions,
- Rate-independent gradient system in damage with plasticity (jointly with RG 1 *Partial Differential Equations*; see [1]),
- Evolution of liquid crystal flows (jointly with RG 1; see [2] and [4]),
- Sharp interface limits of diffuse interface models for tumor growth (see [6]).

### Further activities

The knowledge transfer was developed via the organization of international workshops and the participation of the group members in international conferences and workshop, but also by collaborating with international experts visiting the group, like Pavel Krejčí (Prague) on January 25–29, Arghir Zarnescu (Brighton) on February 7–13, and Eduard Feireisl (Prague) on February 7–13, and



**Fig. 1:** Tumor cross section



**Fig. 2:** Nematic liquid crystals

by organizing international workshops in cooperation with other groups at WIAS and with international experts in the field:

- ERC Workshop on Modeling Materials and Fluids using Variational Methods (MoMatFlu) at WIAS in Berlin, February 22–26, organized with A. Mielke (RG 1),
- Perspectives in Applied PDEs: A Day in Pavia, miniworkshop in Pavia, February 9.



Fig. 3: MoMatFlu

## References

- [1] E. BONETTI, E. ROCCA, R. ROSSI, M. THOMAS, *A rate-independent gradient system in damage coupled with plasticity via structured strains*, in: Gradient Flows: From Theory to Application, B. Düring, C.-B. Schönlieb, M.T. Wolfram, eds., vol. 54 of ESAIM Proceedings and Surveys, 2016, pp. 54–69.
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- [3] P. COLLI, G. GILARDI, E. ROCCA, J. SPREKELS, *Optimal distributed control of a diffuse interface model of tumor growth*, WIAS Preprint no. 2228, 2016.
- [4] M. DAI, E. FEIREISL, E. ROCCA, G. SCHIMPERNA, M.E. SCHONBEK, *On asymptotic isotropy for a hydrodynamic model of liquid crystals*, Asymptot. Anal, **97** (2016), pp. 189–210.
- [5] S. FRIGERI, E. ROCCA, J. SPREKELS, *Optimal distributed control of a nonlocal Cahn–Hilliard/Navier–Stokes system in two dimensions*, SIAM J. Control Optim., **54** (2016), pp. 221–250.
- [6] E. ROCCA, R. SCALA, *A rigorous sharp interface limit of a diffuse interface model related to tumor growth*, arXiv:1606.04663, Cornell University Library, arXiv.org, Ithaca, USA, 2016.

# A Facts and Figures

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

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

## A.1 Professorships, Awards, Habilitations, Ph.D. Theses, Supervision

### A.1.1 Offers of Professorships

1. CH. BAYER, Associate Professorship, October 25, Royal Institute of Technology, Department of Mathematics, Stockholm, Sweden.
2. P. FRIZ, Full Professorship, August 4, Universität Wien, Fakultät für Mathematik, Austria.
3. ———, Full Professorship, August 18, Universität Basel, Fakultät für Mathematik, Switzerland.
4. ———, W3 Professorship, October 21, Rheinisch-Westfälische Technische Hochschule Aachen, Fakultät für Mathematik.
5. E. VALDINOCI, Full Professorship, August 1, University of Melbourne, School of Mathematics and Statistics, Australia.

### A.1.2 Awards and Distinctions

1. M. HINTERMÜLLER, *Chair of the Einstein Center for Mathematics Berlin*.
2. ———, *Member of MATHEON's Executive Board*.
3. ———, *SIAM Fellow, Class of 2016, Society for Industrial and Applied Mathematics, Philadelphia, USA, for contributions to theoretical and numerical optimization, and for their application*.
4. D. HÖMBERG, *Member of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization*.
5. ———, *Vice Chair of Cost Action TD1409 (Mi-NET)*.
6. ———, *President of the European Consortium for Mathematics in Industry (ECMI), 2016/17*.
7. F. DASSI, L. KAMENSKI, H. SI, *International Meshing Roundtable Best Technical Paper Award, September 29, 2016*.
8. W. KÖNIG, *Member of MATHEON's Executive Board*.
9. M. LIERO, *Member of the Executive Board of the Einstein Center for Mathematics Berlin (Scientific Employee Representative)*.
10. A. MIELKE, *Head of the Secretariat of the International Mathematical Union (IMU)*.
11. ———, *Member of MATHEON's Executive Board*.
12. ———, *Member of the Executive Board of the Einstein Center for Mathematics Berlin*.
13. ———, *Member of the IMU Berlin Einstein Foundation Program Committee*.
14. ———, *Treasurer of IMU*.
15. D. PESCHKA, *Member of MATHEON's Executive Board (Scientific Employee Representative)*.
16. E. VALDINOCI, *Selection for Thomson Reuters' "Highly Cited Researchers 2016" list*.

### A.1.3 Habilitations

1. A. CAIAZZO, *On mathematical modeling and simulation of biological flows and tissues*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, July 6.

### A.1.4 Defenses of Ph.D. Theses

1. M. COZZI, *Qualitative properties of solutions of nonlinear anisotropic PDEs in local and nonlocal settings*, Università di Milano, Dipartimento di Matematica, supervisors: Prof. Dr. A. Farina, Prof. Dr. E. Valdinoci, January 11.
2. M. DZIWNIAK, *Dewetting of thin solid films: Modeling, analysis and numerical simulation*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Prof. Dr. B. Wagner, Prof. Dr. A. Münch, March 17.
3. F. EICHENAUER, *Analysis for dissipative Maxwell–Bloch type models*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, June 30.
4. S. GIERE, *Numerical and analytical aspects of POD-based reduced-order modeling in computational fluid dynamics*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 19.
5. M. HOFMANN, *Einfluss dynamischer Resonanzen auf die Wechselwirkung optischer Femtosekunden-Pulse mit transparenten Dielektrika*, Technische Universität Berlin Fakultät II – Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. U. Bandelow, August 30.
6. M. MAURELLI, *Regularization by noise in finite dimension*, Scuola Normale Superiore di Pisa, Dipartimento di Matematica, supervisor: Prof. F. Flandoli, March 18.
7. J. NEUMANN, *Adaptive methods for the Darcy equation with stochastic input data*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 27.
8. M. REDMANN, *Balancing related model order reduction applied to linear controlled evolution equations with Lévy noise*, Otto-von-Guericke Universität Magdeburg, Fachbereich Mathematik, supervisor: Prof. Dr. P. Benner, July 22.

### A.1.5 Supervision of Undergraduate Theses

1. H. AYDIN, *Ein Optimalitätsproblem für Angeln an zwei Orten* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 19.
2. V. BRILZ, *Exponentially-fitted finite volume methods for population balance systems* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, April 27.
3. F. CLAUSS, *Optimalsteuerung von Trocknungsprozessen in der Lebensmittelindustrie* (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, December 2.
4. F. GEBAUER, *Große Abweichungen für Lokalzeiten einer Irrfahrt mit zufälligen Leitfähigkeiten in einer großen Box* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 28.
5. E. GINTAUTAS, *Algebraic stabilizations for scalar convection-diffusion equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, April 13.
6. N. GOLOMBIEWSKI, *Irrfahrten mit zufälligen Leitfähigkeiten in einer Box* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 23.



7. D. GROH, *A bilevel optimization approach to the blind deconvolution problem with total variation regularization* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, January 29.
8. V. HEIDEMANN, *Funktionaler Grenzwertsatz im Edwards-Modell* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 31.
9. A. HINOJOSA CALLEJA, *Interference in ad-hoc telecommunication systems in the high-density limit* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. Ch. Hirsch, August 24.
10. E.J. HINTZE, *Matrixwertige Prozesse und ihre Eigenwerte* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 29.
11. M. HOFFMANN, *Adaptive finite element methods for Stokes–Darcy* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, March 20.
12. K. KARLISCH, *Große Abweichungen für Selbstüberschneidungslokalzeiten von Irrfahrten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 31.
13. M. KOLLOCK, *Calibration in PDE-based option pricing* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, January 11.
14. M. KRAUS, *Modeling of porous metal–electrolyte interfaces* (master's thesis), Ostbayerische Technische Hochschule Regensburg, Fakultät Informatik und Mathematik, supervisor: Dr. M. Landstorfer, November 22.
15. A. KYNAST, *Konvergenzgeschwindigkeit ausgewählter stochastischer Mischverfahren* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 15.
16. S. LING, *Numerical investigations of reduced order models for convection-diffusion equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, March 30.
17. M.H. LY LE, *Extremwertstatistik für stochastische Prozesse* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 23.
18. M. MARSHALL, *Tensor approximation in Bayesian inversion* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. M. Eigel, July 7.
19. M. MÜLLER, *Application of the optimal transport to Bayesian estimation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 28.
20. F. NEUMANN, *Quasi-Optimalität bei einer druckrobusten nichtkonformen Finite-Elemente-Methode für das Stokes-Problem* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. A. Linke, April 27.
21. M. NÖTH, *Numerische Methoden für nichtkonvexe Nash-Gleichgewichtsprobleme mit PDE-Restriktion* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, June 28.
22. L. REICHARD, *Zeitstetige Multityp-Verzweigungsprozesse in zufälligem Medium* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 31.
23. E. ROLLY, *Gibbs-Maße für Trajektorien von Nachrichten in einem Kommunikationsnetzwerk* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 23.

24. M. SCHREIBER, *Koregistrierung von Traktogrammen* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, April 15.
25. S. STACHELHAUS, *Neuronale Netze und Antragsbewertung* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 29.
26. A. STAHN, *Ein Phasenübergang im parabolischen Anderson-Modell mit skaliertem Gauß'schen Potential* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 3.
27. N. TALI, *Signal-to-Interference-Ratio in Kommunikationsnetzwerken mit hoher Dichte* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 11.
28. A. TÓBIÁS, *Highly dense mobile communication networks with random fadings* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. Ch. Hirsch, May 17.
29. TH. TRANG NGUYEN, *Stochastische Analyse des Hausverkaufsproblems und Varianten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 20.
30. J.R. TRANTOW, *Trust-Region SQP Verfahren in der Nichtlinearen Optimierung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, June 29.
31. A. VOGLER, *Multityp-Verzweigungsprozesse in verschiedenen zufälligen Medien* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 6.
32. M. WOLFF, *Finite-Element-Methode für die Stokes-Darcy-Gleichungen in 3D* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, June 2.

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

European Union, Brussels

### ■ Seventh Framework Programme



**ERC Advanced Researcher Grant “AnaMultiScale – Analysis of Multiscale Systems Driven by Functionals”** (Prof. A. Mielke in RG 1)

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

**ERC Consolidator Grant “GPSART – Geometric Aspects in Pathwise Stochastic Analysis and Related Topics”** (Prof. P. Friz in RG 6)

The project ERC-2015-CoG no. 683164 takes part in RG 6 and is funded for the duration from September 2016 to August 2021. Its purpose is to study a number of important problems in stochastic analysis, including the transfer of rough paths ideas to Hairer’s regularity structures, the study of rough volatility in quantitative finance, a pathwise view on stochastic Loewner evolution, and an understanding of the role of geometry in the pathwise analysis of fully nonlinear evolution equations. This project is run jointly with the Technische Universität Berlin.

**ERC Starting Independent Researcher Grant “RPT – Rough Path Theory, Differential Equations and Stochastic Analysis”** (Prof. P. Friz in RG 6)

The project ERC-2010-StG no. 258237 took part in RG 6, was funded by the European Research Council from September 2010 to August 2016. The research was 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”** (Prof. E. Valdinoci in ERC 1)

The ERC-2011-StG no. 277749 was funded by the European Research Council from January 2012 to December 2016. The research topics included partial differential equations (PDEs), nonlocal diffusion, fractional minimal surfaces, and phase transitions. The methods relied on variational techniques, geometric measure theory, asymptotic analysis, and nonlinear PDE tools.

**ERC Starting Grant “EntroPhase – Entropy Formulation of Evolutionary Phase Transitions”** (Prof. E. Rocca in ERC 2)

The ERC-2010-StG no. 256872 has been funded by the European Research Council since April 2011 and lasts for six 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 Marie Skłodowska-Curie Innovative Training Networks – European Industrial Doctorate ITN-EID “MIMESIS – Mathematics and Materials Science for Steel Production and Manufacturing”** (in RG 3 and RG 4)

In October 2015, the Weierstrass Institute saw the launch of the EID project MIMESIS. Driven by the five partners—EFD Induction (Norway), SSAB Europe Oy and Outokumpu Stainless OY (Finland), the University



<sup>1</sup>The research groups (RG) involved in the respective projects are indicated in brackets.

of Oulu (Finland), and WIAS—eight doctoral thesis projects will be jointly carried out, providing a unique interdisciplinary and inter-sectorial training opportunity. The research is focused on three major topics: induction heating, phase transformations in steel alloys, and gas stirring in steelmaking ladles. MIMESIS has a budget of 2.1 million euros and is coordinated by the head of RG 4, Prof. D. Hömberg.

#### EU framework Eurostars (in RG 2)

Eurostars supports international innovative projects of research- and development-performing small- and medium-sized enterprises. It is a joint programme between EUREKA and the European Commission, co-funded from the national budgets of 36 Eurostars participating states and partner countries and by the European Union through Horizon 2020. RG 2 is a full partner within the Eurostars project E!10524 “High power composites of edge emitting semiconductor lasers” (HIP-Lasers, 2016–2019), which aims to improve the quality of high-power laser beams by a specially designed intracavity photonic-crystal-type filter and a novel beam-combining scheme.

#### 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, Teilprojekt H” (Joint project EPILYZE: DNA methylation signatures as innovative biomarkers for the quantitative and qualitative analysis of immune cells, subproject H; in RG 6)

##### ■ Fördermaßnahme “Effiziente Hochleistungs-Laserstrahlquellen” (Funding program: Efficient high-performance laser beam sources, EffiLAS) in the framework of the programme “Photonik Forschung Deutschland” (Photonics Research Germany)

This measure supports enterprises in the research and development of innovative laser beam sources and components with a large application and market potential. RG 2 acts as a subcontractor of Ferdinand Braun Institut für Höchstfrequenztechnik, Berlin, within the projects “Effiziente und brillante Breitstreifendiodenlaser mit hohen Leistungen für den Betrieb bei hohen Umgebungstemperaturen” (Efficient and brilliant high-power broad-area diode lasers for operation at high temperatures, HotLas, 2016–2019) and “Puls-Laser und Scanner für LiDAR-Anwendungen: Automotive, Consumer, Robotic” (Pulse lasers and scanners for LiDAR applications: Automotive, consumer, robotic, PLUS, 2016–2019), both aiming to improve the quality of semiconductor high-power lasers.

##### ■ 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)

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 (BMW). In this framework, WIAS (RG 3) runs from 2013 to 2017 the Subproject „Makroskopische Modellierung von Transport- und Reaktionsprozessen in Magnesium-Luft-Batterien“ (Macroscopic modeling of transport and reaction processes in magnesium-air

**ENERGIESPEICHER**  
Forschungsinitiative der Bundesregierung

batteries) in the Interdisciplinary Research Network “Perspektiven für wiederaufladbare Magnesium-Luft-Batterien” (Perspectives for rechargeable magnesium-air batteries). Project partners are German experimental and theoretical groups in the field of electrochemistry.

- **National strategy for the European Research Area – ERA Fellowship:** For six weeks in Autumn 2016, a colleague from the Alfred Renyi Institute of Mathematics in Budapest, Hungary, came to WIAS to exchange experience with the institute’s administration and colleagues working in scientific coordination about administration aspects of European projects within the Horizon 2020 framework (mainly ERC), like, e.g., financial management and audit organization.

#### **Bundesministerium für Wirtschaft und Technologie (Federal Ministry of Economics and Technology), Berlin**

- **Zentrales Innovationsprogramm Mittelstand (ZIM): Kooperationen (Central Innovation Program for Small and Medium-sized Enterprises: Cooperations)**

Cooperative Project “Entwicklung von In-situ-Messtechnik für die Prozesskontrolle und Strukturbestimmung bei Plasma-Ätzprozessen” (In-situ metrology development for semiconductor processing in etch processes), Subproject “Entwicklung eines hybriden Scattering-Matrix-Algorithmus für die indirekte Vermessung von Oberflächenstrukturen bei Plasma-Ätzprozessen” (Development of hybrid scattering-matrix algorithms for the metrology of surface structures in etch processes; in RG 4)

#### **Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Bonn**

- **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)**

This transregio research center, which has been funded by the DFG since October 2014, focuses on an efficient handling of gas transportation. The Weierstrass Institute participates in the subprojects “Nichtlineare Wahrscheinlichkeitsrestriktionen in Gastransportproblemen” (Nonlinear chance constraints in problems of gas transportation; in RG 4) and “Parameteridentifikation, Sensorlokalisierung und Quantifizierung von Unsicherheiten mit schaltenden Systemen von PDEs” (Parameter identification, sensor localization and quantification of uncertainties in switched PDE systems”; in RG 8).

- **Collaborative Research Center (SFB) 649, Humboldt-Universität zu Berlin “Ökonomisches Risiko” (Economic Risk)**

This research center, which was funded by the DFG from 2005 to 2016, focused on studying economic risk. The Weierstrass Institute participated in the third term in the Subproject 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)**

This collaborative research center began its work on January 1, 2008. In the third funding period (2016–2019), WIAS participates in the subprojects B4: “Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters” (in RG 1 and RG 2) and 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).



Mathematische Modellierung,  
Simulation und Optimierung  
am Beispiel von Gasnetzwerken



■ **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)**

This center, which started in January 2011, involves groups at several institutes in Berlin, most of them working in physics. The Subproject A5 “Musterbildung in mehrskaligen Systemen” (Pattern formation in systems with multiple scales; in 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. Starting from 2015, also the Subproject A3: “Aktivitätsmuster in Systemen mit zeitverzögerten Kopplungen” (Activity patterns in delay-coupled systems; in RG 2) has been treated by WIAS staff members, jointly with TU Berlin.



■ **Collaborative Research Center (SFB) 1114**, Freie Universität Berlin

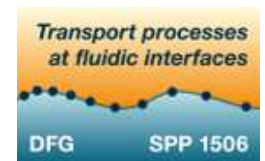
**“Skalenkaskaden in komplexen Systemen” (Scaling Cascades in Complex Systems)**

The center began its work on October 1, 2014 (funding period until June 30, 2018). WIAS members participate in the subprojects: 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), and C08: “Stochastische räumliche koagulierende Partikelprozesse” (Stochastic spatial coagulation particle processes; in RG 5).



■ **Priority Program SPP 1506: “Fluide Grenzflächen” (Transport Processes at Fluidic Interfaces)**, Technische Universität Darmstadt and Rheinisch-Westfälische Technische Hochschule Aachen

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 in the second funding period (October 2013 – September 2016) in the Subproject “Mathematical modeling, analysis, numerical simulation of thin liquid bilayers and validation experiments” (in RG 7) and in 2016 also in the Subproject “Fully adaptive and integrated numerical methods for the simulation and control of variable density multiphase flows governed by diffuse interface models” (in RG 8).



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

This interdisciplinary nationwide priority program aims at the development of new mathematical methods for the study and understanding of an innovative evolution biology. In the prolongation of the Subproject “Branching processes in random environment and their application to population genetics” for 2016–2018 (in RG 5), the interest was concentrated in 2016 on models for branching processes on finite gene sequences and the question how quickly these population processes spread over this space in relation to the length of the gene sequences. Various distributions of the branching rates were compared with each other.



■ **Priority Program SPP 1679: “Dyn-Sim-FP – Dynamische Simulation vernetzter Feststoffprozesse” (Dynamic Simulation of Interconnected Solids Processes)**, Technische Universität Hamburg-Harburg

WIAS participates in this priority program (first two funding periods Oct. 2013 – Sept. 2017) with the Subproject “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). The project aims at assessing and improving numerical methods for population balance systems. The assessment of the methods is based on data from experiments that are conducted by one of the project’s partners. In 2016, this project contributed essentially to the development of the new code *ParMoon*. As a result, it was possible to simulate the time-dependent flow field in the helix geometry that is used in the experiments. In addition, a module for solving systems of evolutionary convection-diffusion equations was implemented.







- **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

RG 1 participates in this priority program with the Subproject “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), which is a collaboration with Universität Freiburg (duration: Oct. 2014 – Sept. 2017). The project puts emphasis on unregularized numerical approaches for the treatment of functions of bounded variations (BV) that lead to sharp approximations of discontinuities on coarse grids and rigorous convergence proofs.



- **Priority Program SPP 1962: “Nichtglatte Systeme und Komplementaritätsprobleme mit verteilten Parametern: Simulation und mehrstufige Optimierung” (Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization)**, Humboldt-Universität zu Berlin

The Director of WIAS, Prof. M. Hintermüller, is the coordinator of this new priority program that was started with the Kick-off Meeting in October 2016 with the aim to help solve some of the most challenging problems in the applied sciences that involve nondifferentiable structures as well as partial differential operators, thus leading to nonsmooth distributed parameter systems.

WIAS participates with the subprojects “Simulation und Steuerung eines nichtglaten Cahn-Hillard-Navier-Stokes-Systems mit variablen Fluidsdichten” (Simulation and control of a nonsmooth Cahn–Hillard Navier–Stokes system with variable fluid densities, in RG 8), “Verallgemeinerte Nash-Gleichgewichtsprobleme mit partiellen Differentialoperatoren: Theorie, Algorithmik und Risikoaversion” (Generalized Nash equilibrium problems with partial differential operators: Theory, algorithms and risk aversion, in RG 8), and “Optimale Steuerung von elliptischen und parabolischen Quasi-Variationsungleichungen” (Optimal control of elliptic and parabolic quasi-variational inequalities, in RG 8).

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

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. RG 6 is studying the convergence and efficiency of such algorithms (second funding period until March 2018) in the Subproject “Semiparametric structural analysis in regression estimation”.



- **Research Unit FOR 2402 “Rough Paths, Stochastic Partial Differential Equations and Related Topics”**, Technische Universität Berlin

This new research unit has been funded since December 2015. One of the two spokesmen is Prof. P. Friz (FG 6). The research unit further develops and investigates innovative methods for applying rough path theory to the analysis of stochastic partial differential equations (SPDEs), like rough flow transformations, paracontrolled distributions, and regularity structures. The goal is to push forward the understanding of the solution theory of various types of SPDEs and the analysis of the most important physical properties of the solution processes. The overall intention is to fully overcome the gap between SPDEs and ordinary differential equations, whose solutions are often much better behaved and much more regular functions of the input parameters.

The central theme in the Subproject TP 3 “Numerische Analysis von rauen partiellen Differentialgleichungen” (Numerical analysis of rough PDEs; in RG 6) are numerical techniques for PDEs driven by deterministic or random rough paths. Two distinct promising techniques are being explored: the application of semi-group theory to rough PDEs connected with Galerkin finite element methods and Feynman–Kac representations combined with spatial regression, aiming at the development of new implementable numerical methods, their error analysis, and computational complexity.

In the Subproject TP5 “Singular SPDEs – Approximation and statistical properties” (in RG 5), two important

and prominent types of equations are studied – the Kardar–Parisi–Zhang (KPZ) equation and the (time-dependent) parabolic Anderson equation. The main goal is the investigation of their most important long-time properties like ageing for the KPZ equation and intermittency of the Anderson equation. Both are studied for rather singular input quantities like Gaussian noises, both time-dependent and static.

#### ■ Normalverfahren (Individual Grants)

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

“Entwicklung von Methoden in der Theorie selbstadjungierter Erweiterungen” (Development of methods in the theory of self-adjoint extensions; in RG 1)

“Freie Randwertprobleme und Level-Set-Verfahren” (Free boundary problems and level-set methods; in RG 8)

“Rauhe stochastische Volatilität und verwandte Themen” (Rough stochastic volatility and related topics; in RG 6)

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

#### Leibniz-Gemeinschaft (Leibniz Association), Berlin

##### ■ Leibniz-Wettbewerb (Leibniz Competition)

“Probabilistische Methoden für Kommunikationsnetzwerke mit mobilen Relais” (Probabilistic methods for communication networks with mobile relays; July 2014 – June 2017, in LG 4)

#### Einstein Stiftung Berlin (Einstein Foundation Berlin)

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

This center was established in 2012 as a platform for mathematical initiatives in Berlin, such as, e.g., the Berlin Mathematical School, the German Centre for Mathematics Teacher Education (DZLM), and the MATHEON (see below).

In December 2016, the Director of WIAS, Prof. M. Hintermüller, was elected Chair of ECMath, Prof. A. Mielke member of the Executive Board, and Dr. M. Liero (RG 1), Scientific Employee Representative.

#### Research Center MATHEON

The highlight of the collaboration with the mathematical institutions in Berlin was again the joint operation of the Research Center MATHEON “Mathematics for key technologies”. Since June 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 September 2016, the reviewing for the second phase was successful, and the funding was extended until December 2018.

In 2016, WIAS again dedicated considerable financial and personal resources to the Center: Its director, Prof. M. Hintermüller (RG 8), and deputy directors, Prof. A. Mielke (RG 1) and Prof. W. König (RG 5), 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 “Energy and Materials”, Priv.-Doz. Dr. U. Bandelow (RG 2), Scientist in Charge of the Application Area D “Electronic and Photonic Devices”, Priv.-Doz. Dr. R. Henrion (RG 4), Scientist in Charge of the Application Area “Networks”; and WIAS members participated in the successful running of the following subprojects:

D-OT1: “Mathematical modeling, analysis, and optimization of strained germanium microbridges” (in RG 1 and RG 8)

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

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



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

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

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

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

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

- A DAAD-Mikhail Lomonosov Programme Fellowship holder (in RG 2); see page 191



#### 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). The project—a cooperation between WIAS and the DHI-WASY GmbH Berlin—was funded from 2014 to 2016 by the Investitionsbank Berlin in the framework of its “Pro FIT” program. Its main purpose was knowledge transfer on modern methods for partial differential equations (PDE) with stochastic coefficients from research to industry. It focused on the assessment of efficient methods for PDEs with stochastic coefficients and the selection of preferred methods to be implemented in the software of the project partner. In addition, the investigation of stochastic methods for inverse problems was started.

#### Helmholtz-Gemeinschaft (Helmholtz Association), Berlin/Bonn

- Virtual Institute: Microstructure Control for Thin-film Solar Cells

In this virtual institute, which is coordinated by the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), the formation of structural defects and related strain during the growth of thin-film solar cells is investigated by combining experimental as well as simulation approaches. The aim is to understand and control the formation of structural defects and strain during the growth of polycrystalline silicon and Cu(In,Ga)Se<sub>2</sub> (CIGSe) thin films by optimized growth parameters. RG 7 participates in the project “Modeling of interdiffusion in Cu-In-Se”.

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

- Three Humboldt Research Fellowship holders (in RG 6, RG 8, and ERC 1); see page 191

#### International projects

- Participation of the head of RG 6, Prof. V. Spokoiny, in the Grant 14-5000150 of the Russian Scientific Foundation at the Institute for Information Transmission Problems (IITP RAS) as a principal investigator and head of the Research Group PreMoLab (<http://premolab.ru/>), which was created within the Mega Grant of the Russian Government (<http://www.p220.ru/en/>)
- Fondation Mathématique Jacques Hadamard (FMJH): Optimisation dans l’incertain pour les problèmes de Unit Commitment (Optimization under uncertainty for unit commitment problems; in RG 4)

**Mission-oriented research (examples)**

- Deloitte & Touche GmbH Wirtschaftsprüfungsgesellschaftung: Development, implementation, and calibration of multiple-curve interest rate models and evaluation of corresponding interest rate products (in RG 6)
- General Electric (Switzerland) GmbH, Baden: “Prozesssimulation bei industriellen Gasturbinen” (Process simulation for industrial gas turbines; in RG 3 and RG 6)
- Mathshop Limited, Salisbury, Wiltshire, UK: Consulting contract (in RG 5)
- Orange Labs Research, Paris, France: “Continuum percolation theory applied to device-to-device” (in LG 4). This one-year research project aims at a deeper understanding of device-to-device networks based on the idea of network “überisation” using continuum percolation theory.
- 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). The aim of this two-year research and development cooperation was the development of improved algorithms and software for hybrid volumetric meshing based on Voronoi diagrams for geological models.
- TRUMPF Laser GmbH, Schemmberg: Consulting contract “Introduction to the simulation of the nonlinear dynamics of edge-emitting broad-area semiconductor lasers using the software BALaser” (in RG 2)



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

1. J. SPREKELS, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
2. ———, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
3. ———, Editorial Board, Advances in Mathematical Sciences and Applications, Gakkōtoshō, Tokyo, Japan.
4. ———, Editorial Board, Applied Mathematics and Optimization, Springer-Verlag, New York, USA.
5. P. FRIZ, Editorial Board, Monatshefte der Mathematik, Springer-Verlag, Berlin.
6. ———, Editorial Board, Stochastic Processes and Applications, Elsevier, Oxford, UK.
7. ———, Editorial Board, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
8. R. HENRION, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
9. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
10. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
11. ———, Editorial Board, Mathematical Programming, Series A, Springer-Verlag, Heidelberg.
12. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
13. M. HINTERMÜLLER, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
14. ———, Editorial Board, Optimization Methods and Software, Taylor & Francis, Oxford, UK.
15. ———, Editorial Board, SIAM Journal on Scientific Computing, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
16. ———, Editorial Board, SIAM Journal on Numerical Analysis, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
17. ———, Series Editor, International Series of Numerical Mathematics, Springer-Verlag, Basel, Switzerland.
18. ———, Series Editor, Handbook of Numerical Analysis, Elsevier, Amsterdam, Netherlands.
19. D. HÖMBERG, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
20. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
21. V. JOHN, Series Editor, Lecture Notes in Mathematical Fluid Mechanics, Birkhäuser Verlag, Basel, Switzerland.
22. W. KÖNIG, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
23. ———, Area Editor, Bernoulli Journal, International Statistical Institute/Bernoulli Society for Mathematical Statistics and Probability, The Hague, Netherlands.
24. ———, Series Editor, Pathways in Mathematics, Birkhäuser, Basel, Switzerland.

<sup>2</sup>Memberships in editorial boards by nonresident members have been listed in front of those by the WIAS staff members.

25. P. MATHÉ, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
26. ———, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, Netherlands.
27. A. MIELKE, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
28. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
29. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
30. ———, Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
31. H. NEIDHARDT, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russian Federation.
32. ———, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
33. ———, Editorial Board, Journal of Operators, Hindawi Publishing Corporation, New York, USA.
34. J. POLZEHL, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
35. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, Netherlands.
36. J.G.M. SCHOENMAKERS, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
37. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
38. ———, Editorial Board, Applied Mathematical Finance, Taylor & Francis, Oxford, UK.
39. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
40. V. SPOKOINY, Editor, Theory of Probability and its Applications, SIAM, Philadelphia, Pennsylvania, USA.
41. B. WAGNER, Editorial Board, Journal of Engineering Mathematics, Springer-Verlag, Dordrecht, Netherlands.
42. 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

1ST LEIBNIZ MMS DAYS

Berlin, January 27–29

Organized by: WIAS

The first Leibniz MMS Days were an activity of the Leibniz Network “Mathematical Modeling and Simulation” (MMS) coordinated by WIAS. It was intended for Leibniz institutions and brought together participants from varied fields from natural to social sciences. Fifty-one scientists from 23 Leibniz institutes took part in the workshop. The goal was to systematically exploit the potential of modern methods of MMS and create synergy effects. In order to account for thematic diversity, the workshop comprised both general plenary discussions and smaller groups focused on specific themes.

Two keynote talks were delivered. Rupert Klein (Freie Universität Berlin) explained “How math helps structuring climate discussions” and Konrad Poltner (also Freie Universität Berlin) talked about “Discrete mathematics for geometry processing”.

ERC WORKSHOP ON MODELING MATERIALS AND FLUIDS USING VARIATIONAL METHODS

Berlin, February 22–26

Organized by: WIAS (RG 1 and ERC 1)

Supported by: ERC Advanced Grant “Analysis of Multiscale Systems Driven by Functionals” and ERC Starting Grant “Entropy Formulation of Evolutionary Phase Transitions”

This workshop was focused on the use of variational methods for the modeling, analysis, and simulation of materials and fluids with heterogeneous and multiscale structures. The program featured 18 invited lectures and 12 additional invited speakers and was attended by 51 participants. The workshop included the topics of

- phase transitions and plasticity in elastic materials
- damage, delamination, adhesion, and contact problems
- nonlinear nonlocal equations modeling interacting fluids dynamics
- bulk-interface interactions, diffuse interface models for special materials like liquid crystals, shape memory materials, polymers, biomaterials, ferromagnetic materials
- chemical reaction-diffusion systems
- mathematical methods for dissipative evolution with a gradient structure, including evolutionary Gamma-convergence



#### WIAS–PGMO WORKSHOP ON NONSMOOTH AND STOCHASTIC OPTIMIZATION WITH APPLICATIONS TO ENERGY MANAGEMENT

Berlin, May 10–12

Organized by: WIAS (RG 4)

Supported by: WIAS, Fondation Mathématique Jacques Hadamard, DFG Collaborative Research Center/Transregio 154 *Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks*, Einstein Center for Mathematics Berlin, Gaspard Monge Program for Optimization and Operations Research (PGMO)

The aim of this workshop was to bring together ideas from nonsmooth optimization/variational analysis and stochastic optimization, which is motivated by many applications in energy management (e.g., analysis of market equilibria, optimal quantization, probabilistic constraints, conditioning of stochastic programs). Altogether, 34 participants from six countries presented talks on various aspects of nonsmooth or stochastic optimization, such as the theory of subdifferentials and multifunctions or optimization problems under probabilistic constraints.

#### NONLINEAR DYNAMICS IN SEMICONDUCTOR LASERS (NDSL2016)

Berlin, June 15–17

Organized by: WIAS (RG 2)

Supported by: DFG Collaborative Research Center (SFB) 787 *Semiconductor Nanophotonics*, WIAS

This workshop was organized with the support of SFB 787 and was focused on the discussion of novel technological trends and modeling approaches in optoelectronics. The aim of the three-day workshop was to bring together applied mathematicians, physicists, and engineers in order to provide them an opportunity to exchange knowledge and latest developments with their colleagues and young scientists by presenting their recent theoretical and experimental results in the field of nonlinear phenomena in optoelectronic devices. The subjects of the workshop included: dynamics of high-power tapered and broad-area lasers and amplifiers, vertical-cavity surface-emitting lasers, micro- and nanolasers, photonic crystal lasers, ring and multisection lasers, mode-locked lasers, lasers with delayed feedback, and synchronization of laser arrays. Special attention was focused on the consideration of the field and carrier dynamics of quantum well and quantum dot lasers and amplifiers, the investigation of spatially and temporally localized structures of light, the application of the bifurcation theory and numerical methods to the analysis of optoelectronic devices, model reduction using the dynamical systems theory, and the application of the singular perturbation theory in the field of nonlinear optics. The program featured 35 invited and contributed talks presented by speakers from 10 countries, 6 poster presentations, and was attended by 53 registered participants.



Fig. 1: NewMET2016

#### NEW METHODS IN EXTENSION THEORY APPLIED TO QUANTUM MECHANICS (NewMET2016)

Berlin, July 14–15

Organized by: Hagen Neidhardt (RG 1), Johannes Brasche (Technische Universität Clausthal)

Supported by: Deutsche Forschungsgemeinschaft (DFG)

NewMET2016 is a part of the DFG project “Development of methods in the theory of self-adjoint extensions”.

Its aim was to bring together mathematicians and physicists interested in mathematical problems of quantum mechanics that are related to extension theory in a very general sense. The idea was to use the workshop to brainstorm for the DFG project, which was very successful. The participants gave a lot of suggestions for the realization of the project in the next years. The workshop was attended by 25 scientists from all over the world. Twenty-two talks were given, among them 17 by invited speakers. The desire was expressed to repeat the workshop in the next year.

#### 5TH ANNUAL ERC BERLIN–OXFORD YOUNG RESEARCHERS MEETING ON APPLIED STOCHASTIC ANALYSIS

Berlin, September 12–15

Organized by: WIAS (RG 6), TU Berlin, Oxford University

Supported by: European Research Council, WIAS

The workshop focused on rough path analysis and its rapidly growing applications in applied stochastic analysis, ranging from the resolution of ill-posed stochastic partial differential equations to new ways of handling high-dimensional data. More precisely, rough paths and related topics nowadays lead to significant progress in a broad variety of fields, such as nonlinear stochastic partial differential equations, regularity structures, scaling limits and discrete approximation for stochastic partial differential equations, expected signatures, stochastic Loewner evolution, statistics and machine learning, Gaussian rough path analysis, and numerical analysis for stochastic and rough differential equations.

The three-day workshop attracted about 35 participants and featured 21 invited speakers, mostly early career researchers from Berlin, Oxford, and Warwick, on topics related to the afore-mentioned fields. It was jointly organized by WIAS RG 6 (Peter Friz – ERC funded, Mario Maurelli), Technische Universität Berlin (Khalil Chouk), and Oxford University (Terry Lyons – ERC funded, Horatio Boedihardjo, Harald Oberhauser). A sixth Berlin–Oxford meeting was announced to take place in Oxford from December 8 to 10, 2016.

#### CONFERENCE IN HONOR OF THE 75TH BIRTHDAY OF S.R.S. VARADHAN

Berlin, August 15–19

Organized by: WIAS (RG 5 and RG 6) and TU Berlin

Supported by: European Research Council, Einstein Center for Mathematics Berlin, Berlin Mathematical School, Research Training Group 1845 *Stochastic Analysis with Applications in Biology, Finance and Physics*, DFG

WIAS had the great honor to be the main organizer of an international workshop in honor of the 75th birthday of one of the most influential and well-known probabilists of our time, S.R.S. Varadhan (Courant Institute New York), whose works on large deviations, stochastic analysis, random media, and much more are renowned. Several of his most important collaborators followed the invitation to celebrate this event by delivering talks on all the subjects to which Prof. Varadhan had given enormous inputs, like homogenization, large deviations, random walks in random environments, statistical mechanics of interacting random motions, and hydrodynamic limits.

This one-week workshop featured about 25 speakers (many of whom from the US and South-America) and attracted about 80 participants from Berlin, various parts of Germany, and from abroad. It took place in the Main Building of the Technische Universität (TU) Berlin with all coffee breaks being held in its beautiful air well (“Lichthof”). The workshop was jointly organized by the WIAS Research Groups RG 6 (Peter Friz) and RG 5 (Wolfgang König and Chiranjib Mukherjee) and the TU Berlin. The external organizer was Stefano Olla (Paris). In particular, the ERC funding by Prof. Friz’ grant is gratefully acknowledged.

#### 1ST LEIBNIZ MMS MINI WORKSHOP ON CFD & GFD

Berlin, September 8–9

Organized by: WIAS (RG 3) and others

Within the Leibniz Network “Mathematical Modelling and Simulation” (MMS), in September 2016 the “1st Leibniz MMS Mini Workshop on CFD & GFD” was organized at WIAS. The idea was developed during the Leibniz MMS Days in January 2016, where it was realized that simulations in Computational Fluid Dynamics (CFD) and

Geophysical Fluid Dynamics (GFD) are regularly performed at several Leibniz institutes and that a number of Leibniz institutes conduct independent research on several aspects of simulation algorithms.

Twenty-three members, from 10 different Leibniz institutes, participated in the workshop, coming from as different disciplines as agriculture, atmospheric physics, geophysics, oceanography, crystal growth, and microelectronics. Thirteen talks and 6 posters were presented to identify open questions, find possible collaborations among Leibniz institutes, and get helpful advice from other participants. Much time was devoted to two discussion rounds in which ideas for exchange and cooperation within the Leibniz Network MMS were developed. The next meeting of the “Special Interest Group CFD & GFD” within the Leibniz MMS Network is planned for February 2017 during the Leibniz MMS Days in Hanover.

The workshop was jointly organized by Erich Becker (IAP K hlungsborn), Georg Feulner (PIK, Potsdam), Oswald Knoth (TROPOS Leipzig), and Alexander Linke (WIAS, RG 3).

#### WIAS/GAMM/TUM SUMMER SCHOOL ON UNCERTAINTY QUANTIFICATION

Berlin, September 12–16

Organized by: International Association of Applied Mathematics and Mechanics (GAMM), Technische Universit t M nchen, WIAS (RG 4)

Supported by: International Research and Training Group Munich–Graz (IGDK 1754), WIAS, Einstein Center for Mathematics Berlin

Quantifying the impact of uncertainties on responses of interest in mathematical models has become an active field of research over the past years in many disciplines such as structural mechanics, materials science, fluid dynamics, geophysics, and systems biology. The main objective of the summer school was to address important mathematical concepts of uncertainty quantification and the related computational and algorithmic challenges arising in the numerous engineering and science disciplines and to introduce these to master and Ph.D. students.

Sixty participants from 11 countries attended the lectures and lab sessions covering low-rank tensor representations, Bayesian inversion, polynomial surrogate models, and modern Monte Carlo methods, which were presented by five internationally renowned researchers.

#### DYNAMICS OF DELAY EQUATIONS, THEORY AND APPLICATIONS

Berlin, October 12–14

Organized by: WIAS (RG 2)

Supported by: Collaborative Research Center (SFB) 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*, WIAS

The aim of this workshop was to discuss recent developments in the field of delay-differential equations. These equations are an important tool for the modeling of dynamical phenomena in various fields of science, including neuroscience, optoelectronics, as well as biological or mechanical systems. They allow for the description of potentially high-dimensional dynamical effects caused by delayed feedback or control, aging, and finite transmission speed. From a mathematical point of view, they represent an important class of dynamical systems and can be studied by advanced mathematical methods, including, e.g., bifurcation theory, singular perturbations, or semigroup theory. The program featured 31 invited and contributed talks presented by speakers from 11 countries and was attended by 39 registered participants.

#### KICK-OFF MEETING OF THE DFG PRIORITY PROGRAMME 1962

Berlin, October 27–28

Organized by: WIAS (RG 8)

Supported by: DFG, WIAS

The event at WIAS on October 27–28 was the first meeting of the members of the new Priority Programme (SPP) *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization*, which is coordinated by the Director of WIAS, Prof. Michael Hinterm ller. The aim of the meeting

was to familiarize the members with each of the 24 projects in the SPP and to meet and network with the other members, initializing the dialogue for possible links and collaborations within the SPP in different projects. Presentations for each project were given describing the aims and goals as well as the first research steps and directions for the continuation of the work, and concrete collaborations were identified. The principal investigators also took part in discussions about the overall structures, activities, and future direction for the new SPP. The two-day event was well attended from members throughout Germany, and plans regarding future activities for the whole SPP group as well as separate activities for Ph.D. students and younger postdocs were discussed.

#### WORKSHOP ON PROBABILISTIC METHODS IN TELECOMMUNICATION

Berlin, November 14–16

Organized by: WIAS (LG 4 and RG 5) and IHP Frankfurt (Oder)

Supported by: Leibniz Association

The interdisciplinary workshop brought together mathematicians and engineers working at the interface of probabilistic spatial models and wireless networks. The three-day event featured presentations from both communities and thereby provided the breeding ground for a lively exchange of ideas.

The scientific program was composed of a mini-course taught by a world-class expert, ten research talks by distinguished invited speakers, and a poster session. In the presentations, the common topic was approached from multiple points of views, including, e.g., random graph theory, graph coloring problems, fading and shadowing analysis, algorithmic efficiency, large deviations, and cell-free massive multiple-input multiple-output approaches.

The workshop was attended by about 50 mostly European participants with backgrounds ranging from mathematics to information theory to telecommunication engineering. It was jointly organized by the WIAS Leibniz Group “Probabilistic Methods for Mobile Ad-hoc Networks” and the Leibniz Institute for Innovative Microelectronics (IHP).

#### AG DANK AUTUMN MEETING 2016

Berlin, November 18–19

Organized by: WIAS (RG 6)

Supported by: Gesellschaft für Klassifikation e.V. (GfKL, Data Science Society), WIAS

In 2016, the annual autumn meeting of the AG DANK took place in Berlin at the Erhard-Schmidt lecture hall of the Weierstrass Institute. As indicated by its name “**D**aten**A**nalyse und **N**umerische **K**lassifikation”, the working group (“AG DANK”) deals with the statistical analysis of data in a broad sense with a focus on supervised and unsupervised classification. The workshop continued the topic of the 2015 meeting held at the Karlsruhe Institute of Technology: recent developments of big data analysis and data science. This time, the focus was mainly directed on statistical problems of (necessary) data preprocessing, such as transformations, variable selection, and dimension reduction in clustering and classification. Here, the aim was to bring together leading statisticians and scientists working in life sciences for discussing applications of classification/clustering to neural sciences, genetics, market research, archaeometry, and the like. The program started with four invited lectures. Altogether, 16 talks were presented. The meeting was attended by 24 participants.

As usual for the autumn meetings, the participants could take part in a competition. This time, the task was statistical clustering of data from a flame plasma electrochemical sensor, i.e., asking for the cluster membership of 120 particulates. The dataset was delivered by Christian Hennig (University College London). The three book prizes were donated by WIAS.

## FREE BOUNDARY, PARTIAL DIFFERENTIAL EQUATIONS AND RELATED TOPICS

Berlin, December 19–20

Organized by: WIAS (ERC 1 and RG 8)

Supported by: European Research Council, Italian Ministry of Education (MIUR)

This workshop was the conclusion of Enrico Valdinoci's ERC Starting Grant "EPSILON – Elliptic Partial Differential Equations and Symmetry of Interfaces and Layers for Odd Nonlinearities", which was organized by him and the WIAS Director, Michael Hintermüller, with the aim to gather distinguished European researchers and promising young mathematicians working in the vast and important fields of free boundary, PDEs, calculus of variations, and related subjects.

In a friendly and stimulating environment, the 17 participants from seven countries shared their results and discussed further developments and open problems. The workshop also linked the past research with the future perspectives and bridged the theory to the applications. Nine invited talks were given.

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

## PATTERNS OF DYNAMICS

Berlin, July 25–29

Organized by: Freie Universität Berlin, WIAS (RG 1), Max Planck Institute for Mathematics in the Sciences, Brown University (Providence/USA), University of Minnesota (USA), Westfälische Wilhelms-Universität Münster, Technische Universität Berlin

Supported by: DFG, FU Berlin, TU Berlin, WIAS, HU Berlin, Collaborative Research Center (SFB) 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*, Collaborative Research Center (SFB) 647 *Space – Time – Matter. Analytic and Geometric Structures*, Berlin Mathematical School (BMS)

The conference was devoted to recent advances of dynamical systems theory and their interplay with a wide range of applications in the sciences and engineering. Speakers from four different continents presented their results related to the mathematical theory on formation, dynamics, and control of spatio-temporal patterns together with various applications to experiments and real-world dynamics.

Overall, 13 keynote, 35 invited and 38 contributed talks, as well as 8 posters were presented. The conference was organized in honor of the 60th birthday of Bernold Fiedler, emphasizing his vital role for the scientific community in this field of science within Berlin and worldwide.

The organizing committee was joining members from Berlin universities and institutions (FU, TU, HU, WIAS, SFB 910, SFB 647, BMS) with outstanding international scientists. The participation of two members of WIAS, Alexander Mielke (RG 1) and Matthias Wolfrum (RG 2), in this group underlines the importance of this mathematical field for WIAS as well as the longstanding connections to Prof. Fiedler and his group.



## OPTIMAL TRANSPORTATION AND APPLICATIONS

Pisa (Italy), November 7–11

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

Supported by: Scuola Normale Superiore de Pisa and ERC Advanced Grant "Analysis of Multiscale Systems Driven by Functionals"

The eighth edition of this traditional meeting in Pisa successfully continued its mission of bringing together leading experts as well as newcomers to discuss new topics, methods, and results in the theory of optimal transport.

Despite being a classical topic, whose origin dates back to the fundamental work of Monge in the late 18th century, optimal transportation theory still has a surprising relevance in modern mathematical disciplines and



applications. In particular, in the workshop novel topics in connection to optimal transport were presented, e.g., mean field games, optimal transport formulation of density functional theory in quantum mechanics, gradient flow structures of Boltzmann equation and dissipative quantum systems, learning and sparse control of multiagent systems, multiphase flows in porous media, evolution of dislocations in crystal lattices, handling of big data in large-scale networks, and (unbalanced) entropy transport problems. However, recent progress in classical questions, such as curvature conditions in metric spaces and their generalizations as well as improved functional inequalities, was addressed, too. Finally, also computational aspects of optimal transport and related problems were extensively discussed. The workshop attracted about 70 participants from the USA, Japan, and Europe and featured 29 invited speakers.

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

WORKSHOP “ROUGH PATHS, REGULARITY STRUCTURES AND RELATED TOPICS”

Mathematisches Forschungsinstitut Oberwolfach, May 1 – 7

Organized by: Thomas Cass (London), Massimiliano Gubinelli (Paris), Peter Friz (PI of the ERC project of the same name, TU Berlin and RG 6)

This workshop took place in early summer 2016, effectively a continuation of the 2012 meeting “Rough Paths and PDEs” remembered for the initial presentation by Martin Hairer (Warwick, Fields Medal 2014) of what is now famously known as *Regularity Structures*. A large part of the 2016 meeting was thus devoted to singular stochastic partial differential equations, now studied either by regularity structures or the competing paracontrolled approach due to Gubinelli, Imkeller, and Perkowski. Another part of the meeting was devoted to “classical” rough path theory à la Terry Lyons. More than 50 invited participants attended the workshop. These scientists came from a diverse set of countries and young mathematicians were especially wellrepresented among them.

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

1. J. SPREKELS, co-organizer, *International INdAM Conference “Optimal Control for Evolutionary PDEs and Related Topics (OCERTO 2016)”*, Cortona, Italy, June 20–24.
2. N. AHMED, co-organizer, *International Conference on Differential Equations and Applications*, Lahore University of Management Sciences, Pakistan, May 26–28.
3. A. CAIAZZO, co-organizer of the Minisymposium 33 “Open Boundary Conditions for Incompressible Flows: Theoretical and Practical Aspects”, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
4. K. DISSER, co-organizer of the Young Researchers’ Minisymposium “Multiscale Evolutionary Problems”, *Joint Annual Meeting of DMV and GAMM*, Technische Universität Braunschweig, March 7–11.
5. P.-É. DRUET, organizer of the Minisymposium 03 “Analysis of Thermodynamically Consistent Models of Electrolytes in the Context of Battery Research”, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
6. M. EIGEL, co-organizer of the Minisymposium 67 “Bayesian Inversion and Low-rank Approximation” (Part I+II), *SIAM Conference on Uncertainty Quantification*, Lausanne, Switzerland, April 5–8.
7. P. FARRELL, D. PESCHKA, N. ROTUNDO, co-organizers of the Minisymposium 23 “Charge Transport in Semiconductor Materials: Emerging and Established Mathematical Topics”, *The 19th European Conference on Mathematics for Industry (ECMI 2016)*, Universidade de Santiago de Compostela, Spain, June 13–17.
8. ———, co-organizers of the Minisymposium 22 “Mathematical Methods for Semiconductors”, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
9. P. FRIZ, organizer, *International Scientific Workshop: Paths to, from and in Renormalisation*, Universität Potsdam, Institut für Mathematik, February 8–12.
10. ———, scientific organizer, *Berlin–Leipzig Workshop in Analysis and Stochastics*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, April 13–15.
11. ———, organizer, *Workshop “Rough Paths, Regularity Structures and Related Topics”*, Mathematisches Forschungsinstitut Oberwolfach, May 1–7.
12. ———, organizer, *Rough Volatility Meeting*, Imperial College London, Department of Mathematics, UK, October 7–8.
13. ———, organizer, *6th Berlin–Oxford Meeting*, University of Oxford, Mathematics Department, UK, December 8–10.
14. J. FUHRMANN, organizer of the Minisymposium “Generalized Drift-Diffusion Equations in Semiconductors, Electrochemical Systems and Beyond: Models, Algorithms and Open Questions”, *Conference on Scientific Computing (ALGORITMY 2016)*, Slovak University of Technology, Department of Mathematics and Descriptive Geometry, Podbanské, Slovakia, March 14–18.
15. M. HINTERMÜLLER, co-organizer of the Minisymposia “Non-Convex Regularization Methods in Image Restoration – Part I and II”, *SIAM Conference on Imaging Science*, Albuquerque, USA, May 23–26.
16. ———, co-organizer, *BMS Summer School “Mathematical and Numerical Methods in Image Processing”*, Berlin Mathematical School, Technische Universität Berlin, Humboldt-Universität zu Berlin, July 25 – August 5.

<sup>3</sup>Membership in organizing committees of non-WIAS meetings by nonresident members have been listed in front of those by the WIAS staff members.

17. ———, co-organizer, *Imaging with Modulated/Incomplete Data 2016*, SFB Research Center: Mathematical Optimization and Applications in Biomedical Sciences (MOBIS), Graz, Austria, September 22–24.
18. D. HÖMBERG, co-organizer of the Minisymposium 38 “Maths in HORIZON 2020 and Beyond”, *The 19th European Conference on Mathematics for Industry (ECMI 2016)*, Universidade de Santiago de Compostela, Spain, June 13–17.
19. ———, member of the Scientific Committee, *The 19th European Conference on Mathematics for Industry (ECMI 2016)*, Universidade de Santiago de Compostela, Spain, June 13–17.
20. ———, organizer of the Minisymposium 37 “Maths for the Digital Factory”, *The 19th European Conference on Mathematics for Industry (ECMI 2016)*, Universidade de Santiago de Compostela, Spain, June 13–17.
21. ———, member of the Program Committee, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
22. ———, member of the Organizing Committee, *Math Meets Industry*, Trondheim, Norway, September 22–23.
23. V. JOHN, organizer of the Minisymposium “Finite Element Methods for Convection-Dominated Problems”, *15th Conference on the Mathematics of Finite Elements and Applications 2016 (Brunel MAFELAP 2016)*, Brunel University London, Uxbridge, UK, June 14–17.
24. O. KLEIN, member of the Steering Committee, *Murphys-HSFS 2016 Workshop*, Centre de Recerca Matemàtica, Barcelona, Spain, June 13–17.
25. W. KÖNIG, member of the Local Organizing Committee, the Grant Committee, and the Satellite Event Committee, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
26. ———, co-organizer, *Conference in Honor of the 75th Birthday of S.R.S. Varadhan*, Technische Universität Berlin, August 15–19.
27. TH. KOPRUCKI, member of the Steering Committee, *16th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD16)*, University of Sydney, Australia, July 11–15.
28. A. MIELKE, co-organizer, *Program “Nonlinear Flows” with a lecture series (May – June 2016) and two workshops*, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, May 30 – July 15.
29. ———, co-organizer, *Workshop “Entropy Methods, Dissipative Systems, and Applications” in the Program “Nonlinear Flows” (May 30 to July 17, 2016)*, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, June 13–17.
30. ———, co-organizer, *Berlin Dresden Prague Würzburg Workshop “Homogenization and Related Topics”*, Technische Universität Dresden, Fachbereich Mathematik, June 22.
31. ———, co-organizer, *Workshop “Variational and Hamiltonian Structures: Models and Methods” in the Program “Nonlinear Flows” (May 30 to July 17, 2016)*, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, July 11–15.
32. ———, member of the Scientific Committee, the Local Organizing Committee, and the Program Committee, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
33. ———, co-organizer of the Minisymposium “Deformation Accumulation in Seismic Faults and Networks”, *SCCS Days, CRC 1114 “Complex Processes Involving Cascades of Scales”*, Ketzin, October 10–12.
34. ———, co-organizer, *Berlin Dresden Prague Würzburg Workshop “Mathematics of Continuum Mechanics”*, Technische Universität Dresden, Fachbereich Mathematik, December 5.
35. M. MITTENZWEIG, course tutor, *Eine Naturwissenschaftliche Reise hinter das Display eines Smartphones*, Deutsche Schülerakademie, Braunschweig, July 4–8.

36. CH. MUKHERJEE, co-organizer, *Conference in Honor of the 75th Birthday of S.R.S. Varadhan*, Technische Universität Berlin, August 15–19.
37. S. REICHEL, co-organizer, *International Conference on Control of Complex Systems and Networks*, SFB 910 “Control of Self-Organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, Heringsdorf/Usedom, September 4–8.
38. E. ROCCA, co-organizer, *Perspectives in Applied PDEs: A Day in Pavia*, Università di Pavia, Italy, February 9.
39. ———, co-organizer, *International INdAM Conference “Optimal Control for Evolutionary PDEs and Related Topics (OCERTO 2016)”*, Cortona, Italy, June 20–24.
40. H. SI, member of the Organizing Committee, *25th International Meshing Roundtable and User Forum*, Sandia National Laboratories, Washington, DC, USA, September 27–30.
41. V. SPOKOINY, co-organizer, *Workshop on Modern Statistics and Optimization*, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, February 23–24.
42. ———, member of the Program Committee, *Information Technology and Systems 2016*, Russian Academy of Sciences, Institute for Information Transmission Problems, St. Petersburg, September 25–30.
43. M. THOMAS, co-organizer of the Special Session 68 “Rate-dependent and Rate-independent Evolution Problems in Continuum Mechanics: Analytical and Numerical Aspects”, *The 11th AIMS Conference on Dynamical Systems, Differential Equations and Applications*, The American Institute of Mathematical Sciences, Orlando (Florida), USA, July 1–5.
44. ———, co-organizer of the Minisymposium 29 “Nonsmooth PDEs in the Modeling Damage, Delamination, and Fracture”, *7th European Congress of Mathematics (7ECM)*, Technische Universität Berlin, July 18–22.
45. N. TOGOBYTSKA, co-organizer of the Minisymposium 26 “Stochastic Inverse Problems”, *The 19th European Conference on Mathematics for Industry (ECMI 2016)*, Universidade de Santiago de Compostela, Spain, June 13–17.
46. E. VALDINOCI, co-organizer, *Otto-von-Guericke-School in Partial Differential Equations*, Otto-von-Guericke-Universität Magdeburg, March 14–16.
47. ———, co-organizer, *Research Meeting on Non-Local Operators (RMNLO)*, Università di Cagliari, Italy, October 6–8.
48. ———, co-organizer, *Workshop on Recent Trends in the Analysis of PDEs*, IMATI-CNR, Pavia, Italy, October 19–21.
49. B. WAGNER, member of the Scientific Committee, *The 19th European Conference on Mathematics for Industry (ECMI 2016)*, Universidade de Santiago de Compostela, Spain, June 13–17.
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51. ———, co-organizer, *European Summer School in Modelling, Analysis and Simulation: Crime and Image Processing*, University of Oxford, Mathematical Institute, UK, July 4–8.

## A.6 Publications

### A.6.1 Monographs

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- [2] W. KÖNIG, *The Parabolic Anderson Model – Random Walks in Random Potential*, Pathways in Mathematics, Birkhäuser, Basel, 2016, xi+192 pages.
- [3] C. BUCUR, E. VALDINOCI, *Nonlocal Diffusion and Applications*, no. 20 in Lecture Notes of the Unione Matematica Italiana, Springer International Publishing Switzerland, Cham, 2016, xii+155 pages.

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- [1] M. DIMIAN, P. GUREVICH, O. KLEIN, D. KNEES, D. RACHINSKII, S. TIKHOMIROV, eds., *MURPHYS-HSFS-2014: 7th International Workshop on Multi-Rate Processes and HYSteresis (MURPHYS) & 2nd International Workshop on Hysteresis and Slow-Fast Systems (HSFS)*, vol. 727 of Journal of Physics: Conference Series, no. 1, IOP Publishing, 2016, 252 pages. Open Access: <http://iopscience.iop.org/issue/1742-6596/727/1>.
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### A.6.3 Outstanding Contributions to Monographs

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A.6.4 Articles in Refereed Journals<sup>4</sup>

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## A.7 Preprints, Reports

### A.7.1 WIAS Preprints Series<sup>5</sup>

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- [4] ———, *Distributed optimal control of a nonstandard nonlocal phase field system with double obstacle potential*, Preprint no. 2277, WIAS, Berlin, 2016.
- [5] ———, *Global existence for a nonstandard viscous Cahn–Hilliard system with dynamic boundary condition*, Preprint no. 2284, WIAS, Berlin, 2016.
- [6] ———, *Optimal boundary control of a nonstandard viscous Cahn–Hilliard system with dynamic boundary condition*, Preprint no. 2307, WIAS, Berlin, 2016.
- [7] S. OLMI, A. TORCINI, *Chimera states in pulse coupled neural networks: The influence of dilution and noise*, Preprint no. 2305, WIAS, Berlin, 2016.
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- [10] N. AHMED, S. BECHER, G. MATTHIES, *Higher-order discontinuous Galerkin time stepping and local projection stabilization techniques for the transient Stokes problem*, Preprint no. 2253, WIAS, Berlin, 2016.
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- [13] N. AHMED, V. JOHN, G. MATTHIES, J. NOVO, *A local projection stabilization/continuous Galerkin–Petrov method for incompressible flow problems*, Preprint no. 2347, WIAS, Berlin, 2016.
- [14] A. ALPHONSE, CH.M. ELLIOTT, J. TERRA, *A coupled ligand-receptor bulk-surface system on a moving domain: Well posedness, regularity and convergence to equilibrium*, Preprint no. 2357, WIAS, Berlin, 2016.
- [15] V. AVANESOV, J. POLZEHL, K. TABELOW, *Consistency results and confidence intervals for adaptive  $l_1$ -penalized estimators of the high-dimensional sparse precision matrix*, Preprint no. 2229, WIAS, Berlin, 2016.
- [16] A. ANKIEWICZ, D.J. KEDZIORA, A. CHOWDURY, U. BANDELOW, N. AKHMEDIEV, *Infinite hierarchy of nonlinear Schrödinger equations and their solutions*, Preprint no. 2208, WIAS, Berlin, 2016.
- [17] CH. BAYER, M. SIEBENMORGEN, R. TEMPONE, *Smoothing the payoff for efficient computation of basket option prices*, Preprint no. 2280, WIAS, Berlin, 2016.
- [18] S. BIRKHOLZ, C. BRÉE, I. VESELIĆ, A. DEMIRCAN, G. STEINMEYER, *Ocean rogue waves and their phase space dynamics in the limit of a linear interference model*, Preprint no. 2335, WIAS, Berlin, 2016.

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- [58] H. HEITSCH, H. LEÖVEY, W. RÖMISCH, *Are quasi-Monte Carlo algorithms efficient for two-stage stochastic programs?*, Preprint no. 2245, WIAS, Berlin, 2016.
- [59] L. ADAM, R. HENRION, J. OUTRATA, *On  $M$ -stationarity conditions in MPECs and the associated qualification conditions*, Preprint no. 2215, WIAS, Berlin, 2016.



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- [62] R. HILDEBRAND, *Copositive matrices with circulant zero pattern*, Preprint no. 2241, WIAS, Berlin, 2016.
- [63] L. ADAM, M. HINTERMÜLLER, TH.M. SUROWIEC, *A semismooth Newton method with analytical path-following for the  $H^1$ -projection onto the Gibbs simplex*, Preprint no. 2340, WIAS, Berlin, 2016.
- [64] M. HINTERMÜLLER, M. HINZE, CH. KAHLE, T. KEIL, *A goal-oriented dual-weighted adaptive finite element approach for the optimal control of a nonsmooth Cahn–Hilliard–Navier–Stokes system*, Preprint no. 2311, WIAS, Berlin, 2016.
- [65] M. HINTERMÜLLER, K. PAPAFITSOROS, C.N. RAUTENBERG, *Analytical aspects of spatially adapted total variation regularisation*, Preprint no. 2293, WIAS, Berlin, 2016.
- [66] M. HINTERMÜLLER, C.N. RAUTENBERG, *On the uniqueness and numerical approximation of solutions to certain parabolic quasi-variational inequalities*, Preprint no. 2237, WIAS, Berlin, 2016.
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- [68] M. HINTERMÜLLER, C.N. RAUTENBERG, M. MOHAMMADI, M. KANITSAR, *Optimal sensor placement: A robust approach*, Preprint no. 2287, WIAS, Berlin, 2016.
- [69] M. HINTERMÜLLER, C.N. RAUTENBERG, S. RÖSEL, *Density of convex intersections and applications*, Preprint no. 2333, WIAS, Berlin, 2016.
- [70] M. HINTERMÜLLER, C.N. RAUTENBERG, T. WU, A. LANGER, *Optimal selection of the regularization function in a generalized total variation model. Part II: Algorithm, its analysis and numerical tests*, Preprint no. 2236, WIAS, Berlin, 2016.
- [71] D. COUPIER, CH. HIRSCH, *Coalescence of Euclidean geodesics on the Poisson–Delaunay triangulation*, Preprint no. 2243, WIAS, Berlin, 2016.
- [72] CH. HIRSCH, B. JAHNEL, P. KEELER, R.I.A. PATTERSON, *Traffic flow densities in large transport networks*, Preprint no. 2221, WIAS, Berlin, 2016.
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- [74] M. HOFMANN, C. BRÉE, *Adiabatic Floquet model for the optical response in femtosecond filaments*, Preprint no. 2217, WIAS, Berlin, 2016.
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- [76] D. HÖMBERG, O. ROTT, K. STURM, *Discretisation and error analysis for a mathematical model of milling processes*, Preprint no. 2364, WIAS, Berlin, 2016.
- [77] T. ABBAS, H. AMMARI, G. HU, A. WAHAB, J.C. YE, *Elastic scattering coefficients and enhancement of nearly elastic cloaking*, Preprint no. 2275, WIAS, Berlin, 2016.
- [78] G. BAO, G. HU, T. YIN, J. SUN, *Direct and inverse elastic scattering from anisotropic media*, Preprint no. 2348, WIAS, Berlin, 2016.
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- [80] G. HU, M. SALO, E.V. VESALAINEN, *Shape identification in inverse medium scattering problems with a single far-field pattern*, Preprint no. 2222, WIAS, Berlin, 2016.

- [81] T. YIN, G. HU, L. XU, B. ZHANG, *Near-field imaging of obstacles with the factorization method: Fluid-solid interaction*, Preprint no. 2224, WIAS, Berlin, 2016.
- [82] J. ELSCHNER, G. HU, *Acoustic scattering from corners, edges and circular cones*, Preprint no. 2242, WIAS, Berlin, 2016.
- [83] B. JAHNEL, CH. KÜLSKE, *The Widom–Rowlinson model under spin flip: Immediate loss and sharp recovery of quasilocality*, Preprint no. 2297, WIAS, Berlin, 2016.
- [84] W. HUANG, L. KAMENSKI, *On the mesh nonsingularity of the moving mesh PDE method*, Preprint no. 2218, WIAS, Berlin, 2016.
- [85] M. KANTNER, TH. KOPRUCKI, *Numerical simulation of carrier transport in semiconductor devices at cryogenic temperatures*, Preprint no. 2296, WIAS, Berlin, 2016.
- [86] P. KEELER, N. ROSS, A. XIA, B. BŁASZCZYŚZYN, *Stronger wireless signals appear more Poisson*, Preprint no. 2327, WIAS, Berlin, 2016.
- [87] A. STIVALA, P. KEELER, *Another phase transition in the Axelrod model*, Preprint no. 2352, WIAS, Berlin, 2016.
- [88] O. KLEIN, *Uncertainty quantification for hysteresis operators and a model for magneto-mechanical hysteresis*, Preprint no. 2246, WIAS, Berlin, 2016.
- [89] M. BISKUP, W. KÖNIG, R. SOARES DOS SANTOS, *Mass concentration and aging in the parabolic Anderson model with doubly-exponential tails*, Preprint no. 2295, WIAS, Berlin, 2016.
- [90] TH. KOPRUCKI, K. TABELOW, *Mathematical models: A research data category?*, Preprint no. 2267, WIAS, Berlin, 2016.
- [91] CH. KRAUS, M. RADSZUWEIT, *Modeling and simulation of non-isothermal rate-dependent damage processes in inhomogeneous materials using the phase-field approach*, Preprint no. 2299, WIAS, Berlin, 2016.
- [92] M. LANDSTORFER, *Boundary conditions for electrochemical interfaces*, Preprint no. 2361, WIAS, Berlin, 2016.
- [93] ———, *The partial molar volume and area of solvated ions and some aspects of partial charge transfer*, Preprint no. 2337, WIAS, Berlin, 2016.
- [94] M. ERBAR, M. FATHI, V. LASCHOS, A. SCHLICHTING, *Gradient flow structure for McKean–Vlasov equations on discrete spaces*, Preprint no. 2219, WIAS, Berlin, 2016.
- [95] M. LIERO, A. MIELKE, G. SAVARÉ, *Optimal entropy-transport problems and a new Hellinger–Kantorovich distance between positive measures*, Preprint no. 2207, WIAS, Berlin, 2016.
- [96] A. LINKE, CH. MERDON, *Pressure-robustness and discrete Helmholtz projectors in mixed finite element methods for the incompressible Navier–Stokes equations*, Preprint no. 2250, WIAS, Berlin, 2016.
- [97] P.L. LEDERER, A. LINKE, CH. MERDON, J. SCHÖBERL, *Divergence-free reconstruction operators for pressure-robust Stokes discretizations with continuous pressure finite elements*, Preprint no. 2288, WIAS, Berlin, 2016.
- [98] E. MECA ÁLVAREZ, V.B. SHENOY, J. LOWENGRUB, *H<sub>2</sub>-dependent attachment kinetics and shape evolution in chemical vapor deposition graphene growth*, Preprint no. 2358, WIAS, Berlin, 2016.
- [99] E. MECA ÁLVAREZ, A. MÜNCH, B. WAGNER, *Sharp-interface formation during lithium intercalation into silicon*, Preprint no. 2257, WIAS, Berlin, 2016.
- [100] ———, *Thin-film electrodes for high-capacity lithium-ion batteries: Influence of phase transformations on stress*, Preprint no. 2254, WIAS, Berlin, 2016.

- [101] A. MIELKE, *Uniform exponential decay for reaction-diffusion systems with complex-balanced mass-action kinetics*, Preprint no. 2326, WIAS, Berlin, 2016.
- [102] A. MIELKE, R. ROSSI, G. SAVARÉ, *Global existence results for viscoplasticity at finite strain*, Preprint no. 2304, WIAS, Berlin, 2016.
- [103] A. MIELKE, T. ROUBÍČEK, *Rate-independent elastoplasticity at finite strains and its numerical approximation*, Preprint no. 2210, WIAS, Berlin, 2016.
- [104] J. HASKOVEC, S. HITTMEIR, P. MARKOWICH, A. MIELKE, *Decay to equilibrium for energy-reaction-diffusion systems*, Preprint no. 2233, WIAS, Berlin, 2016.
- [105] A. MIELKE, M. MITTNENZWEIG, *Convergence to equilibrium in energy-reaction-diffusion systems using vector-valued functional inequalities*, Preprint no. 2349, WIAS, Berlin, 2016.
- [106] A. MIELKE, D. PESCHKA, N. ROTUNDO, M. THOMAS, *Gradient structure for optoelectronic models of semiconductors*, Preprint no. 2317, WIAS, Berlin, 2016.
- [107] M. MITTNENZWEIG, A. MIELKE, *An entropic gradient structure for Lindblad equations and GENERIC for quantum systems coupled to macroscopic models*, Preprint no. 2320, WIAS, Berlin, 2016.
- [108] N. BERGER, CH. MUKHERJEE, K. OKAMURA, *Quenched large deviations for simple random walks on percolation clusters including long-range correlations*, Preprint no. 2360, WIAS, Berlin, 2016.
- [109] H. NEIDHARDT, A. STEPHAN, V.A. ZAGREBNOV, *Convergence rate estimates for Trotter product approximations of solution operators for non-autonomous Cauchy problems*, Preprint no. 2356, WIAS, Berlin, 2016.
- [110] O. OMEL'CHENKO, L. RECKE, V. BUTUZOV, N. NEFEDOV, *Time-periodic boundary layer solutions to singularly perturbed parabolic problems*, Preprint no. 2300, WIAS, Berlin, 2016.
- [111] O. OMEL'CHENKO, M. WOLFRUM, *Is there an impact of small phase lags in the Kuramoto model?*, Preprint no. 2234, WIAS, Berlin, 2016.
- [112] ST. PATRIZI, E. VALDINOCI, *Long-time behavior for crystal dislocation dynamics*, Preprint no. 2302, WIAS, Berlin, 2016.
- [113] R.I.A. PATTERSON, D.R.M. RINGER, *Dynamical large deviations of countable reaction networks under a weak reversibility condition*, Preprint no. 2273, WIAS, Berlin, 2016.
- [114] ST. BOMMER, R. SEEMANN, S. JACHALSKI, D. PESCHKA, B. WAGNER, *Liquid-liquid dewetting: Morphologies and rates*, Preprint no. 2346, WIAS, Berlin, 2016.
- [115] S. PICKARTZ, U. BANDELOW, S. AMIRANASHVILI, *Adiabatic theory of champion solitons*, Preprint no. 2276, WIAS, Berlin, 2016.
- [116] ———, *Asymptotically stable compensation of soliton self-frequency shift*, Preprint no. 2343, WIAS, Berlin, 2016.
- [117] ———, *Efficient all-optical control of solitons*, Preprint no. 2298, WIAS, Berlin, 2016.
- [118] D. DAVINO, P. KREJČÍ, A. PIMENOV, D. RACHINSKII, C. VISIONE, *Analysis of an operator-differential model for magnetostrictive energy harvesting*, Preprint no. 2225, WIAS, Berlin, 2016.
- [119] A. PIMENOV, S. SLEPNEVA, G. HUYET, A.G. VLADIMIROV, *Dispersive time-delay dynamical systems*, Preprint no. 2324, WIAS, Berlin, 2016.
- [120] M. RADZIUNAS, *Modeling and efficient simulations of broad-area edge-emitting semiconductor lasers and amplifiers*, Preprint no. 2292, WIAS, Berlin, 2016.
- [121] ———, *A multi-mode delay differential equation model for lasers with optical feedback*, Preprint no. 2294, WIAS, Berlin, 2016.
- [122] ———, *Traveling wave modeling of nonlinear dynamics in multisection semiconductor lasers*, Preprint no. 2261, WIAS, Berlin, 2016.

- [123] M. REDMANN, M.A. FREITAG, *Balanced truncation and singular perturbation approximation model order reduction for stochastically controlled linear systems*, Preprint no. 2339, WIAS, Berlin, 2016.
- [124] D. HORSTMANN, J. REHBERG, H. MEINLSCHMIDT, *The full Keller–Segel model is well-posed on fairly general domains*, Preprint no. 2312, WIAS, Berlin, 2016.
- [125] H. MEINLSCHMIDT, CH. MEYER, J. REHBERG, *Optimal control of the thermistor problem in three spatial dimensions*, Preprint no. 2238, WIAS, Berlin, 2016.
- [126] S. REICHEL, *Corrector estimates for a class of imperfect transmission problems*, Preprint no. 2354, WIAS, Berlin, 2016.
- [127] ———, *Error estimates for elliptic equations with not exactly periodic coefficients*, Preprint no. 2260, WIAS, Berlin, 2016.
- [128] A. MUNTEAN, S. REICHEL, *Corrector estimates for a thermo-diffusion model with weak thermal coupling*, Preprint no. 2310, WIAS, Berlin, 2016.
- [129] P. COLLI, G. GILARDI, E. ROCCA, J. SPREKELS, *Optimal distributed control of a diffuse interface model of tumor growth*, Preprint no. 2228, WIAS, Berlin, 2016.
- [130] B. ALBERS, P. KREJČÍ, E. ROCCA, *Solvability of an unsaturated porous media flow problem with thermomechanical interaction*, Preprint no. 2211, WIAS, Berlin, 2016.
- [131] A. ROGGENSACK, CH. KRAUS, *Existence of weak solutions for the Cahn–Hilliard reaction model including elastic effects and damage*, Preprint no. 2231, WIAS, Berlin, 2016.
- [132] L. HELTAI, N. ROTUNDO, *Error estimates in weighted Sobolev norms for finite element immersed interface methods*, Preprint no. 2323, WIAS, Berlin, 2016.
- [133] G. SCHMIDT, *Scattering of general incident beams by diffraction gratings*, Preprint no. 2355, WIAS, Berlin, 2016.
- [134] F. LANZARA, V. MAZ'YA, G. SCHMIDT, *A fast solution method for time dependent multidimensional Schrödinger equations*, Preprint no. 2279, WIAS, Berlin, 2016.
- [135] D. BELOMESTNY, J.G.M. SCHOENMAKERS, *Projected particle methods for solving McKean–Vlasov equations*, Preprint no. 2341, WIAS, Berlin, 2016.
- [136] R. HILDEBRAND, J.G.M. SCHOENMAKERS, J. ZHANG, F. DICKMANN, *Regression based duality approach to optimal control with application to hydro electricity storage*, Preprint no. 2330, WIAS, Berlin, 2016.
- [137] S. DIPIERRO, J. SERRA, E. VALDINOCI, *Improvement of flatness for nonlocal phase transitions*, Preprint no. 2345, WIAS, Berlin, 2016.
- [138] ———, *Nonlocal phase transitions: Rigidity results and anisotropic geometry*, Preprint no. 2334, WIAS, Berlin, 2016.
- [139] H. EGGER, TH. KUGLER, N. STROGIES, *Parameter identification in a semilinear hyperbolic system*, Preprint no. 2278, WIAS, Berlin, 2016.
- [140] M. THOMAS, CH. ZANINI, *Cohesive zone-type delamination in visco-elasticity*, Preprint no. 2350, WIAS, Berlin, 2016.
- [141] R. ROSSI, M. THOMAS, *From adhesive to brittle delamination in visco-elastodynamics*, Preprint no. 2259, WIAS, Berlin, 2016.
- [142] B. ABDELLAOUI, A. DIEB, E. VALDINOCI, *A nonlocal concave-convex problem with nonlocal mixed boundary data*, Preprint no. 2344, WIAS, Berlin, 2016.
- [143] L. CAFFARELLI, S. DIPIERRO, E. VALDINOCI, *A logistic equation with nonlocal interactions*, Preprint no. 2216, WIAS, Berlin, 2016.

- [144] S. DIPIERRO, E. VALDINOCI, *Nonlocal minimal surfaces: Interior regularity, quantitative estimates and boundary stickiness*, Preprint no. 2281, WIAS, Berlin, 2016.
- [145] S. DIPIERRO, A. KARAKHANYAN, E. VALDINOCI, *A class of unstable free boundary problems*, Preprint no. 2212, WIAS, Berlin, 2016.
- [146] ———, *A nonlinear free boundary problem with a self-driven Bernoulli condition*, Preprint no. 2325, WIAS, Berlin, 2016.
- [147] S. DIPIERRO, L. LOMBARDINI, P. MIRAGLIO, E. VALDINOCI, *The Phillip Island penguin parade (a mathematical treatment)*, Preprint no. 2342, WIAS, Berlin, 2016.
- [148] S. DIPIERRO, F. MAGGI, E. VALDINOCI, *Asymptotic expansions of the contact angle in nonlocal capillarity problems*, Preprint no. 2315, WIAS, Berlin, 2016.
- [149] S. DIPIERRO, M. NOVAGA, E. VALDINOCI, *Rigidity of critical points for a nonlocal Ohta–Kawasaki energy*, Preprint no. 2252, WIAS, Berlin, 2016.
- [150] S. DIPIERRO, O. SAVIN, E. VALDINOCI, *Definition of fractional Laplacian for functions with polynomial growth*, Preprint no. 2318, WIAS, Berlin, 2016.
- [151] ———, *Local approximation of arbitrary functions by solutions of nonlocal equations*, Preprint no. 2303, WIAS, Berlin, 2016.
- [152] S. DIPIERRO, N. SOAVE, E. VALDINOCI, *On fractional elliptic equations in Lipschitz sets and epigraphs: Regularity, monotonicity and rigidity results*, Preprint no. 2256, WIAS, Berlin, 2016.
- [153] A. FARINA, E. VALDINOCI, *Anisotropic nonlocal operators regularity and rigidity theorems for a class of anisotropic nonlocal operators*, Preprint no. 2213, WIAS, Berlin, 2016.
- [154] F. MAGGI, E. VALDINOCI, *Capillarity problems with nonlocal surface tension energies*, Preprint no. 2274, WIAS, Berlin, 2016.
- [155] J. SPREKELS, E. VALDINOCI, *A new type of identification problems: Optimizing the fractional order in a nonlocal evolution equation*, Preprint no. 2214, WIAS, Berlin, 2016.
- [156] A.G. VLADIMIROV, G. HUYET, A. PIMENOV, *Effect of chromatic dispersion on multimode laser dynamics: Delay differential model*, Preprint no. 2240, WIAS, Berlin, 2016.
- [157] A. MÜNCH, B. WAGNER, L.P. COOK, R.R. BRAUN, *Apparent slip for an upper convected Maxwell fluid*, Preprint no. 2255, WIAS, Berlin, 2016.
- [158] W. WAGNER, O. MUSCATO, *A class of stochastic algorithms for the Wigner equation*, Preprint no. 2239, WIAS, Berlin, 2016.
- [159] U. WILBRANDT, C. BARTSCH, N. AHMED, N. ALIA, F. ANKER, L. BLANK, A. CAIAZZO, S. GANESAN, S. GIERE, G. MATTHIES, R. MEESALA, A. SHAMIM, J. VENKATENSAN, V. JOHN, *ParMoon – A modernized program package based on mapped finite elements*, Preprint no. 2316, WIAS, Berlin, 2016.

### A.7.2 WIAS Technical Reports Series

- [1] J. BORCHARDT, P. MATHÉ, G. PRINTSYPAR, *Calibration methods for gas turbine performance models*, WIAS Technical Report no. 16, WIAS, Berlin, 2016.
- [2] H. GAJEWSKI, M. LIERO, R. NÜRNBERG, H. STEPHAN, *WIAS-TeSCA – Two-dimensional semi-conductor analysis package*, WIAS Technical Report no. 14, WIAS, Berlin, 2016.
- [3] M. RADZIUNAS, *Mathematical modeling and numerical simulations of diode lasers with micro-integrated external resonators*, WIAS Technical Report no. 15, WIAS, Berlin, 2016.

### A.7.3 Preprints/Reports in other Institutions

- [1] V. AVANESOV, N. BUZUN, *Change-point detection in high-dimensional covariance structure*, arXiv:1610.03783, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [2] L. BOGOLUBSKY, P. DVURECHENSKY, A. GASNIKOV, G. GUSEV, Y. NESTEROV, A. RAIGORODSKII, A. TIKHONOV, M. ZHUKOVSKII, *Learning supervised PageRank with gradient-based and gradient-free optimization methods*, arXiv:1603.00717, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [3] A. CHERNOV, P. DVURECHENSKY, A. GASNIKOV, *Fast primal-dual gradient method for strongly convex minimization problems with linear constraints*, arXiv:1605.02970, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [4] P. DVURECHENSKY, A. GASNIKOV, E. GASNIKOVA, S. MATSIEVSKY, A. RODOMANOV, I. USIK, *Primal-dual method for searching equilibrium in hierarchical congestion population games*, arXiv:1606.08988, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [5] J.-D. DEUSCHEL, P. FRIZ, M. MAURELLI, M. SLOWIK, *The enhanced Sanov theorem and propagation of chaos*, arxiv:1602.08043, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [6] J. BLATH, A. GONZÁLEZ CASANOVA SOBERÓN, N. KURT, M. WILKE-BERENGUER, *A new coalescent for seed-bank models*, arxiv.org:1411.4747, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [7] A. GONZÁLEZ CASANOVA SOBERÓN, N. KURT, A. WAKOLBINGER, L. YUAN, *An individual-based model for the Lenski experiment, and the deceleration of the relative fitness*, arxiv.org:1505.01751, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [8] G.R. BARRENECHEA, V. JOHN, P. KNOBLOCH, *An algebraic flux correction scheme satisfying the discrete maximum principle and linearity preservation on general meshes*, Preprint no. 2016-06, Nečas Center for Mathematical Modeling, Prague, Czech Republic, 2016.
- [9] S. LU, P. MATHÉ, S. PEREVERZEV, *Balancing principle in supervised learning for a general regularization scheme*, Preprint no. 2016-38, RICAM Reports, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, 2016.
- [10] P. MATHÉ, S. PEREVERZEV, *Complexity of linear ill-posed problems in Hilbert space*, Preprint no. 2016-09, RICAM Reports, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, 2016.
- [11] R. PLATO, P. MATHÉ, B. HOFMANN, *Optimal rates for Lavrentiev regularization with adjoint source conditions*, Preprint no. 03, Technische Universität Chemnitz, Fakultät für Mathematik, 2016.
- [12] ST. BÜRGER, P. MATHÉ, *Discretized Lavrent'ev regularization for the autoconvolution equation*, arXiv:1604.03275, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [13] J. BEHRNDT, M.M. MALAMUD, H. NEIDHARDT, *Scattering matrices and Dirichlet-to-Neumann maps*, arXiv:1511.02376v2, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [14] R.I.A. PATTERSON, S. SIMONELLA, W. WAGNER, *Kinetic theory of cluster dynamics*, arXiv: 1601.05838, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [15] E. ROCCA, R. SCALA, *A rigorous sharp interface limit of a diffuse interface model related to tumor growth*, arXiv:1606.04663, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
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- [17] X. ROS-OTON, J. SERRA, *The structure of the free boundary in the fully nonlinear thin obstacle problem*, arXiv:1603.09292, Cornell University Library, arXiv.org, Ithaca, USA, 2016.
- [18] P. KRAVETC, D. RACHINSKII, A.G. VLADIMIROV, *Pulsating dynamics of slow-fast population models with delay*, arxiv.org:1601.06452, Cornell University Library, arXiv.org, Ithaca, USA, 2016.



- [19] K.F. LEE, M. DOSTA, A.D. MCGUIRE, S. MOSBACH, W. WAGNER, ST. HEINRICH, M. KRAFT, *Development of a multi-compartment population balance model for high-shear wet granulation with Discrete Element Method*, Technical report no. 170, c4e-Preprint Series, Cambridge, UK, 2016.
- [20] M. KRAFT, W. WAGNER, *A numerical scheme for the Random Cloud Model*, Technical report no. 173, c4e-Preprint Series, Cambridge, UK, 2016.

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

### A.8.1 Main and Plenary Talks

1. J. SPREKELS, *On a nonstandard Cahn–Hilliard system with dynamic boundary condition*, INdAM-ISIMM Workshop on Trends on Applications of Mathematics to Mechanics, September 5–9, The International Society for the Interaction of Mechanics and Mathematics (ISIMM), Rome, Italy, September 9.
2. U. BANDELOW, *Ultrashort solitons that do not want to be too short in duration*, XIX Conference on Nonequilibrium Statistical Mechanics and Nonlinear Physics (MEDYFINOL 2016), Universidad de los Andes, Universidad de Mar del Plata, and Instituto Tecnológico de Buenos Aires, Valdivia, Chile, December 7.
3. P. FRIZ, *Option pricing in the moderate deviations regime*, Vienna Congress on Mathematical Finance – VCMF 2016, September 12–14, Vienna University of Economics and Business, Austria, September 12.
4. R. HENRION, *Calmness of the perturbation mappings for MPECs in original and enhanced form*, International Conference on Bilevel Optimization and Related Topics, May 4–6, Dresden, May 6.
5. M. HINTERMÜLLER, *Recent trends in optimal control problems with nonsmooth structures*, Computational Methods for Control of Infinite-dimensional Systems, March 14–18, Institute for Mathematics and its Applications, Minneapolis, USA, March 14.
6. ———, *Towards sharp stationarity conditions for classes of optimal control problems for variational inequalities of the second kind*, International INdAM Conference “Optimal Control for Evolutionary PDEs and Related Topics (OCERTO 2016)”, June 20–24, Cortona, Italy, June 20.
7. ———, *Nonsmooth structures in PDE constrained optimization*, 66th Workshop “Advances in Convex Analysis and Optimization”, July 5–10, International Centre for Scientific Culture “E. Majorana”, School of Mathematics “G. Stampacchia”, Erice, Italy, July 9.
8. ———, *Bilevel optimization and applications in imaging*, Imaging, Vision and Learning based on Optimization and PDEs, August 29 – September 1, Bergen, Norway, August 30.
9. D. HÖMBERG, *Math for steel production and manufacturing*, MACSI10 – Empowering Industrial Mathematical and Statistical Modelling for the Future, December 8–9, University of Limerick, Ireland, December 9.
10. A. LINKE, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Advanced Numerical Methods: Recent Developments, Analysis, and Applications, October 3–7, Institut Henri Poincaré, Paris, France, October 6.
11. V. SPOKOINY, *Clustering using adaptive weights*, Information Technology and Systems 2016, September 26, Russian Academy of Sciences, Institute for Information Transmission Problems, St. Petersburg, September 26.

### A.8.2 Scientific Talks (Invited)

1. J. SPREKELS, *A new identification problem: Optimizing the order in a nonlocal evolution equation*, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, September 13.
2. ———, *On a nonstandard viscous Cahn–Hilliard system: Existence and optimal control*, Congress of the Italian Society of Industrial and Applied Mathematics (SIMAI 2016), September 13–16, Politecnico di Milano, Italy, September 14.
3. ———, *On a nonstandard viscous Cahn–Hilliard system with dynamic boundary conditions*, Mathematical Institute of the Czech Academy of Sciences, Prague, December 6.

4. N. AHMED, *A review of VMS methods for the simulation of turbulent incompressible flows*, International Conference on Differential Equations and Applications, May 26–28, Lahore University of Management Sciences, Pakistan, May 27.
5. S. AMIRANASHVILI, *How to become a champion soliton*, International Conference on Wave Interaction (WIN-2016), Johannes Kepler Universität Linz, Austria, April 27.
6. ———, *Extreme solitons in optical fibers*, Workshop on Abnormal Wave Events, University of Nice Sophia Antipolis, Nice, France, June 15.
7. U. BANDELOW, *Solitons that do not want to be too short in duration*, International Conference on Wave Interaction (WIN-2016), Johannes Kepler Universität Linz, Austria, April 27.
8. ———, *Heteroclinic connections and limiting cases in integrable NLS-type equations*, 618. WE-Heraeus-Seminar: Extreme Events and Rogue Waves – 2016, Wilhelm und Else Heraeus-Stiftung, Bad Honnef, June 3.
9. ———, *Solitons on a background, rogue waves, and classical soliton solutions of extended nonlinear Schrödinger equations*, International Tandem Workshop on Pattern Dynamics in Nonlinear Optical Cavities, August 15–19, Max-Planck-Institut für Physik komplexer Systeme, Dresden, August 15.
10. ———, *Nonlinear dynamical effects in photonics: Modeling, simulation and analysis*, Coloquio del Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, December 14.
11. ———, *Ultrashort solitons, rogue waves and event horizons in nonlinear dispersive optical media*, Coloquio de la Facultad de Ingeniería y Ciencias Aplicadas, Universidad de los Andes, Santiago, Chile, December 15.
12. CH. BAYER, *The forward-reverse method for conditional Markov processes*, Bayes in Paris, École Nationale de la Statistique et de l'Administration Économique, Paris, France, January 28.
13. ———, *SDE based regression for random PDEs*, Workshop “Rough Paths, Regularity Structures and Related Topics”, May 1–7, Mathematisches Forschungsinstitut Oberwolfach, May 3.
14. ———, *Pricing under rough volatility*, Stochastic Analysis and Mathematical Finance – A Fruitful Partnership, May 22–27, Banff International Research Station for Mathematical Innovation and Discovery, Oaxaca, Mexico, May 24.
15. ———, *Pricing under rough volatility*, Statistics for Differential Equations driven by Rough Paths, September 7–8, University of Warwick, Centre for Research in Statistical Methodology, Coventry, UK, September 7.
16. ———, *Pricing under rough volatility*, Vienna Congress on Mathematical Finance – VCMF 2016, September 12–14, Vienna University of Economics and Business, Austria, September 12.
17. ———, *Pricing under rough volatility*, Czech, Slovenian, Austrian, Slovak and Catalan Mathematical Societies Joint Meeting 2016, September 20–23, Societat Catalana de Matemàtiques, Institut d'Estudis Catalans, Barcelona, Spain, September 20.
18. ———, *Short dated option prices under rough volatility*, Rough Volatility Meeting, October 7–8, Imperial College London, Department of Mathematics, UK, October 7.
19. ———, *Smoothing the payoff for efficient computation of basket option*, Stochastik Seminar, Technische Universität Wien, Institut für Stochastik und Wirtschaftsmathematik, Austria, December 1.
20. ———, *Smoothing the payoff for efficient computation of basket option*, Seminar, École Polytechnique CNRS, Centre de Mathématiques Appliquées, Palaiseau, France, December 12.
21. ———, *Short dated option pricing under rough volatility*, Bachelier seminar, École Polytechnique CNRS, Centre de Mathématiques Appliquées, Palaiseau, France, December 16.

22. C. BRÉE, *Adiabatic Floquet model for the optical response in femtosecond filaments*, group seminar, Leibniz Universität Hannover, Institut für Quantenoptik, February 11.
23. ———, *Adiabatic Floquet model for the optical response in sub-picosecond optical filamentation*, III International Symposium “Advances in Nonlinear Photonics” (ANPh’2016), September 29 – October 1, Belarusian State University, Minsk, Belarus, September 30.
24. N. BUZUN, *Multiplier bootstrap for change point detection*, Mathematical Statistics and Inverse Problems, February 8–12, Faculté des Sciences de Luminy, France, February 11.
25. A. CAIAZZO, *Backflow stabilization methods for open boundaries*, Christian-Albrechts-Universität zu Kiel, Angewandte Mathematik, Kiel, May 19.
26. E. CINTI, *Quantitative flatness results and BV-estimates for nonlocal minimal surfaces*, Seminario di Equazioni Differenziali, Università degli Studi di Roma “Tor Vergata”, Italy, April 19.
27. ———, *Quantitative flatness results and BV-estimates for nonlocal minimal surfaces*, Bruxelles-Torino talks in PDE’s, May 2–5, Università degli Studi di Torino, Dipartimento di Matematica “Giuseppe Peano”, Italy, May 3.
28. ———, *Quantitative flatness results and BV-estimates for nonlocal minimal surfaces*, 9th European Conference on Elliptic and Parabolic Problems, May 23–27, University of Zurich, Institute of Mathematics, Gaeta, Italy, May 23.
29. ———, *Quantitative flatness results and BV estimates for nonlocal minimal surfaces*, Workshop “Calculus of Variations”, July 11–15, Mathematisches Forschungsinstitut Oberwolfach, July 12.
30. A. CIPRIANI, *Extremes of some Gaussian random interfaces*, Seminar Series in Probability and Statistics, Delft University of Technology, Department of Applied Probability, Netherlands, January 21.
31. ———, *The membrane model*, seminar, Delft University of Technology, Department of Applied Probability, Netherlands, September 5.
32. ———, *The membrane model*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, September 29.
33. F. DASSI, *A novel anisotropic mesh adaption strategy*, Politecnico di Milano, Dipartimento di Matematica “F. Brioschi”, Milano, Italy, February 23.
34. K. DISSER, *Zhukovskys Theorem in der Fluid-Struktur-Interaktion*, Universität Augsburg, Institut für Mathematik, July 4.
35. P. DVURECHENSKY, *Accelerated primal-dual gradient method for composite optimization with unknown smoothness parameter*, VIII Moscow International Conference on Operations Research (ORM2016), November 18–21, Lomonosov Moscow State University, Faculty of Computational Mathematics and Cybernetics, Russian Federation, October 19.
36. M. EIGEL, *Adaptive stochastic Galerkin FEM with hierarchical tensor representations*, Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2016), January 5–10, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia, January 8.
37. ———, *Adaptive stochastic Galerkin FEM with hierarchical tensor representations*, Joint Annual Meeting of DMV and GAMM, Section 18 “Numerical Methods of Differential Equations”, March 7–11, Technische Universität Braunschweig, March 10.
38. ———, *Bayesian inversion using hierarchical tensor approximations*, SIAM Conference on Uncertainty Quantification, Minisymposium 67 “Bayesian Inversion and Low-rank Approximation (Part II)”, April 5–8, Lausanne, Switzerland, April 6.
39. ———, *Adaptive stochastic Galerkin FEM with hierarchical tensor representations*, 15th Conference on the Mathematics of Finite Elements and Applications (Brunel MAFELAP 2016), Minisymposium “Uncer-

- tainty Quantification Using Stochastic PDEs and Finite Elements”, June 14–17, Brunel University London, Uxbridge, UK, June 14.
40. ———, *Some aspects of adaptive random PDEs*, Oberseminar, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, July 21.
  41. P. FARRELL, *Finite volume schemes for non-Boltzmann statistics*, Friedrich-Alexander Universität Erlangen-Nürnberg, Fachbereich Mathematik, May 12.
  42. ———, *Multilevel collocation with radial basis function*, Friedrich-Alexander Universität Erlangen-Nürnberg, Fachbereich Mathematik, May 12.
  43. ———, *Scharfetter–Gummel schemes for non-Boltzmann statistics*, The 19th European Conference on Mathematics for Industry (ECMI2016), Minisymposium 23 “Charge Transport in Semiconductor Materials: Emerging and Established Mathematical Topics”, June 13–17, Universidade de Santiago de Compostela, Spain, June 14.
  44. M.H. FARSHBAF SHAKER, *A phase field approach for optimal boundary control of damage processes in two-dimensional viscoelastic media*, International INdAM Conference “Optimal Control for Evolutionary PDEs and Related Topics (OCERTO 2016)”, June 20–24, Cortona, Italy, June 21.
  45. F. FLEGEL, *Spectral localization vs. homogenization in the random conductance model*, Summer School 2016, August 21–26, Research Training Group (RTG) 1845 “Stochastic Analysis with Applications in Biology, Finance and Physics”, Hejnice, Czech Republic, August 22.
  46. ———, *Spectral localization vs. homogenization in the random conductance model*, Probability Seminar at UCLA, University of California, Los Angeles, Department of Mathematics, Los Angeles, USA, October 13.
  47. S.P. FRIGERI, *On a diffuse interface model of tumor growth*, 9th European Conference on Elliptic and Parabolic Problems, May 23–27, University of Zurich, Institute of Mathematics, Gaeta, Italy, May 23.
  48. ———, *Optimal distributed control for nonlocal Cahn–Hilliard/Navier–Stokes systems in 2D*, International INdAM Conference “Optimal Control for Evolutionary PDEs and Related Topics (OCERTO 2016)”, June 20–24, Cortona, Italy, June 24.
  49. ———, *On some nonlocal diffuse-interface models for binary fluids: Regularity results and applications*, Congress of the Italian Society of Industrial and Applied Mathematics (SIMAI 2016), September 13–16, Politecnico di Milano, Italy, September 14.
  50. P. FRIZ, *A regularity structure for rough volatility*, Stochastic Analysis, Rough Paths, Geometry, January 7–9, Imperial College London, UK, January 7.
  51. ———, *The enhanced Sanov theorem and propagation of chaos*, Probabilistic Models – From Discrete to Continuous, March 29 – April 2, University of Warwick, Mathematics Institute, UK, March 31.
  52. ———, *Support theorem for the (generalized) parabolic Anderson model*, Stochastic Partial Differential Equations, May 16–20, Stony Brook University, Simons Center for Geometry and Physics, USA, May 18.
  53. ———, *Support theorem for singular SPDEs: The case of gPAM*, Stochastic Partial Differential Equations and Applications, May 29 – June 3, Centro Internazionale per la Ricerca Matematica (CIRM), Levico, Italy, May 31.
  54. ———, *Option pricing in the moderate deviations regime*, At the Frontiers of Quantitative Finance, June 27–30, University of Edinburgh, UK, June 28.
  55. ———, *Malliavin calculus for regularity structures: The case of gPAM*, Stochastic Partial Differential Equations and Related Fields, October 10–14, Universität Bielefeld, Fakultät für Mathematik, October 13.
  56. ———, *Signatures, rough paths and probability*, Stochastics and Finance Seminar, University of Amsterdam, Korteweg-de Vries Institute for Mathematics, Netherlands, October 18.

57. ———, *From rough paths to regularity structures and back*, Colloquium, November 8–12, Instituto de Ciencias Matemáticas (ICMAT), Madrid, Spain, November 8.
58. A. GLITZKY,  *$p(x)$ -Laplace thermistor models for electrothermal feedback in organic semiconductor devices*, 9th European Conference on Elliptic and Parabolic Problems, May 23–27, University of Zurich, Institute of Mathematics, Gaeta, Italy, May 23.
59. ———,  *$p(x)$ -Laplace thermistor models for electrothermal effects in organic semiconductor devices*, 7th European Congress of Mathematics (7ECM), Minisymposium 22 “Mathematical Methods for Semiconductors”, July 18–22, Technische Universität Berlin, July 22.
60. A. GONZÁLEZ CASANOVA SOBERÓN, *Modeling the Lenski experiment*, Mathematical and Computational Evolutionary Biology, June 12–16, Le Laboratoire d'Informatique, de Robotique et de Microélectronique de Montpellier (LIRMM), Hameau de l'Etoile, France, June 14.
61. ———, *The seedbank coalescent*, World Congress in Probability and Statistics, Invited Session “Stochastic Models of Evolution”, July 11–15, Fields Institute, Toronto, Canada, July 5.
62. ———, *The seed bank model*, 3 talks, VIII School on Probability and Stochastic Processes, September 12–16, Centro de Investigación en Matemáticas (CIMAT), Department of Probability and Statistics, Guanajuato, Mexico, September 12–15.
63. ———, *Fixation in a  $X_i$  coalescent with selection*, Miniworkshop on Probabilistic Models in Evolutionary Biology, November 24–25, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, November 25.
64. ———, *Fixation in a  $X_i$  coalescent model with selection*, Probability seminar, University of Warwick, Mathematics Institute, Warwick, UK, November 30.
65. C. GUHLKE, *Continuum thermodynamics in the immediate vicinity of an electrode-electrolyte interface*, Soft Matter at Interfaces 2016, February 28 – March 2, Schloss Ringberg, Kreuth, February 28.
66. ———, *Impact of stress on the electrical double layer*, 2016 MRS Spring Meeting & Exhibit, Symposium EE7 “Mechanics of Energy Storage and Conversion – Batteries, Thermoelectrics and Fuel Cells”, March 28 – April 1, Phoenix, USA, March 31.
67. M. HEIDA, *On homogenization of rate-independent systems*, MATHEON Multiscale Seminar, Technische Universität Berlin, February 17.
68. ———, *Large deviation principle for a stochastic Allen–Cahn equation*, 9th European Conference on Elliptic and Parabolic Problems, May 23–27, University of Zurich, Institute of Mathematics, Gaeta, Italy, May 25.
69. ———, *Stochastic homogenization of rate-independent systems*, Berlin Dresden Prague Würzburg Workshop “Homogenization and Related Topics”, Technische Universität Dresden, Fachbereich Mathematik, June 22.
70. ———, *Stochastic homogenization of 1-homogeneous functionals*, 7th European Congress of Mathematics (7ECM), Minisymposium 29 “Nonsmooth PDEs in the Modeling Damage, Delamination, and Fracture”, July 18–22, Technische Universität Berlin, July 22.
71. CH. HEINEMANN, *Global-in-time well-posedness for a phase field system describing rate-dependent damage phenomena*, ERC Workshop on Modeling Materials and Fluids using Variational Methods, February 22–26, WIAS, Berlin, February 23.
72. ———, *Analysis of optimality conditions for a PDE system modeling damage processes*, 7th European Congress of Mathematics (7ECM), Minisymposium 29 “Nonsmooth PDEs in the Modeling Damage, Delamination, and Fracture”, July 18–22, Technische Universität Berlin, July 21.



73. H. HEITSCH, *Optimization in gas transport networks using nonlinear probabilistic constraints*, XIV International Conference on Stochastic Programming (ICSP 2016), Thematic Session: Probabilistic Constraints: Applications and Theory, June 25 – July 1, Búzios, Brazil, June 28.
74. R. HENRION, *Aspects of nondifferentiability for probability functions*, 7th International Seminar on Optimization and Variational Analysis, June 1–3, Universidad de Alicante, Spain, June 2.
75. ———, *(Sub-)Gradient formulae for Gaussian probability functions*, XIV International Conference on Stochastic Programming (ICSP 2016), Thematic Session: Probabilistic Constraints: Applications and Theory, June 25 – July 1, Búzios, Brazil, June 28.
76. ———, *Formules du gradient pour des fonctions probabilistes Gaussiennes*, Workshop on Offshore Wind Generation, September 9, Electricité de France R&D, Paris, France, September 9.
77. ———, *Robust-stochastic optimization problems in stationary gas networks*, Conference “Mathematics of Gas Transport”, October 6–7, Zuse Institut Berlin, October 6.
78. ———, *Initiation aux problèmes d’optimisation sous contraintes en probabilité*, Workshop “Optimisation en Milieu Aléatoire”, November 8, Institut des Sciences Informatiques et de leurs Interactions, GdR 720 ISIS (Information, Signal, Image et ViSion), Paristech Télécom, Paris, France, November 8.
79. ———, *Aspects of nonsmoothness for Gaussian probability functions*, PGMO Days 2016 – Gaspard Monge Program for Optimization and Operations Research, November 8–9, Electricité de France, Palaiseau, France, November 9.
80. ———, *Optimisation sous contraintes en probabilité*, Séminaire du Groupe de Travail “Modèles Stochastiques en Finance”, Ecole Nationale Supérieure des Techniques Avancées (ENSTA) ParisTech, Palaiseau, France, November 28.
81. R. HILDEBRAND, *Periodic discrete dynamical systems and copositive matrices with circulant zero patterns*, Optimization Without Borders, February 7–12, Les Houches, France, February 11.
82. ———, *Periodic discrete dynamical systems and copositive matrices with circulant zero patterns*, International Conference on Optimization: SIGOPT 2016, April 6–8, Universität Trier, Fachbereich Mathematik, April 6.
83. ———, *Canonical barriers on convex cones*, Oberseminar Geometrische Analysis, Johann Wolfgang Goethe-Universität Frankfurt am Main, Fachbereich Mathematik, April 26.
84. ———, *Barriers on symmetric cones*, Bridging Gaps: The CORE@50 Conference, May 23–25, Université Catholique de Louvain, Louvain-la-Neuve, Belgium, May 23.
85. M. HINTERMÜLLER, *Adaptive finite elements in total variation based image denoising*, SIAM Conference on Imaging Science, Minisymposium “Leveraging Ideas from Imaging Science in PDE-constrained Optimization”, May 23–26, Albuquerque, USA, May 24.
86. ———, *Optimal selection of the regularisation function in a localised TV model*, SIAM Conference on Imaging Science, Minisymposium “Analysis and Parameterisation of Derivative Based Regularisation”, May 23–26, Albuquerque, USA, May 24.
87. ———, *Bilevel optimization for a generalized total-variation model*, SIAM Conference on Imaging Science, Minisymposium “Non-Convex Regularization Methods in Image Restoration”, May 23–26, Albuquerque, USA, May 26.
88. ———, *Optimal control of multiphase fluids and droplets*, Salzburg Mathematics Colloquium, Universität Salzburg, Fachbereich Mathematik, Austria, June 9.
89. ———, *Shape and topological sensitivities in mathematical image processing*, 2 talks, BMS Summer School “Mathematical and Numerical Methods in Image Processing”, July 25 – August 5, Berlin Mathematical School, Technische Universität Berlin, Humboldt-Universität zu Berlin, Berlin, August 4.

90. ———, *Optimal control of multiphase fluids and droplets*, The Fifth International Conference on Continuous Optimization, Session: “Recent Developments in PDE-constrained Optimization I”, August 6–11, Tokyo, Japan, August 10.
91. CH. HIRSCH, *Large deviations in relay-augmented wireless networks*, Workshop on Dynamical Networks and Network Dynamics, January 17–22, International Centre for Mathematical Science, Edinburgh, UK, January 18.
92. ———, *From heavy-tailed Boolean models to scale-free Gilbert graphs*, Workshop on Continuum Percolation, January 26–29, University Lille 1, Science et Technologies, France, January 28.
93. ———, *Large deviations in relay-augmented wireless networks*, 12th German Probability and Statistics Days 2016 – Bochumer Stochastik-Tage, February 29 – March 4, Ruhr-Universität Bochum, Fakultät für Mathematik, March 3.
94. ———, *On maximal hard-core thinnings of stationary particle processes*, Oberseminar Wahrscheinlichkeitstheorie, Ludwig-Maximilians-Universität München, Fakultät für Mathematik, April 18.
95. D. HÖMBERG, *Modelling and simulation of multi-frequency induction hardening*, Fifth Chilean Workshop on Numerical Analysis of Partial Differential Equations (WONAPDE 2016), January 11–15, Universidad de Concepción, Chile, January 14.
96. ———, *Multifrequency induction hardening – Modelling and simulation*, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, May 17.
97. ———, *European collaboration in Industrial and Applied Mathematics*, The 19th European Conference on Mathematics for Industry (ECMI 2016), Minisymposium 38 “Maths in HORIZON 2020 and Beyond”, June 13–17, Universidade de Santiago de Compostela, Spain, June 15.
98. ———, *Analysis and simulation of Joule heating problems*, Mathematisches Kolloquium, Bergische Universität Wuppertal, Fachgruppe Mathematik und Informatik, June 21.
99. G. HU, *Uniqueness in inverse medium scattering problems*, Workshop “Theory and Numerics of Inverse Scattering Problems”, September 18–24, Mathematisches Forschungsinstitut Oberwolfach, September 20.
100. ———, *Inverse medium scattering problems*, Workshop on Inverse Problems and their Applications, November 18–20, Southeast University, Nanjing, China, November 20.
101. ———, *Direct and inverse problems in elastodynamics*, Workshop “Theory, Numerics and Application of Partial Differential Equations”, December 10, Chinese Academy of Sciences, Beijing, December 10.
102. B. JAHNEL, *Classes of nonergodic interacting particle systems with unique invariant measure*, Romanian Academy of Sciences, Institute of Mathematical Statistics and Applied Mathematics, Bucharest, February 22.
103. ———, *Attractor properties for irreversible and reversible interacting particle systems*, 12th German Probability and Statistics Days 2016 – Bochumer Stochastik-Tage, February 29 – March 4, Ruhr-Universität Bochum, Fakultät für Mathematik, March 3.
104. ———, *GnG transitions for the continuum Widom–Rowlinson model under spin flip: Immediate loss and sharp recovery of quasilocality*, Transformations in Statistical Mechanics: Pathologies and Remedies, October 9–14, Lorentz Center – International Center for Scientific Workshops, Leiden, Netherlands, October 11.
105. V. JOHN, *A survey on the analysis and numerical analysis of some turbulence models*, Technische Universität Darmstadt, Fachbereich Mathematik, January 20.
106. ———, *Ein weites Feld – Wissenschaftliche Beiträge von Prof. Dr. Lutz Tobiska*, Festkolloquium aus Anlass des 65. Geburtstags von Prof. Dr. Lutz Tobiska, Universität Magdeburg, Institut für Analysis und Numerik, March 31.

107. ———, *On the divergence constraint in mixed finite element methods for incompressible flows*, 5th European Seminar on Computing (ESCO 2016), June 5–10, Pilsen, Czech Republic, June 7.
108. ———, *On the divergence constraint in mixed finite element methods for incompressible flows*, Beijing Computational Science Research Center, China, August 23.
109. ———, *The role of the pressure in finite element methods for incompressible flow problems*, 4 talks, Summer School 2016 “Fluids under Pressure” and Workshop, August 29 – September 2, Nečas Center for Mathematical Modeling, Prague, Czech Republic, September 1–2.
110. ———, *Analytical and numerical results for algebraic flux correction schemes*, Conference on Recent Advances in Analysis and Numerics of Hyperbolic Conservation Laws, September 8–10, Otto-von-Guericke Universität Magdeburg, September 9.
111. P. KEELER, *Signal-to-interference ratio in wireless communication networks*, Workshop on Dynamical Networks and Network Dynamics, January 17–24, International Centre for Mathematical Science, Edinburgh, UK, January 18.
112. ———, *Wireless network models: Geometry OR signal-to-interference ratio (SIR)*, Telecom Orange Paris, Paris, France, June 3.
113. ———, *A random walk through the history of random terms*, Weekly Seminar, The University of Melbourne, Department of Mathematics and Statistics, Australia, October 3.
114. O. KLEIN, *Uncertainty quantification for hysteresis operators*, 7th European Congress of Mathematics (7ECM), Minisymposium 29 “Nonsmooth PDEs in the Modeling Damage, Delamination, and Fracture”, July 18–22, Technische Universität Berlin, July 22.
115. ———, *On uncertainty quantification for hysteresis operators*, Silesian University, Mathematical Institute, Opava, Czech Republic, December 7.
116. W. KÖNIG, *Connection times in large ad-hoc mobile networks*, Workshop on Dynamical Networks and Network Dynamics, January 18–21, International Centre for Mathematical Science, Edinburgh, UK, January 18.
117. ———, *A variational formula for the free energy of an interacting many-body system*, Workshop “Variational Structures and Large Deviations for Interacting Particle Systems and Partial Differential Equations”, March 15–18, European Institute for Statistics, Probability, Stochastic Operations Research and their Applications (EURANDOM), Eindhoven, Netherlands, March 17.
118. ———, *The mean-field polaron model*, Workshop on Stochastic Processes in honour of Erwin Bolthausen’s 70th birthday, September 14–16, Universität Zürich, Institut für Mathematik, Switzerland, September 15.
119. ———, *The spatially discrete parabolic Anderson model with time-dependent potential*, “Guided Tour: Random Media” — Special occasion to celebrate the 60th birthday of Frank den Hollander, December 14–16, EURANDOM, Eindhoven, Netherlands, December 16.
120. TH. KOPRUCKI, *Mathematical research data: How the WIAS handles mathematical research data*, Joint Annual Meeting of DMV and GAMM, Zentralblatt Meeting on Mathematical Knowledge Management “Mathematics on the WEB – Information and Communication in Mathematics”, March 7–11, Technische Universität Braunschweig, March 9.
121. M. LIERO, *On  $p(x)$ -Laplace thermistor models describing eletrothermal feedback in organic semiconductors*, The 19th European Conference on Mathematics for Industry (ECMI 2016), Minisymposium 23 “Charge Transport in Semiconductor Materials: Emerging and Established Mathematical Topics”, June 13–17, Universidade de Santiago de Compostela, Spain, June 15.
122. ———, *Gradient structures for reaction-diffusion systems and optimal entropy-transport problems*, Workshop “Variational and Hamiltonian Structures: Models and Methods”, July 11–15, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, July 11.

123. ———, *On entropy-transport problems and the Hellinger–Kantorovich distance*, Follow-up Workshop to Junior Hausdorff Trimester Program “Optimal Transportation”, August 29 – September 2, Hausdorff Research Institute for Mathematics, Bonn, August 30.
124. ———, *On geodesic curves and convexity of functionals with respect to the Hellinger–Kantorovich distance*, Workshop “Optimal Transport and Applications”, November 7–11, Scuola Normale Superiore, Dipartimento di Matematica, Pisa, Italy, November 10.
125. ———, *On electrothermal feedback in organic light-emitting diodes*, Berlin Dresden Prague Würzburg Workshop “Mathematics of Continuum Mechanics”, Technische Universität Dresden, Fachbereich Mathematik, December 5.
126. A. LINKE, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Universität Rostock, Leibniz-Institut für Atmosphärenphysik, Kühlungsborn, July 14.
127. ———, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Workshop “Modelling, Model Reduction, and Optimization of Flows”, September 26–30, Shanghai University, China, September 27.
128. ———, *Robust discretization of advection-diffusion-reaction equations and the incompressible Navier–Stokes equations*, Technische Universiteit Eindhoven, Department of Mathematics and Computer Science, Netherlands, November 24.
129. ———, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Technische Universität Kaiserslautern, Scientific Computing, December 15.
130. P. MATHÉ, *Discrepancy based model selection in statistical inverse problems*, Mathematical Statistics and Inverse Problems, February 8–12, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, February 11.
131. ———, *Complexity of linear ill-posed problems in Hilbert space*, IBC on the 70th anniversary of Henryk Wozniakowski, August 29 – September 2, Banach Center, Bedlewo, Poland, August 31.
132. ———, *Complexity of linear ill-posed problems in Hilbert space*, Chemnitz Symposium on Inverse Problems, September 22–23, Technische Universität Chemnitz, Fakultät für Mathematik, September 22.
133. M. MAURELLI, *Regularization by noise for linear SPDE’s*, Oberseminar Analysis – Probability, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 26.
134. ———, *Enhanced Sanov theorem and robust propagation of chaos*, Berlin–Leipzig Workshop in Analysis and Stochastics, April 13–15, Max Planck Institut für Mathematik in den Naturwissenschaften, Leipzig, April 13.
135. ———, *Enhanced Sanov theorem and large deviations for interacting particles*, Workshop “Rough Paths, Regularity Structures and Related Topics”, May 1–7, Mathematisches Forschungsinstitut Oberwolfach, May 5.
136. ———, *Regularization by noise for continuity equation via Young drivers*, Stochastic Partial Differential Equations and Applications, May 30 – June 2, Centro Internazionale per la Ricerca Matematica (CIRM), Levico, Italy, May 30.
137. ———, *Regularization by noise for transport-type equations via stochastic exponentials*, Workshop in Stochastic Analysis, June 28–30, Universidade Estadual de Campinas, Instituto de Matemática, Estatística e Computação Científica, Campinas, Brazil, June 29.
138. ———, *Regularization by noise for stochastic scalar conservation laws*, The 11th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 41 “Stochastic Partial Differential Equations”, July 1–5, The American Institute of Mathematical Science, Orlando (Florida), USA, July 4.

139. ———, *Regularization by noise for scalar conservation laws*, Mathematical Finance and Stochastic Analysis Seminars, University of York, UK, October 26.
140. E. MECA ÁLVAREZ, *Si electrodes for Li-ion batteries: Phase-field modeling*, University of Oxford, Mathematical Institute, UK, February 18.
141. CH. MERDON, *Pressure-robust finite element methods for the Navier–Stokes equations and mass conservative coupling to transport processes*, Friedrich-Alexander Universität Erlangen–Nürnberg, Fachbereich Mathematik, May 11.
142. ———, *Pressure-robust mixed finite element methods for transient Navier–Stokes discretisations*, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, December 14.
143. A. MIELKE, *Evolutionary relaxation for a rate-independent phase-transformation model*, Workshop “Mechanics of Materials: Mechanics of Interfaces and Evolving Microstructure”, March 14–18, Mathematisches Forschungszentrum Oberwolfach, March 14.
144. ———, *On a model for the evolution of microstructures in solids – Evolutionary relaxation*, KTGU-IMU Mathematics Colloquia, March 30–31, Kyoto University, Department of Mathematics, Japan, March 31.
145. ———, *Gradient structures and dissipation distances for reaction-diffusion equation*, Mathematisches Kolloquium, Westfälische Wilhelms-Universität, Institut für Mathematik, Münster, April 28.
146. ———, *On entropic gradient structures for classical and quantum Markov processes with detailed balance*, Pure Analysis and PDEs Seminar, Imperial College London, Department of Mathematics, UK, May 11.
147. ———, *Optimal transport versus reaction – On the geometry of reaction-diffusion equations*, Pure Analysis and PDEs Seminar, Imperial College London, Department of Mathematics, UK, May 12.
148. ———, *Mutual recovery sequences and evolutionary relaxation of a two-phase problem*, 2nd Workshop on CENTRAL Trends in Analysis and Numerics for PDEs, May 26–28, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, May 27.
149. ———, *Multiscale modeling via evolutionary Gamma convergence*, 3rd PhD Workshop, May 30–31, International Research Training Group of the Collaborative Research Center (SFB) 1114 “Scaling Cascades in Complex Systems”, Güstrow, May 30.
150. ———, *Rate-independent microstructure evolution via relaxation of a two-phase model*, Workshop “Advances in the Mathematical Analysis of Material Defects in Elastic Solids”, June 6–10, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, June 10.
151. ———, *Global existence for finite-strain viscoplasticity via the energy-dissipation principle*, Seminar “Analysis & Mathematical Physics”, Institute of Science and Technology Austria (IST Austria), Vienna, Austria, July 7.
152. ———, *Exponential decay into thermodynamical equilibrium for reaction-diffusion systems with detailed balance*, Workshop “Patterns of Dynamics”, July 25–29, Freie Universität Berlin, Fachbereich Mathematik und Informatik, July 28.
153. ———, *Evolutionary Gamma-convergence*, 3 talks, 2nd CENTRAL School on Analysis and Numerics for Partial Differential Equations, August 29 – September 2, Humboldt-Universität zu Berlin, Institut für Mathematik, August 31 – September 2.
154. ———, *On the geometry of reaction and diffusion*, INdAM-ISIMM Workshop on Trends on Applications of Mathematics to Mechanics, September 5–8, The International Society for the Interaction of Mechanics and Mathematics (ISIMM), Rome, Italy, September 7.
155. ———, *On the Hellinger–Kantorovich distance for reaction and diffusion*, Workshop “Interactions between Partial Differential Equations & Functional Inequalities”, September 12–16, The Royal Swedish Academy of Sciences, Institut Mittag–Leffler, Stockholm, Sweden, September 12.

156. ———, *Entropy-entropy production estimates for energy-reaction diffusion systems*, Workshop “Front of PDEs: Modelling, Analysis and Numerics”, December 12–14, Technische Universität Wien, Institut für Analysis and Scientific Computing, Austria, December 13.
157. M. MITTENZWEIG, *Gradient structures for Lindblad equations satisfying detailed balance*, 3rd PhD Workshop, May 30–31, International Research Training Group of the Collaborative Research Center (SFB) 1114 “Scaling Cascades in Complex Systems”, Güstrow, May 31.
158. ———, *Zwischen Flüssigkristallen und Informationstheorie*, 12 talks, Kurs “Eine naturwissenschaftliche Reise hinter das Display eines Smartphones”, Deutsche Schülerakademie, Braunschweig, July 4–8.
159. H.-J. MUCHA, *Big data clustering: Is subsampling better than fast pre-clustering?*, 5th German-Japanese Workshop, September 11–13, Wissenschaftszentrum Schloss Reinsburg, Günzburg, September 13.
160. CH. MUKHERJEE, *Compactness, large deviations, and the polaron problem*, 12th German Probability and Statistics Days 2016 – Bochumer Stochastik-Tage, February 29 – March 4, Ruhr-Universität Bochum, Fakultät für Mathematik, March 3.
161. ———, *Occupation measures, compactness and large deviations*, Young European Probabilists Workshop “Large Deviations for Interacting Particle Systems and Partial Differential Equations” (YEP XIII), March 6–11, European Institute for Statistics, Probability, Stochastic Operations Research and their Applications (EURANDOM), Eindhoven, Netherlands, March 7.
162. ———, *On some aspects of large deviations*, Mathematics Colloquium, West Virginia University, Department of Mathematics, Morgantown, USA, March 17.
163. ———, *Compactness and large deviations*, Mathematisches Kolloquium, Universität Konstanz, Fachbereich Mathematik und Statistik, May 18.
164. ———, *Compactness, large deviations and statistical mechanics*, Seminar des Fachbereichs Mathematik und Statistik, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, October 17.
165. ———, *Compactness and large deviations*, Probability Seminar, University of California at Berkeley, Department of Statistics, USA, October 19.
166. ———, *Weak/strong disorder for stochastic heat equation*, Analysis Seminar, University of California at Berkeley, Department of Mathematics, USA, October 21.
167. ———, *Polaron problem*, Probability Seminar, University of California at Irvine, Department of Mathematics, USA, October 25.
168. ———, *Weak/strong disorder for stochastic heat equation*, Probability and Mathematical Physics Seminar, University of California at Los Angeles, Department of Mathematics, USA, October 27.
169. ———, *Compactness, large deviations and the polaron*, Probability Seminar, University of Washington, Department of Mathematics, Seattle, USA, October 31.
170. ———, *Compactness, large deviations and the polaron*, The University of Arizona, Department of Mathematics, USA, November 2.
171. ———, *Quenched large deviations for random walks on supercritical percolation clusters*, Probability and Mathematical Physics Seminar, Courant Institute, New York, Department of Mathematics, USA, November 4.
172. ———, *Weak/strong disorder for stochastic heat equation*, City University of New York, Department of Mathematics, USA, November 8.
173. ———, *Compactness and large deviations*, Probability Seminar, Stanford University, Department of Mathematics and Statistics, USA, November 14.



174. ———, *The polaron problem*, Rutgers University, Department of Mathematics, New Brunswick, USA, November 17.
175. R. MÜLLER, *The Lippmann equation for liquid metal electrodes*, 11th DFG-CNRS Workshop “Micro-Macro Modeling and Simulation of Liquid-Vapor Flows”, March 2–4, Université Pierre et Marie Curie, Laboratoire Jacques-Louis Lions, Paris, France, March 3.
176. H. NEIDHARDT, *To the spectral theory of vector-valued Sturm–Liouville operators with summable potentials and point interactions*, Workshop “Mathematical Challenge of Quantum Transport in Nanosystems” (Pierre Duclos Workshop), November 14–15, Saint Petersburg National Research University of Informational Technologies, Mechanics, and Optics, Russian Federation, November 15.
177. J. NEUMANN, *Adaptive SDE based sampling for random PDE*, SIAM Conference on Uncertainty Quantification, Minisymposium 142 “Error Estimation and Adaptive Methods for Uncertainty Quantification in Computational Sciences – Part II”, April 5–8, Lausanne, Switzerland, April 8.
178. ———, *The phase field approach for topology optimization under uncertainties*, ZIB Computational Medicine and Numerical Mathematics Seminar, Konrad-Zuse-Zentrum für Informationstechnik Berlin, August 25.
179. O. OMEL’CHENKO, *Chimera states in nonlocally coupled oscillators: Their variety and control*, 4th International Conference on Complex Dynamical Systems and Applications, National Institute of Technology, Durgapur, India, February 16.
180. ———, *Nonuniversal transitions to synchrony in globally coupled phase oscillator*, International Workshop on Nonlinear Complex Dynamical Systems, Indian Statistical Institute, Kolkata, February 19.
181. ———, *Spike solutions to singularly perturbed elliptic problems*, The 13th Annual Workshop on Numerical Methods for Problems with Layer Phenomena, Lomonosov Moscow State University, Russian Federation, April 7.
182. ———, *Creative control for chimera states*, Workshop on Synchronization and Oscillators with Generalized Coupling, University of Exeter, UK, April 21.
183. ———, *Mean-field equation for coherence-incoherence patterns*, 7th European Congress of Mathematics (7ECM), Minisymposium 37 “Propagation Phenomena in Discrete Media”, July 18–22, Technische Universität Berlin, July 22.
184. ———, *On the limitations of the Kuramoto model*, Dynamics Days Latin America and the Caribbean, Benemérita Universidad Autónoma de Puebla, Mexico, October 28.
185. ———, *Asymptotics of traveling coherence-incoherence patterns*, Contemporary Problems of Mathematical Physics and Computational Mathematics, Lomonosov Moscow State University, Russian Federation, November 2.
186. A. PANDEY, *Meshfree method for fluctuating hydrodynamics*, International Conference on Advances in Scientific Computing, November 28–30, Indian Institute of Technology, Department of Mathematics, Madras, November 30.
187. R.I.A. PATTERSON, *Simulations of flame generated particles*, Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2016), January 5–10, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia, January 5.
188. ———, *Monte Carlo simulation of soot*, King Abdullah University of Science and Technology (KAUST), Clean Combustion Research Center, Thuwal, Saudi Arabia, January 11.
189. ———, *Pathwise LDPs for chemical reaction networks*, 12th German Probability and Statistics Days 2016 – Bochumer Stochastik-Tage, February 29 – March 4, Ruhr-Universität Bochum, Fakultät für Mathematik, March 4.

190. ———, *Population balance simulation*, University of Cambridge, Department for Chemical Engineering and Biotechnology, UK, May 5.
191. J. PELLERIN, *Simultaneous meshing and simplification of complex 3D geometrical models using Voronoi diagrams*, Université Catholique de Louvain, Institute of Mechanics, Materials and Civil Engineering, Louvain-la-Neuve, Belgium, June 30.
192. D. PESCHKA, *Thin film free boundary problems — Modeling of contact line dynamics with gradient formulations*, CeNoS-Kolloquium, Westfälische Wilhelms-Universität Münster, Center for Nonlinear Science, January 12.
193. ———, *A free boundary problem for the motion of viscous liquids*, 7th European Congress of Mathematics (7ECM), Minisymposium 29 “Nonsmooth PDEs in the Modeling Damage, Delamination, and Fracture”, July 18–22, Technische Universität Berlin, July 22.
194. ———, *Multi-phase flows with contact lines: Solid vs liquid substrates*, Industrial and Applied Mathematics Seminar, University of Oxford, Mathematical Institute, UK, October 27.
195. ———, *Scientific computing and applied mathematics for optoelectronics and soft matter problems*, Universiteit Twente, Departement of Mathematics, Enschede, Netherlands, November 8.
196. TH. PETZOLD, *The MIMESIS project – An example for an interdisciplinary research project*, Leibniz-Kolleg for Young Researchers: Chances and Challenges of Interdisciplinary Research, Thematic Workshop “Models and Modelling”, November 9–11, Leibniz-Gemeinschaft, Berlin, November 9.
197. J. POLZEHL, *Modeling high resolution MRI: Statistical issues*, Mathematical and Statistical Challenges in Neuroimaging Data Analysis, January 31 – February 5, Banff International Research Station (BIRS), Banff, Canada, February 1.
198. ———, *Assessing dynamics in learning experiments*, Novel Statistical Methods in Neuroscience, June 22–24, Otto-von-Guericke-Universität Magdeburg, Institut für Mathematische Stochastik, June 22.
199. G. PRINTSYPAR, *Modeling of membranes for forward osmosis at different scales*, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Strömungs- und Materialsimulation, Kaiserslautern, May 19.
200. M. RADSZUWEIT, *A non-isothermal phase field model for damage in heterogeneous materials*, Seminar “Nichtlineare Dynamik und Strukturbildung”, Technische Universität Berlin, Institut für Theoretische Physik, February 3.
201. M. RADZIUNAS, *A multi-mode delay differential equation model for lasers with optical feedback*, Research Seminar, Macquarie University, Department of Physics and Astronomy, Sydney, Australia, July 15.
202. M. REDMANN, *Model reduction for stochastic differential equations*, Stochastic Analysis Seminar, University of Oxford, Mathematical Institute, UK, October 31.
203. J. REHBERG, *On optimal elliptic Sobolev regularity*, Oberseminar Analysis, Technische Universität Clausthal, Institut für Mathematik, Clausthal-Zellerfeld, January 20.
204. ———, *On non-smooth parabolic equations*, Oberseminar Analysis, Universität Kassel, Institut für Mathematik, May 2.
205. ———, *On non-smooth parabolic equations*, Oberseminar Analysis, Leibniz Universität Hannover, Institut für Angewandte Mathematik, May 10.
206. ———, *On Hölder continuity for elliptic and parabolic problems*, 8th Singular Days, June 27–30, University of Lorraine, Department of Sciences and Technologies, Nancy, France, June 29.
207. S. REICHELT, *On periodic homogenization*, 20. Harz-Seminar zur Strukturbildung in Chemie und Biophysik, February 21–22, Physikalisch-Technische Bundesanstalt, Hahnentklee, February 22.

208. ———, *Homogenization of Cahn–Hilliard-type equations via evolutionary  $\Gamma$ -convergence*, Joint Annual Meeting of DMV and GAMM, Young Researchers’ Minisymposium “Multiscale Evolutionary Problems”, March 7–11, Technische Universität Braunschweig, March 7.
209. ———, *Error estimates for elliptic and parabolic equations with oscillating coefficients*, Karlstad Applied Analysis Seminar, Karlstad University, Department of Mathematics and Computer Science, Sweden, April 13.
210. ———, *Error estimates for elliptic equations with not exactly periodic coefficients*, Berlin Dresden Prague Würzburg Workshop “Homogenization and Related Topics”, Technische Universität Dresden, Fachbereich Mathematik, June 22.
211. ———, *Homogenization of Cahn–Hilliard-type equations via gradient structures*, The 11th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 2 “Emergence and Dynamics of Patterns in Nonlinear Partial Differential Equation”, July 1–5, The American Institute of Mathematical Sciences, Orlando (Florida), USA, July 3.
212. D.R.M. RINGER, *Large deviations for reacting particle systems: The empirical and ensemble process*, Young European Probabilists Workshop “Large Deviations for Interacting Particle Systems and Partial Differential Equations” (YEP XIII), March 6–11, European Institute for Statistics, Probability, Stochastic Operations Research and their Applications (EURANDOM), Eindhoven, Netherlands, March 7.
213. ———, *Functions of bounded variation with an infinite-dimensional codomain*, Meeting in Applied Mathematics and Calculus of Variations, September 13–16, Università di Roma “La Sapienza”, Dipartimento di Matematica “Guido Castelnuovo”, Italy, September 16.
214. N. ROTUNDO, *On some extension of energy-drift-diffusion models*, The 19th European Conference on Mathematics for Industry (ECMI 2016), Minisymposium 34 “Mathematical Modeling of Charge Transport in Graphene and Low Dimensional Structure”, June 13–18, Universidade de Santiago de Compostela, Spain, June 14.
215. ———, *Numerical methods for drift-diffusion models*, Seminar “Angewandte Mathematik”, Ernst Moritz Arndt Universität Greifswald, Institut für Mathematik und Informatik, June 28.
216. ———, *Thermodynamic modeling of optoelectronic semiconductor devices*, Mathematical Models for Quantum and Classical Mechanics (SEMOTAY2016), November 17–18, Università degli Studi di Firenze, Dipartimento di Matematica, Florence, Italy, November 18.
217. J.G.M. SCHOENMAKERS, *Uniform approximation of the Cox–Ingersoll–Ross process*, Frontiers in Stochastic Modelling for Finance, February 2–6, Università degli Studi di Padova, Padua, Italy, February 5.
218. ———, *Financial Mathematics*, 5 talks, The 9th Summer School in Financial Mathematics 2016, February 18–20, African Institute for Mathematical Sciences South Africa (AIMS), Cape Town, February 18–20.
219. ———, *Uniform approximation methods for the C.I.R. process*, Stochastic Seminar, Charles University, Prague, Czech Republic, April 6.
220. H. SI, *Some geometric problems in tetrahedral mesh generation*, Fifth Workshop on Grid Generation for Numerical Computations (Tetrahedron V), July 4–5, University of Liège, Montefiore Institute, Department of Electrical Engineering and Computer Science, Belgium, July 5.
221. ———, *On tetrahedralizations of reduced Chazelle polyhedra with interior Steiner points*, 25th International Meshing Roundtable and User Forum, September 27–30, Sandia National Laboratories, Washington, DC, USA, September 27.
222. ———, *An introduction to Delaunay-based mesh generation and adaptation*, University of Kansas, Department of Mathematics, Lawrence, USA, October 5.
223. ———, *TetGen, a Delaunay-based quality tetrahedral mesh generator*, Old Dominion University, Department of Computer Science, Norfolk, USA, October 7.

224. ———, *An introduction to Delaunay-based mesh generation and adaptation*, State University of New York, Department of Computer Science, Stony Brook, USA, October 11.
225. ———, *On 3D irreducible and indecomposable polyhedra and the number of interior Steiner points*, International Conference “Numerical Geometry, Grid Generation and Scientific Computing” (NUMGRID 2016), October 31 – November 2, Russian Academy of Sciences, Federal Research Center of Information and Control, Moscow, October 31.
226. R. SOARES DOS SANTOS, *Random walk on random walks*, Rhein-Main Kolloquium Stochastik, Johannes-Gutenberg Universität, Institut für Mathematik, Mainz, May 13.
227. ———, *Random walk on random walks*, Seminar, Leiden University, Institute of Mathematics, Netherlands, May 16.
228. ———, *Random walk on random walks*, University College London, Department of Mathematics, London, UK, June 15.
229. V. SPOKOINY, *Inference for Structural Nonparametrics*, 6 talks, Open Access: [http://www.mathnet.ru/php/conference.phtml?option\\_lang=eng&eventID=25&confid=872](http://www.mathnet.ru/php/conference.phtml?option_lang=eng&eventID=25&confid=872), Independent University of Moscow (IUM), Russian Federation, February 15 – March 1.
230. ———, *Deviation bounds for quadratic forms with applications*, Monash Probability Conference in Honor of Robert Liptser’s 80th Birthday, April 25–29, Monash University, School of Mathematical Sciences, Prato, Italy, April 27.
231. ———, *Self-normalized deviation bound for a martingale*, Modern Problems of Stochastic Analysis and Statistics, May 29 – June 2, Higher School of Economics, International Laboratory of Stochastic Analysis and its Applications, Moscow, Russian Federation, May 31.
232. ———, *Adaptive weights clustering*, 2nd International Scientific Conference “Science of the Future”, September 20–23, The Ministry of Science and Education of the Russian Federation, Kazan, September 21.
233. ———, *Clustering using adaptive weights*, Yandex, Moscow, Russian Federation, October 28.
234. ———, *Adaptive weights clustering*, Mathematisches Kolloquium, Universität Ulm, Institut für Analysis, November 18.
235. ———, *Inference for structured regression*, Meeting in Mathematical Statistics 2016 “Advances in Nonparametric and High-dimensional Statistics”, December 12–16, Fréjus, France, December 15.
236. ———, *Clustering using adaptive weights*, The 3rd Professor Day Academic Conference, December 19–20, Huawei Research Centre (RRC), Moscow, Russian Federation, December 19.
237. B. STEMPER, *MOTM option pricing under rough volatility*, 6th Berlin–Oxford Meeting, December 8–10, University of Oxford, Mathematics Department, UK, December 10.
238. A. SUVORIKOVA, *Multiscale change point detection*, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, November 9.
239. ———, *Bootstrap confidence sets for Wasserstein barycenters*, Meeting in Mathematical Statistics 2016 “Advances in Nonparametric and High-dimensional Statistics”, December 12–16, Fréjus, France, December 16.
240. K. TABELOW, *Mathematical models: A research data category?*, The 5th International Congress on Mathematical Software, July 11–14, Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), July 13.
241. ———, *Denosing brain images: A clinical need and a mathematical idea*, Leibniz-Kolleg for Young Researchers: Challenges and Chances of Interdisciplinary Research, November 9–11, Leibniz-Gemeinschaft, Berlin, November 9.

242. ———, *Functional magnetic resonance imaging: Processing large dataset*, AG DANK Autumn Meeting 2016, November 18–19, Gesellschaft für Klassifikation, Arbeitsgruppe “Datenanalyse und Numerische Klassifikation”, WIAS Berlin, November 18.
243. M. THOMAS, *Non-smooth PDEs in material failure: Towards dynamic fracture*, Joint Annual Meeting of DMV and GAMM, Section 14 “Applied Analysis”, March 7–11, Technische Universität Braunschweig, March 10.
244. ———, *Coupling rate-independent and rate-dependent processes: Delamination models in visco-elastodynamics*, Oberseminar “Mathematik in den Naturwissenschaften”, Universität Würzburg, Institut für Mathematik, June 10.
245. ———, *Analysis and optimization for edge-emitting semiconductor heterostructures*, The 11th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 2 “Emergence and Dynamics of Patterns in Nonlinear Partial Differential Equation”, July 1–5, The American Institute of Mathematical Sciences, Orlando (Florida), USA, July 3.
246. ———, *Rate-independent evolution of sets*, INdAM-ISIMM Workshop on Trends on Applications of Mathematics to Mechanics, September 5–8, The International Society for the Interaction of Mechanics and Mathematics (ISIMM), Rome, Italy, September 6.
247. ———, *Energetic concepts for coupled rate-independent and rate-dependent processes: Damage & delamination in visco-elastodynamics*, 2 talks, International Conference “Mathematical Analysis of Continuum Mechanics and Industrial Applications II” (CoMFoS16), October 22–24, Kyushu University, Fukuoka, Japan, October 23–24.
248. ———, *Rate-independent evolution of sets & application to fracture processes*, Seminar on Analysis, Kanazawa University, Institute of Science and Engineering, Kanazawa, Japan, October 28.
249. N. TOGOBYTSKA, *Uncertainty quantification in environmental simulations*, The 19th European Conference on Mathematics for Industry (ECMI 2016), Minisymposium 26 “Stochastic Inverse Problems”, June 13–17, Universidade de Santiago de Compostela, Spain, June 13.
250. E. VALDINOCI, *Nonlocal minimal surfaces, a geometric and analytic insight*, Seminar on Differential Geometry and Analysis, Otto-von-Guericke-Universität Magdeburg, January 18.
251. ———, *Nonlocal minimal surface*, Justus-Liebig-Universität Gießen, Fakultät für Mathematik, February 10.
252. ———, *Interior and boundary properties of nonlocal minimal surfaces*, Calcul des Variations & EDP, Université Aix-Marseille, Institut de Mathématiques de Marseille, France, February 25.
253. ———, *Nonlocal minimal surfaces and phase transitions*, Seminar, University of Leeds, School of Mathematics, UK, April 19.
254. ———, *Superfici minime e transizioni di fase (non)locali*, EDP e Dintorni II Incontro, Università di Bari, Dipartimento di Matematica, Italy, May 13.
255. ———, *Nonlocal equations and applications*, Calculus of Variations and Nonlinear Partial Differential Equations, May 16–27, Columbia University, Department of Mathematics, New York, USA, May 25.
256. ———, *Nonlocal equations from various perspectives*, PIMS Workshop on Nonlocal Variational Problems and PDEs, June 13–17, University of British Columbia, Vancouver, Canada, June 13.
257. ———, *A notion of fractional perimeter and nonlocal minimal surfaces*, Seminar, Università del Salento, Dipartimento di Matematica e Fisica “Ennio de Giorgi”, Lecce, Italy, June 22.
258. ———, *Interior and boundary properties on nonlocal minimal surfaces*, 3rd Conference on Nonlocal Operators and Partial Differential Equations, June 27 – July 1, Bedlewo, Poland, June 27.
259. ———, *Nonlocal minimal surfaces*, Analysis, PDEs, and Geometry Seminar, Monash University, Clayton, Australia, August 9.

260. ———, *Nonlocal equations from different points of view*, Research Seminar, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, August 31.
261. ———, *Capillarity problems with nonlocal surface tension energies*, Columbia Geometry & Analysis Seminar, Columbia University in the City of New York, Department of Mathematics, USA, September 16.
262. ———, *Planelike solutions in periodic media*, Asymptotic Patterns in Variational Problems: PDE and Geometric Aspects, September 25–30, Banff International Research Station for Mathematical Innovation and Discovery, Oaxaca, Mexico, September 28.
263. W. VAN ZUIJLEN, *Mean field Gibbs-non-Gibbs transitions*, 6th Berlin–Oxford Meeting, December 8–10, University of Oxford, Mathematics Department, UK, December 9.
264. A.G. VLADIMIROV, *Delay differential models in multimode laser dynamics: Taking chromatic dispersion into account*, SPIE Photonics Europe 2016, Conference 9892 “Semiconductor Lasers and Laser Dynamics”, Session 5, April 3–7, SPIE, Brussels, Belgium, April 5.
265. ———, *Distributed delay differential equation models in laser dynamics*, Volga Neuroscience Meeting 2016, July 24–30, from Saint Petersburg to Nizhny Novgorod, Russian Federation, July 28.
266. ———, *Interaction of temporal cavity solitons in driven fiber resonators and mode-locked lasers*, International Tandem Workshop on Pattern Dynamics in Nonlinear Optical Cavities, August 15–19, Max-Planck-Institut für Physik komplexer Systeme, Dresden, August 15.
267. B. WAGNER, *Concentrated suspensions: A multiscale analysis*, University of Limerick, Mathematics Applications Consortium for Science and Industry, Ireland, April 1.
268. ———, *Thin films and complex liquids for industrial application*, Leibniz-Kolleg for Young Researchers: Challenges and Chances of Interdisciplinary Research, Thematic Workshop “Models and Modelling”, Leibniz-Gemeinschaft, Berlin, November 9.
269. M. WOLFRUM, *Emergence of collective behavior in coupled oscillator systems*, Wednesdays@NICO, Northwestern University, Northwestern Institute on Complex Systems, Evanston, USA, January 20.
270. ———, *Emergence of collective behavior in coupled oscillator systems*, Workshop “Dynamics in Networks with Special Properties”, January 25–29, Mathematical Biosciences Institute (MBI), Columbus, USA, January 27.
271. ———, *Synchronization transitions in systems of coupled phase oscillators*, Arbeitsgruppenseminar “Chemische Physik fern vom Gleichgewicht”, Technische Universität München, Fachbereich Physik, March 18.
272. ———, *Synchronization transitions in systems of coupled phase oscillators*, Workshop on Synchronization and Oscillators with Generalized Coupling, April 20–22, University of Exeter, UK, April 21.
273. ———, *Synchronization transitions in systems of coupled phase oscillators*, Oberseminar Angewandte Mathematik, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, June 22.
274. T. WU, *Bilevel optimization and applications in imaging sciences*, 2 talks, Shanghai Jiao Tong University, Institute of Natural Sciences, China, August 24–25.
275. M. ZHILOVA, *Choosing the number of samples in a Monte Carlo simulation using bootstrap*, Workshop on Applied Statistics 2016, March 10–11, Technische Universität Dresden, Institut für Wirtschaft & Verkehr, March 10.
276. ———, *Some new non-asymptotic results about accuracy of the weighted bootstrap*, Stochastics Seminar, Georgia Institute of Technology, School of Mathematics, Atlanta, USA, April 28.



## A.8.3 Talks for a More General Public

1. F. ANKER, *Fraktale: Ordnung im Chaos*, 21. Berliner Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
2. A. CIPRIANI, *Das Teilungsproblem*, MathInside – Mathematik ist überall, Urania, Berlin, March 15.
3. CH. D'ALONZO, *Spaß an Mathe und Programmieren: Die MATSE-Ausbildung, Part I*, Girls' Day, WIAS Berlin, April 28.
4. ———, *Mathematische Spielerei mit der Gaußschen Summenformel, III*, 21. Berliner Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
5. F. FLEGEL, *Kuriositäten aus der Wahrscheinlichkeitsrechnung*, Girls' Day 2016, WIAS Berlin, April 28.
6. CH. HEINEMANN, *Eine Exkursion in die Welt des unendlich Kleinen in der Mathematik*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2016, WIAS at Leibniz Association Headquarters, Berlin, June 11.
7. B. JAHNEL, *Die Entropie des tippenden Affen*, 21. Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
8. ———, *Die Poesie der Logik*, Tag der Mathematik, Universität Regensburg, Fakultät für Mathematik, July 15.
9. W. KÖNIG, *Murphys Gesetz, tippende Affen und Unendlichkeit in der Wahrscheinlichkeitstheorie*, Berliner Mathematische Gesellschaft e.V., Vorträge zur Göttinger Modellsammlung und zur Wahrscheinlichkeit, Freie Universität Berlin, February 18.
10. ———, *Murphys Gesetz, tippende Affen und Unendlichkeit in der Wahrscheinlichkeitsrechnung*, 21. Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
11. ———, *Universalität der Fluktuationen: Warum ist alles Gauß-verteilt?*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2016, WIAS at Leibniz Association Headquarters, Berlin, June 11.
12. ———, *Unendlichkeit in der Wahrscheinlichkeitsrechnung, Murphys Gesetz und tippende Affen*, Tag der Mathematik, Ellen-Key-Schule, Berlin, September 6.
13. ———, *Auf Leibniz' Spuren in der Mathematik*, introduction to the event “Auf Leibniz' Spuren in der Mathematik” (meaning: on Leibniz's traces in mathematics) organized by WIAS in the Leibniz Association Headquarters, Berlin, November 29.
14. ———, *Universalität der Fluktuationen: Warum ist alles Gauß-verteilt?*, 2 talks, Tag der Wissenschaften 2016, Weinberg-Gymnasium Kleinmachnow, December 6.
15. S. REICHELT, *Konvergenz und Homogenisierung*, 21. Berliner Tag der Mathematik (21st Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
16. G. REINHARDT, *Mathematische Spielerei mit der Gaußschen Summenformel, I*, 21. Berliner Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
17. D.R.M. RINGER, *The truth is out there... it's called math!*, Nerd Nite Amsterdam: “Nerd Nite Greatest Hits – Five years of Talks and Beers”, Netherlands, April 15.
18. P. SÖLDNER, *Spaß an Mathe und Programmieren: Die MATSE-Ausbildung, Part II*, Girls' Day 2016, WIAS Berlin, April 28.
19. ———, *Mathematische Spielerei mit der Gaußschen Summenformel, II*, 21. Berliner Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
20. H. STEPHAN, *Die Multiplikation als Dualität in Mathematik, Physik und Erkenntnistheorie*, 21. Berliner Tag der Mathematik (21th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.

21. ———, *Mathematik, Physik und Erkenntnistheorie*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2016, WIAS at Leibniz Association Headquarters, Berlin, June 11.

#### A.8.4 Posters

1. N. ALIA, V. JOHN, *Optimal control of ladle stirring*, 1st Leibniz MMS Mini Workshop on CFD & GFD, WIAS Berlin, September 8–9.
2. L. BOGOLUBSKY, P. DVURECHENSKY, A. GASNIKOV, G. GUSEV, Y. NESTEROV, A.M. RAIGORODSKII, A. TIKHONOV, M. ZHUKOVSKII, *Learning supervised PageRank with gradient-based and gradient-free optimization methods*, The Thirtieth Annual Conference on Neural Information Processing Systems (NIPS), Barcelona, Spain, December 4–10.
3. S. EYDAM, *Mode-locking in systems of phase oscillators with higher harmonic interaction*, Workshop on Synchronization and Oscillators with Generalized Coupling, Exeter, UK, April 20–22.
4. ———, *Mode-locking in systems of phase oscillators with higher harmonic coupling*, International Conference on Control of Complex Systems and Networks, SFB 910 “Control of Self-Organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, Heringsdorf/Usedom, September 4–8.
5. F. FLEGEL, *Spectral localization in the random conductance model*, 2nd Berlin Dresden Prague Würzburg Workshop on Mathematics of Continuum Mechanics, Technische Universität Dresden, Fachbereich Mathematik, December 5.
6. TH. FRENZEL, *Evolutionary Gamma-convergence for amplitude equations and for wiggly energy models*, Winter School 2016: Calculus of Variations in Physics and Materials Science, Würzburg, February 15–19.
7. ———, *Examples of evolutionary Gamma-convergence*, Workshop on Industrial and Applied Mathematics 2016, 5th Symposium of German SIAM Student Chapters, Hamburg, August 31 – September 2.
8. ———, *EDP-convergence for delamination and a wiggly energy model*, 2nd Berlin Dresden Prague Würzburg Workshop on Mathematics of Continuum Mechanics, Technische Universität Dresden, Fachbereich Mathematik, Dresden, December 5.
9. M. BECKER, TH. FRENZEL, TH. NIEDERMAYER, S. REICHEL, M. BÄR, A. MIELKE, *Competing patterns in anti-symmetrically coupled Swift–Hohenberg equations*, International Conference on Control of Complex Systems and Networks, SFB 910 “Control of Self-Organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, Heringsdorf/Usedom, September 4–8.
10. J. FUHRMANN, W. DREYER, C. GUHLKE, M. LANDSTORFER, R. MÜLLER, A. LINKE, CH. MERDON, *Modeling and numerics for electrochemical systems*, Micro Battery and Capacitive Energy Harvesting Materials – Results of the MatFlexEnd Project, Universität Wien, Austria, September 19.
11. J. FUHRMANN, A. LINKE, CH. MERDON, M. KHODAYARI, H. BALTRUSCHAT, *Detection of solubility, transport and reaction coefficients from experimental data by inverse modelling of thin layer flow cells*, 1st Leibniz MMS Mini Workshop on CFD & GFD, WIAS Berlin, September 8–9.
12. J. FUHRMANN, A. LINKE, CH. MERDON, W. DREYER, C. GUHLE, M. LANDSTORFER, R. MÜLLER, *Numerical methods for electrochemical systems*, 2nd Graz Battery Days, Graz, Austria, September 27–28.
13. J. FUHRMANN, CH. MERDON, *A thermodynamically consistent numerical approach to Nernst–Planck–Poisson systems with volume constraints*, The 67th Annual Meeting of the International Society of Electrochemistry, Den Haag, Netherlands, August 21–26.
14. C. GUHLKE, W. DREYER, R. MÜLLER, M. LANDSTORFER, *Models of lithium-ion batteries: A paradigm for consistent modelling*, 1st Leibniz MMS Days, WIAS Berlin, January 27–29.
15. C. GUHLKE, W. DREYER, R. MÜLLER, M. LANDSTORFER, J. FUHRMANN, *Beyond Newman’s battery model*, 2nd Graz Battery Days, Graz, Austria, September 27–28.

16. C. GUHLKE, J. FUHRMANN, W. DREYER, R. MÜLLER, M. LANDSTORFER, *Modeling of batteries*, Batterieforum Deutschland 2016, Berlin, April 6–8.
17. M. HEIDA, A. MIELKE, CH. KRAUS, M. THOMAS, *Effective models for interfaces with many scales*, SCCS Days, CRC 1114 “Complex Processes involving Cascades of Scales”, Ketzin, October 10–12.
18. M. HINTERMÜLLER, K. PAPAITSOROS, C. RAUTENBERG, *A fine scale analysis of spatially adapted total variation regularisation*, Imaging, Vision and Learning based on Optimization and PDEs, Bergen, Norway, August 29 – September 1.
19. M. HINTERMÜLLER, S. HAJIAN, N. STROGIES, *Subproject B02 – Parameter id., sensor localization and quantification of uncertainties in switched PDE systems*, Annual Meeting of the Collaborative Research Center/Transregio (TRR) 154 “Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks”, Technische Universität Berlin, October 4–5.
20. ———, *Subproject B02 – Parameter id., sensor localization and quantification of uncertainties in switched PDE systems*, Conference “Mathematics of Gas Transport”, Konrad-Zuse-Zentrum für Informationstechnik Berlin, October 6–7.
21. M. LANDSTORFER, *Towards a model based understanding of cyclic voltammetry*, Electrochemistry 2016, Gesellschaft Deutscher Chemiker e.V. (GDCh), Goslar, September 26–28.
22. A. LINKE, CH. MERDON, *Pressure-robustness and acceleration of Navier–Stokes solvers*, 1st Leibniz MMS Days, WIAS Berlin, January 27–29.
23. ———, *Pressure-robustness and acceleration of Navier–Stokes solvers*, 37th Northern German Colloquium on Applied Analysis and Numerical Mathematics (NoKo 2016), Universität zu Lübeck, April 22–23.
24. CH. MERDON, J. FUHRMANN, A. LINKE, A. ABD-EL-LATIF, M. KHODAYARI, P. REINSBERG, H. BALTRUSCHAT, *Inverse modelling of thin layer flow cells and RRDEs*, The 67th Annual Meeting of the International Society of Electrochemistry, Den Haag, Netherlands, August 21–26.
25. K. KRAUS, J. DOLATA, T. SCHADE, H.-J. MUCHA, H.-G. BARTEL, *Werkstoffuntersuchungen an einem barocken Kanal im Mainzer Bleichenviertel*, Jahrestagung Archäometrie und Denkmalpflege 2016, Göttingen, September 27 – October 1.
26. R. MÜLLER, W. DREYER, J. FUHRMANN, C. GUHLKE, *New insights into Butler–Volmer kinetics from thermodynamic modeling*, The 67th Annual Meeting of the International Society of Electrochemistry, Den Haag, Netherlands, August 21–26.
27. O. OMEL'CHENKO, *Regular and irregular patterns of self-localized excitation in arrays of coupled phase oscillators*, International Conference on Control of Complex Systems and Networks, SFB 910 “Control of Self-Organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, Heringsdorf/Usedom, September 4–8.
28. S. PICKARTZ, S. AMIRANASHVILI, *Champion solitons that come from nowhere*, 618. WE-Heraeus-Seminar: Extreme Events and Rogue Waves – 2016, Wilhelm und Else Heraeus-Stiftung, Bad Honnef, May 30 – June 3.
29. S. PICKARTZ, U. BANDELOW, S. AMIRANASHVILI, *Numerical optimization of all-optical switching*, 16th International Conference on Numerical Simulation of Optoelectronic Devices, Sydney, Australia, July 11–15.
30. S. REICHELT, *Homogenization of Cahn–Hilliard-type equations via evolutionary Gamma-convergence*, Workshop “Patterns of Dynamics”, Freie Universität Berlin, Fachbereich Mathematik und Informatik, July 25–29.
31. ———, *Competing patterns in anti-symmetrically coupled Swift–Hohenberg equations*, International Conference on Control of Complex Systems and Networks, SFB 910 “Control of Self-Organizing Nonlinear Systems: Theoretical Methods and Concepts of Application”, Heringsdorf/Usedom, September 4–8.
32. A. ROGGENSACK, *Analysis of the Cahn–Hilliard reaction system including a rate-dependent damage process*, PIRE-CNA 2016 Summer School “New Frontiers in Analysis for Materials”, Carnegie Mellon University, Pittsburgh, USA, June 2–10.

33. K. TABELOW, V. AVANESOV, M. DELIANO, R. KÖNIG, A. BRECHMANN, J. POLZEHL, *Assessing dynamics in learning experiments*, Challenges in Computational Neuroscience: Transition Workshop, Research Triangle Park, North Carolina, USA, May 4–6.
34. K. TABELOW, CH. D'ALONZO, J. POLZEHL, M.F. CALLAGHAN, L. RUTHOTTO, N. WEISKOPF, S. MOHAMMADI, *How to achieve very high resolution quantitative MRI at 3T?*, 22th Annual Meeting of the Organization of Human Brain Mapping (OHBM 2016), Geneva, Switzerland, June 26–30.

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

1. N. AHMED, Technische Universität Dresden, Institut für Numerische Mathematik, February 8–11.
2. ———, Lahore University of Management Sciences, Centre for Advanced Studies in Mathematics, Pakistan, May 20–25.
3. N. ALIA, University of Oulu, Faculty of Technology, Finland, November 1 – December 31.
4. M.J. ARENAS JAÉN, University of Oulu, Faculty of Technology, Finland, November 4, 2016 – January 31, 2017.
5. CH. BAYER, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering Division, Thuwal, Saudi Arabia, January 5–12.
6. ———, École Nationale de la Statistique et de l'Administration Économique, Laboratory of Statistics, Malakoff, France, January 26–29.
7. ———, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering Division, Thuwal, Saudi Arabia, February 7–15.
8. ———, Imperial College London, Department of Mathematics, UK, October 3–7.
9. ———, Technische Universität Wien, Institut für Stochastik und Wirtschaftsmathematik, Austria, November 28 – December 2.
10. ———, École Polytechnique CNRS, Centre de Mathématiques Appliquées, Palaiseau, France, December 12–16.
11. N. BUZUN, Moscow Institute of Physics and Technology, Department of Applied Mathematics and Control, Dolgoprudny, Moscow Region, Russian Federation, May 13–23.
12. A. CAIAZZO, University of St Andrews, Mathematical Institute, Scotland, UK, October 10–13.
13. L. CAPONE, University of Oulu, Faculty of Technology, Finland, November 7, 2016 – January 31, 2017.
14. A. CIPRIANI, Delft University of Technology, Department of Applied Probability, Netherlands, January 18–22.
15. ———, University of Bath, Department of Mathematical Sciences, UK, June 15–18.
16. ———, University of Lancaster, Department of Mathematics and Statistics, UK, July 18–22.
17. ———, Delft University of Technology, Department of Applied Probability, Netherlands, August 29 – September 10.
18. ———, University of Bath, Department of Mathematical Sciences, UK, October 2–8.
19. F. DASSI, Politecnico di Milano, Dipartimento di Matematica “F. Brioschi”, Italy, February 18–24.
20. F. FLEGEL, University of California at Los Angeles, Department of Mathematics, USA, October 6–27.
21. S.P. FRIGERI, Politecnico di Milano, Dipartimento di Matematica, Italy, January 18–22.
22. ———, March 21–24.
23. ———, Università di Pavia, Dipartimento di Matematica, Italy, May 2–6.
24. ———, Politecnico di Milano, Dipartimento di Matematica, Italy, May 17–20.
25. ———, Università di Pavia, Dipartimento di Matematica, Italy, June 13–17.

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

26. P. FRIZ, University of Amsterdam, Korteweg-de Vries Institute for Mathematics, Netherlands, October 17–21.
27. A. GONZÁLEZ CASANOVA SOBERÓN, University of Oxford, Mathematical Institute, UK, April 6–13.
28. ———, Centro de Investigación en Matemáticas, Department of Probability and Statistics, Guanajuato, Mexico, September 9 – November 15.
29. ———, Universidad Nacional Autónoma de México, Institute of Mathematics, Mexico City, October 16–21.
30. ———, University of Warwick, Mathematics Institute, UK, November 26 – December 3.
31. CH. HEINEMANN, Università di Pavia, Dipartimento di Matematica; Università di Brescia, Dipartimento di Ingegneria Civile Ambiente Territorio Architettura e Matematica, Italy, May 9–13.
32. R. HILDEBRAND, Université Joseph Fourier, Laboratoire Jean Kuntzmann, Grenoble, France, January 4–11.
33. CH. HIRSCH, Ludwig-Maximilians-Universität München, Fakultät für Mathematik, April 18–22.
34. ———, Telecom Orange Paris, France, June 7–10.
35. D. HÖMBERG, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, February 2–11.
36. ———, September 19–23.
37. ———, October 24 – November 10.
38. B. JAHNEL, Telecom Orange Paris, France, June 7–10.
39. V. JOHN, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, April 3–8.
40. ———, Beijing Computational Science Research Center, China, August 20–24.
41. L. KAMENSKI, Technische Universität Darmstadt, Fachbereich Mathematik, June 28 – July 2.
42. ———, July 25–28.
43. P. KEELER, University of Cambridge, Faculty of Mathematics, UK, May 10–14.
44. ———, Telecom Orange Paris, France, June 6–13.
45. ———, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, September 19–22.
46. ———, The University of Melbourne, Department of Mathematics and Statistics, Australia, September 25 – October 31.
47. ———, Institut National de Recherche en Informatique et en Automatique (INRIA), Research Team DYOGENE – Dynamics of Geometric Networks, Paris, France, November 22–26.
48. O. KLEIN, Silesian University, Mathematical Institute, Opava, Czech Republic, December 5–9.
49. W. KÖNIG, Universität zu Köln, Mathematisches Institut, July 31 – August 7.
50. ———, November 20–24.
51. M. LANDSTORFER, Ostbayerische Technische Universität Regensburg, Fakultät Informatik und Mathematik, August 26–29.
52. V. LASCHOS, Università di Pavia, Dipartimento di Matematica, Italy, November 15–22.
53. P. MATHÉ, Österreichische Akademie der Wissenschaften, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, August 9–12.
54. ———, Fudan University, The School of Mathematical Sciences, Shanghai, China, October 31 – November 11.



55. M. MAURELLI, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 25–29.
56. ———, Universidade Estadual de Campinas, Instituto de Matemática, Estatística e Computação Científica, Campinas, Brazil, June 20–27.
57. ———, University of York, Department of Mathematics, UK, October 19–28.
58. E. MECA ÁLVAREZ, University of California at Irvine, Department of Mathematics, USA, April 18 – May 2.
59. CH. MERDON, Technische Universität Wien, Institut für Analysis und Scientific Computing, December 12–16.
60. A. MIELKE, Technische Universität München, Zentrum Mathematik, February 11–14.
61. ———, Erwin Schrödinger International Institute for Mathematics and Physics (ESI), Vienna, Austria, July 4–8.
62. ———, The Royal Swedish Academy of Sciences, Institute Mittag-Leffler, Stockholm, September 19–23.
63. M. MITTENZWEIG, CDJ Christophorisschule Braunschweig, July 4–8.
64. CH. MUKHERJEE, Courant Institute of Mathematical Sciences, Department of Mathematics, New York, USA, January 1 – August 31.
65. ———, University of California at Berkeley, Department of Mathematics and Statistics, USA, October 18–24.
66. ———, University of Seattle, Department of Mathematics, USA, October 28 – November 1.
67. ———, Courant Institute, Department of Mathematics, New York, USA, November 3–17.
68. R.I.A. PATTERSON, University of Cambridge, Department for Chemical Engineering and Biotechnology, UK, April 28 – May 11.
69. ———, Technische Universität München, Zentrum Mathematik, May 21–25.
70. ———, University of Cambridge, Department for Chemical Engineering and Biotechnology, UK, December 14–18.
71. J. PELLERIN, Sorbonne Universités, Institut du Calcul et de la Simulation, Paris, France, January 27–31.
72. ———, École Nationale Supérieure de Géologie, RING Team – Research for Integrative Numerical Geology, Vandoeuvre-les-Nancy, France, May 4–11.
73. ———, TOTAL E&P RECHERCHE DEVELOPPEMENT SAS, Pau, France, July 18–21.
74. D. PESCHKA, University of Oxford, Mathematical Institute, UK, October 24–28.
75. J. POLZEHL, University of Minnesota, School of Statistics, Minneapolis, USA, February 8–18.
76. ———, May 7–27.
77. S. REICHEL, Karlstad University, Department of Mathematics and Computer Science, Sweden, April 12–15.
78. N. ROTUNDO, International School of Advanced Studies (SISSA), Mathematics, Trieste, Italy, April 18–22.
79. ———, June 30 – July 12.
80. ———, October 17–24.
81. H. SI, University of Liège, Montefiore Institute, Department of Electrical Engineering and Computer, Belgium, March 14–18.
82. ———, State University of New York, Department of Computer Science, Stony Brook, USA, October 9–14.
83. R. SOARES DOS SANTOS, Johannes-Gutenberg Universität, Institut für Mathematik, Mainz, May 11–14.

84. ———, Leiden University, Institute of Mathematics, Netherlands, May 14–17.
85. ———, University College London, Department of Mathematics, UK, June 12–19.
86. V. SPOKOINY, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, February 22 – March 2.
87. ———, September 1–30.
88. ———, October 26–29.
89. ———, November 26–30.
90. M. THOMAS, Kanazawa University, Institute of Science and Engineering, Japan, October 24–29.
91. ———, Vietnam Institute for Advanced Study in Mathematics, Hanoi, November 7–11.
92. E. VALDINOCI, African Institute for Mathematical Sciences (AIMS), Mbour, Senegal, February 14–23.
93. ———, Université Aix-Marseille, Institut de Mathématiques de Marseille, France, February 23–27.
94. ———, Queen Mary University of London, School of Mathematical Sciences, UK, April 3–7.
95. ———, The University of Edinburgh, School of Mathematics, UK, April 9–16.
96. ———, University of Texas at Austin, Mathematics Department, USA, May 28 – June 8.
97. ———, Università di Bari, Dipartimento di Matematica, Italy, June 18–24.
98. W. VAN ZUIJLEN, Leiden University, Institute of Mathematics, Netherlands, November 19–28.
99. ———, December 19–23.
100. M. WOLFRUM, Northwestern University, Department of Engineering Sciences and Applied Mathematics, Chicago, USA, January 18–24.
101. ———, Westfälische Wilhelms-Universität Münster, Institut für Angewandte Mathematik, June 21–24.
102. M. ZHILOVA, Moscow Institute of Physics and Technology, PreMoLab, Russian Federation, February 18 – March 8.
103. ———, Georgia Institute of Technology, School of Mathematics, Atlanta, USA, April 25 – May 6.

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

### Winter Semester 2015/2016

1. S. AMIRANASHVILI, U. BANDELOW, *Nichtlineare Dynamik in der Photonik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
2. L. RECKE, U. BANDELOW, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
3. M. EIGEL, *Tensor Product Approximation in Uncertainty Quantification* (lecture), Technische Universität Berlin, 4 SWS.
4. P. FRIZ, *Rough Paths and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
5. ———, *Stochastic Analysis and Quantitative Finance* (seminar), Technische Universität Berlin, 2 SWS.
6. D. BECHERER, J. BLATH, P. FRIZ, W. KÖNIG, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
7. M. ELLER, A. GLITZKY, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
8. R. HENRION, *Stochastische Optimierung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
9. J. BLATH, W. KÖNIG, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
10. A. MIELKE, K. DISSER, *Mehrdimensionale Variationsrechnung/BMS Advanced Course on Multidimensional Calculus of Variations* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
11. ———, *Mehrdimensionale Variationsrechnung/BMS Advanced Course on Multidimensional Calculus of Variations* (practice), Humboldt-Universität zu Berlin, 2 SWS.
12. R.I.A. PATTERSON, *Stochastic Process Convergence* (lecture), Technische Universität Berlin, 2 SWS.
13. J.G.M. SCHOENMAKERS, *Berechnungs- und Simulationmethoden in der Finanzmathematik* (lecture), Humboldt-Universität zu Berlin, 3 SWS.
14. V. SPOKOINY, W. HÄRDLE, M. REISS, G. BLANCHARD, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
15. K. TABELOW, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
16. M. WOLFRUM, B. FIEDLER, P. GUREVICH, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/DFG Research Unit 1735, 2 SWS.

### Summer Semester 2016

1. L. RECKE, U. BANDELOW, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. CH. BAYER, A. PAPANTOLEON, *Computational Finance* (lecture), Technische Universität Berlin, 4 SWS.
3. K. DISSER, *Analysis II für Mathematiker (stand-in for regular lecturer from May 23 to June 20, 9 lectures)* (lecture), Technische Universität Berlin, 4 SWS.
4. P. FRIZ, *Rough Paths and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.

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

5. D. BECHERER, J. BLATH, P. FRIZ, W. KÖNIG, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
6. A. GLITZKY, *Einführung in die Kontrolltheorie und optimale Steuerung/Introduction to Control Theory and Optimal Control* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
7. ———, *Einführung in die Kontrolltheorie und optimale Steuerung/Introduction to Control Theory and Optimal Control* (practice), Humboldt-Universität zu Berlin, 1 SWS.
8. M. ELLER, A. GLITZKY, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
9. M. HINTERMÜLLER, TH. SUROWIEC, *Mathematische Optimierung* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
10. D. HÖMBERG, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
11. V. JOHN, *Numerical Methods for Convection-Dominated Problems* (lecture), Freie Universität Berlin, 2 SWS.
12. ———, *Numerical Methods for Convection-Dominated Problems* (practice), Freie Universität Berlin, 2 SWS.
13. W. KÖNIG, *Maß- und Integrationstheorie* (lecture), Technische Universität Berlin, 4 SWS.
14. W. KÖNIG, K. FACKELDEY, *Moderne Anwendungen der Theorie der Markovketten* (seminar), Technische Universität Berlin, 1 SWS.
15. J. BLATH, W. KÖNIG, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
16. CH. MERDON, *Lineare Algebra für Ingenieurwissenschaften* (lecture), Technische Universität Berlin, 2 SWS.
17. A. MIELKE, *Ausgewählte Themen der Variationsrechnung/BMS Advanced Course "Selected Topics of the Calculus of Variations"* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
18. V. SPOKOINY, *Mathematische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
19. ———, *Mathematische Statistik* (practice), Humboldt-Universität zu Berlin, 2 SWS.
20. V. SPOKOINY, W. HÄRDLE, M. REISS, G. BLANCHARD, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
21. K. TABELOW, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
22. M. THOMAS, *Evolutionsprobleme in der Kontinuumsmechanik/BMS Advanced Course "Evolution Problems in Continuum Mechanics"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
23. ———, *Evolutionsprobleme in der Kontinuumsmechanik/BMS Advanced Course "Evolution Problems in Continuum Mechanics"* (practice), Humboldt-Universität zu Berlin, 1 SWS.
24. N. TOGOBYTSKA, *Analysis I* (lecture), Hochschule für Technik und Wirtschaft, 3 SWS.
25. ———, *Analysis I* (practice), Hochschule für Technik und Wirtschaft, 4 SWS.
26. M. WOLFRUM, B. FIEDLER, ST. LIEBSCHER, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

### Winter Semester 2016/2017

1. L. RECKE, U. BANDELOW, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. M. EIGEL, *Tensor Product Approximation in Uncertainty Quantification* (lecture), Technische Universität Berlin, 2 SWS.

3. P. FRIZ, *Rough Paths and Regularity Structures* (lecture), Technische Universität Berlin, 2 SWS.
4. D. BECHERER, J. BLATH, P. FRIZ, W. KÖNIG, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
5. J. FUHRMANN, *Wissenschaftliches Rechnen (Scientific Computing)* (lecture), Technische Universität Berlin, 4 SWS.
6. A. GLITZKY, A. MIELKE, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
7. M. HINTERMÜLLER, *Nichtlineare Optimierung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
8. M. HINTERMÜLLER, C. SCHILLINGS, *Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
9. D. HÖMBERG, *Variational Calculus and Optimal Control of Ordinary Differential Equations (13 two-hour lectures from Oct. 24 to Nov. 10, 2016)* (lecture), Norwegian University of Science and Technology, Trondheim, – SWS.
10. ———, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
11. V. JOHN, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
12. ———, *Numerik II* (practice), Freie Universität Berlin, 2 SWS.
13. J. BLATH, W. KÖNIG, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
14. M. MAURELLI, *Numerische Mathematik II für Ingenieure* (practice), Technische Universität Berlin, 2 SWS.
15. A. MIELKE, *Analysis I\** (lecture), Humboldt-Universität zu Berlin, 5 SWS.
16. V. SPOKOINY, W. HÄRDLE, M. REISS, G. BLANCHARD, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
17. H. STEPHAN, *Funktionalanalytische Methoden in der klassischen Physik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
18. ———, *Funktionalanalytische Methoden in der klassischen Physik* (practice), Humboldt-Universität zu Berlin, 1 SWS.
19. K. TABELOW, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
20. M. THOMAS, *Gamma-Convergence Methods for Statics and Evolution (15 one-hour lectures from Nov. 7 to 11, 2016)* (lecture), Vietnam Institute for Advanced Study in Mathematics, – SWS.
21. M. WOLFRUM, B. FIEDLER, P. GUREVICH, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

## A.11 Weierstrass Postdoctoral Fellowship Program

In 2005, the Weierstrass Institute launched the *Weierstrass Postdoctoral Fellowship Program* (see <https://www.wias-berlin.de/jobs/fellowship.jsp?lang=1>). The institute offered postgraduate fellowships with a duration of six to twelve months. These fellowships were 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.

In 2016, Dr. Franco Dassi (Berlin), Dr. Simona Olmi (Consiglio Nazionale delle Ricerche, Institute for Complex Systems, Florence, Italy), and Dr. Anamika Pandey (Universität Mannheim, Institut für Mathematik) worked as fellowship holders at WIAS.



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

### A.12.1 Guests

1. L. ADAM, Humboldt-Universität zu Berlin, Institut für Mathematik, April 29 – December 31.
2. L. ADAMYAN, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, Berlin, December 1, 2015 – December 31, 2016.
3. V. AGOSTINIANI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), mathLab, Trieste, Italy, July 4–7.
4. G. AKAGI, Tohoku University, Mathematical Institute, Sendai, Japan, May 4–7.
5. H. ANTIL, George Mason University, Department of Mathematical Sciences, Fairfax, USA, February 29 – March 4.
6. A. ARAÚJO, University of Coimbra, Department of Mathematics, Coimbra, Portugal, February 25 – March 1.
7. C. BERTOGLIO, Universidad de Chile, Center for Mathematical Modeling, Santiago, Chile, February 18–23.
8. ———, July 12–22.
9. U. BESSI, Università degli Studi di Roma, Dipartimento di Matematica e Fisica, Italy, January 19–22.
10. A. BRADJI, Université Badji Mokhtar – Annaba, Département des Mathématiques, Annaba, Algeria, June 9–16.
11. A. CARPENTIER, Universität Potsdam, Institut für Mathematik, Potsdam, January 1 – December 31.
12. M. CHAPLAIN, University of St Andrews, Mathematical Institute, Scotland, UK, July 24–27.
13. A. CHIARINI, Aix-Marseille Université (I2M), Institut de Mathématiques de Marseille, France, November 1–5.
14. R. ČIEGIS, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, January 10–22.
15. ———, November 6–11.
16. G. CONFORTI, Universität Leipzig, Fakultät für Mathematik und Informatik, Leipzig, November 1–5.
17. P. DAS, EFD Induction AS, Skien, Norway, May 1 – July 31.
18. B. DE RIJK, Universiteit Leiden, Mathematisch Instituut, Leiden, Netherlands, May 17–20.
19. TH. DICKHAUS, Universität Bremen, Institut für Statistik, Bremen, November 15–20.
20. A. DIEB, Ibn Khaldoun University, Department of Mathematics, Tiaret, Algeria, November 22, 2015 – January 31, 2016.
21. A. DREWITZ, Universität zu Köln, Mathematisches Institut, Köln, March 8–11.
22. E. FEIREISL, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, Czech Republic, January 25–29.
23. ———, February 8–12.
24. J. FENG, University of Kansas, Department of Mathematics, Kansas, USA, September 12–17.
25. I. FRANOVIC, University of Belgrade, Institute of Physics Belgrade, Serbia, May 8–14.

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

26. A. GOLDENSCHLUGER, University of Haifa, Department of Statistics, Haifa, Israel, August 22–31.
27. R. GRANDE, University of Salento, Dipartimento di Matematica e Fisica, Lecce, Italy, March 2 – May 31.
28. N. GUILLOTIN-PLANTARD, Université Claude Bernard Lyon 1, Institut Camille Jordan, Villeurbanne, France, April 20–24.
29. S. HAJIAN, Humboldt-Universität zu Berlin, Institut für Mathematik, April 29 – December 31.
30. J. HÄPPÖLÄ, King Abdullah University of Science and Technology (KAUST), Department of Computer, Electrical and Mathematical Sciences & Engineering, Thuwal, Saudi Arabia, June 2–27.
31. M. HEINKENSCHLOSS, Rice University, Department of Computational and Applied Mathematics, Houston, Texas, USA, July 11–18.
32. L. HELTAI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, February 12–19.
33. ———, May 17–20.
34. ———, July 29 – August 4.
35. ———, September 19–27.
36. ———, November 21–29.
37. R. HILDEBRAND, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, Saint Martin d'Hères, France, July 6–29.
38. CH. HIRSCH, Ludwig-Maximilians-Universität München, Mathematisches Institut, November 13–19.
39. W. HUANG, University of Kansas, Department of Mathematics, Lawrence, USA, June 23–28.
40. D. IVANOV, EFD Induction AS, Skien, Norway, August 8–11.
41. V. JAVAHERI, University of Oulu, Faculty of Technology, Finland, May 2 – July 31.
42. B. JIN, University College London, Department of Computer Science, UK, August 1–5.
43. M. KANITSAR, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Graz, Austria, November 3–30.
44. D. KARP, Far Eastern Federal University, Department of Informatics in Business and Mathematical Methods in Economics, Vladivostok, Russian Federation, May 19 – August 13.
45. S. KAYA MERDAN, Middle East Technical University, Department of Mathematics, Ankara, Turkey, May 23–27.
46. T. KEIL, Humboldt-Universität zu Berlin, Institut für Mathematik, April 29 – December 31.
47. G. KITAVTSEV, University of Bristol, School of Mathematics, UK, December 12–15.
48. Y. KLOCHKOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, Berlin, January 1 – December 31.
49. E. KNOBLOCH, University of California at Berkeley, Department of Physics, Berkeley, USA, January 10–16.
50. S. KOLLI, University of Oulu, Faculty of Technology, Finland, May 2 – July 31.
51. R. KRAAIJ, Delft University of Technology, Department of Applied Probability, Netherlands, May 31 – June 3.
52. M. KRAFT, University of Cambridge, Department of Chemical Engineering and Biotechnology, Cambridge, UK, August 22 – September 23.

53. M. KRAUS, Ostbayrische Technische Hochschule Regensburg, Fakultät Informatik und Mathematik, April 3–7.
54. P. KREJČÍ, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, April 18–29.
55. P. LEDERER, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, August 1–5.
56. C. LÖBHARD, Humboldt-Universität zu Berlin, Institut für Mathematik, May 1 – June 30.
57. C. MACNAMARA, University of St Andrews, Mathematical Institute, Scotland, UK, July 24–27.
58. M.M. MALAMUD, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Slavyansk, Ukraine, March 23 – April 22.
59. ———, July 16–22.
60. A. MANTILE, Université de Reims, Laboratoire de Mathématiques, Reims, France, July 4–16.
61. Y. MAXIMOV, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russian Federation, May 15–26.
62. L. MAZZIERI, Università di Trento, Dipartimento di Matematica, Trento, Italy, July 4–7.
63. ST. MELCHIONNA, University of Vienna, Faculty of Mathematics, Vienna, Austria, April 13 – May 20.
64. J. MODERSITZKI, Universität zu Lübeck, Institute of Mathematics and Image Computing, August 1–5.
65. A. MÜNCH, University of Oxford, Mathematical Institute, UK, December 6–9.
66. O. MUSCATO, Università degli Studi di Catania, Dipartimento di Matematica e Informatica (DMI), Catania, Italy, July 31 – August 11.
67. A. NAUMOV, Lomonosov Moscow State University, Faculty of Computational Mathematics and Cybernetics, Moscow, Russian Federation, January 4–8.
68. ———, June 5–11.
69. ———, July 10–14.
70. P. NELSON, Johannes Gutenberg-Universität, Institut für Mathematik, Mainz, June 27 – July 1.
71. J. NOVO, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Madrid, Spain, November 14–18.
72. B. O'SHAUGHNESSY, Tyndall National Institute, Centre for Advanced Photonics & Process Analysis, Cork, Ireland, June 19–24.
73. F.S. PATACCHINI, Imperial College London, Department of Mathematics, London, UK, January 17–20.
74. P. PEREZ-AROS, Universidad de Chile, Center for Mathematical Modeling, Santiago de Chile, Chile, April 13 – May 31.
75. M. PIŠTĚK, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, May 13–20.
76. TH. POCK, Technische Universität Graz, Institut für Maschinelles Sehen und Darstellen, Graz, Austria, August 1–5.
77. E. RAMASETTI, University of Oulu, Faculty of Technology, Finland, May 1 – July 31.
78. S. RAMESH BABU, SSAB Europe Oy, Raase, Finland, May 2 – July 31.
79. S. RAUCH, TRUMPF Laser GmbH, Schramberg, March 1 – May 31.
80. C. RAUTENBERG, Humboldt-Universität zu Berlin, Institut für Mathematik, April 29 – December 31.

81. D. RESHETOVA, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russian Federation, May 22–26.
82. T. ROUBÍČEK, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, November 14 – December 14.
83. W. RUSZEL, Delft University of Technology, Department of Applied Mathematics, Delft, Netherlands, April 25–29.
84. G. SAVARÉ, Università di Pavia, Dipartimento di Matematica, Pavia, Italy, February 27 – March 4.
85. C. SCHILLINGS, University of Warwick, Mathematics Institute, UK, March 7–10.
86. CH. SEIS, Universität Bonn, Institut für angewandte Mathematik, Bonn, January 19–22.
87. J. SHEWCHUK, University of California at Berkeley, Computer Science Division, California, USA, August 31 – September 19.
88. J. SIEBER, University of Exeter, College of Engineering, Mathematics and Physical Sciences, Exeter, UK, December 19–22.
89. S. SIMONELLA, Technische Universität München, Zentrum Mathematik, M5, München, July 18–22.
90. C. SINISTRARI, Università di Roma “Tor Vergata”, Dipartimento di Matematica, Rome, Italy, April 26–29.
91. K. STURM, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, February 21 – March 4.
92. ———, April 3–8.
93. K. STURM, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 13–18.
94. A. SUVORIKOVA, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, Berlin, October 1, 2014 – July 31, 2016.
95. D. TURAEV, Imperial College London, Department of Mathematics, London, UK, July 24–30.
96. V. ULYANOV, Lomonosov Moscow State University, Department of Mathematical Statistics, Probability Theory, Statistics, Russian Federation, January 10–14.
97. ———, July 4–22.
98. W. VAN ACKOOIJ, Electricité de France R&D, Palaiseau, France, December 6–9.
99. M. VARGA, Technische Universität Dresden, Institut für Mathematik, Dresden, August 29 – September 2.
100. CH. WANG, Northeastern University, State Key Laboratory of Synthetical Automation for Process Industries, Shenyang, China, June 11–15.
101. V. ZAGREBNOV, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, Marseille, France, July 18–22.

### A.12.2 Scholarship Holders

1. F. DASSI, WIAS, Weierstrass Postdoctoral Fellowship Program, June 1–30.
2. T. DEL VISCIO, Alfred Renyi Institute of Mathematics, Budapest, Hungary, ERA Fellowship, September 1 – October 15.
3. S. DIPIERRO, University of Edinburgh, School of Mathematics, UK, Humboldt Research Fellowship, May 1 – June 30.

4. A. MORYAKOVA, Demidov Yaroslavl State University, Department of Mathematical Modeling, Russian Federation, DAAD-Mikhail Lomonosov Programme, October 1, 2015 – March 31, 2016.
5. S. OLMI, Consiglio Nazionale delle Ricerche, Institute for Complex Systems, Florence, Italy, Weierstrass Postdoctoral Fellowship Program, August 1, 2016 – July 31, 2017.
6. A. PANDEY, Universität Mannheim, Institut für Mathematik, Weierstrass Postdoctoral Fellowship Program, January 1 – December 31.
7. K. PAPAITSOROS, University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK, Humboldt Research Fellowship, April 1, 2016 – October 31, 2017.
8. V. ULYANOV, Lomonosov Moscow State University, Department of Mathematical Statistics, Probability Theory, Statistics, Russian Federation, Humboldt Research Fellowship, July 4–22.

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

1. L. ADAMYAN, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – December 31.
2. J. BRASSEUR, Université Aix-Marseille, Institut de Mathématiques de Marseille, supervisor: Prof. Dr. E. Valdinoci, doctoral candidate, January 1 – December 31.
3. J.A. BRÜGGEMANN, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
4. C. BUCUR, Università di Milano, Dipartimento di Matematica, supervisor: Prof. Dr. E. Valdinoci, doctoral candidate, January 1 – December 31.
5. K. EFIMOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – December 31.
6. T. GONZÁLEZ GRANDÓN, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. R. Henrion, doctoral candidate, January 1 – December 31.
7. M. KANITSAR, Karl-Franzens-Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, supervisor: Prof. Dr. M. Hintermüller, doctoral candidate, January 1 – November 30.
8. T. KEIL, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
9. E. KLOCHKOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – December 31.
10. L. LOMBARDINI, Università di Milano, Dipartimento di Matematica, supervisor: Prof. Dr. E. Valdinoci, doctoral candidate, January 1 – December 31.
11. P. MIRAGLIO, Università di Milano, Dipartimento di Matematica, supervisor: Prof. Dr. E. Valdinoci, doctoral candidate, January 1 – December 31.
12. S. RAUCH, TRUMPF Laser GmbH, supervisor: Dr. M. Radziunas, doctoral candidate, March 1 – May 31.
13. S. ROCKEL, Freie Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. V. John, Helmholtz-Kolleg GEOSIM, doctoral candidate, January 1 – November 30.
14. S. RÖSEL, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, doctoral candidate, January 1 – December 31.

15. Y. SUN, Technische Universität Berlin, Berlin Mathematical School, supervisor: Prof. Dr. V. Spokoiny, doctoral candidate, October 1 – December 31.
16. A. SUVORIKOVA, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – December 31.



## A.13 Guest Talks

1. L. ADAM, Humboldt-Universität zu Berlin, Institut für Mathematik, *A multi-material phase field approach for the optimal design of germanium-on-silicon microbridges*, May 31.
2. V. AGOSTINIANI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), mathLab, Trieste, Italy, *Monotonicity formulas for electrostatic potentials and static metrics: Part I*, July 6.
3. G. AKAGI, Tohoku University, Mathematical Institute, Sendai, Japan, *Stability and instability of asymptotic profiles for the fast diffusion equation*, May 4.
4. B. ALBERS, Universität Bonn, Institut für Angewandte Mathematik, *Variational analysis of microstructures in low-hysteresis shape memory alloys*, December 19.
5. A. ALPHONSE, University of Warwick, Mathematics Institute, Coventry, UK, *Parabolic PDEs on evolving spaces and some applications*, June 30.
6. H. AMMARI, Eidgenössische Technische Hochschule Zürich, D-MATH, Zürich, Switzerland, *Effective admittivity imaging of biological tissues: Challenges and future trends*, January 28.
7. H. ANTIL, George Mason University, Department of Mathematical Sciences, Fairfax, USA, *Optimal control of free boundary problems*, March 2.
8. TH. APEL, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, Neubiberg, *Anisotropic mesh refinement in polyhedral domains: Error estimates with data in  $L^2(\Omega)$* , April 21.
9. A. ARAÚJO, University of Coimbra, Department of Mathematics, Coimbra, Portugal, *Modelling light scattering in the human retina*, February 26.
10. F. BACH, Institut National de Recherche en Informatique et en Automatique, École Normale Supérieure, Département d'Informatique, Paris, France, *Beyond stochastic gradient descent for large-scale machine learning*, July 20.
11. M. BACHMAYR, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, *Representations of Gaussian random fields and sparse approximation of lognormal diffusion problems*, April 20.
12. P. BELLEC, Centre de Recherche en Economie et en Statistique, Malakoff, France, *Slope meets lasso: Improved oracle bounds and optimality*, June 8.
13. L. BERLYAND, Pennsylvania State University, Department of Mathematics, State College, USA, *Phase field model of cell motility: Sharp interface limit and traveling waves*, May 10.
14. C. BERTOGLIO, Universidad de Chile, Center for Mathematical Modeling, Santiago, Chile, *Noninvasive pressure drop estimation in blood flows*, February 23.
15. U. BESSI, Università degli Studi Roma Tre, Dipartimento di Matematica e Fisica, Italy, *The stochastic value function in metric spaces*, January 21.
16. ST. BIALONSKI, Max-Planck-Institut für Physik komplexer Systeme, Dresden, *Predicting and preventing extreme events in a spatially extended excitable system*, July 7.
17. A. BIANCHI, Università degli Studi di Padova, Dipartimento di Matematica Pura e Applicata, Padova, Italy, *Limiting dynamics of the condensate in the reversible inclusion process on a finite set*, February 3.
18. J. BISCHOFF, Max-Planck-Institut für Sonnensystemforschung, Göttingen/OSIRES – Optical Engineering and Software, Ilmenau, *Modal diffraction methods and selected applications*, November 22.
19. E. BOLTHAUSEN, Universität Zürich, Institut für Mathematik, Zürich, Switzerland, *Green's function estimates for weakly self-avoiding walks*, June 13.

20. A. BRADJI, Université Badji Mokhtar – Annaba, Département des Mathématiques, Algeria, *On the convergence order of gradient schemes for time dependent partial differential equations*, June 14.
21. L. CALATRONI, Ecole Polytechnique, Université Paris-Saclay, Centre de Mathématiques Appliquées (CMAP), France, *Infimal convolution of data discrepancies for mixed noise removal in images*, December 6.
22. A. CARPENTIER, Universität Potsdam, Institut für Mathematik, *Sequential sampling and uncertainty quantification*, July 11.
23. S. CHEN, Humboldt-Universität zu Berlin, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series Analysis”, *Network dynamics of high-frequency trading data: Evidence from NASDAQ market*, November 23.
24. A. CHERN, Technische Universität Berlin, Fachbereich Mathematik, *Fluid simulation using incompressible Schrödinger flow*, August 18.
25. O. CHVARTATSKYI, Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, *NLS breathers, rogue waves, and solutions of the Lyapunov equation*, September 22.
26. R. ČIEGIS, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, *On stability analysis of some non-classical schemes for the Schrödinger equation*, November 10.
27. G. CONFORTI, Universität Leipzig, Fakultät für Mathematik und Informatik, Leipzig, *Fluctuations of bridges, reciprocal characteristics and concentration of measure*, April 6.
28. M.N. CRUZ-BOURNAZOU, Technische Universität Berlin, Institut für Biotechnologie, *Online optimal experimental design in liquid handling robots for fast and reliable parameter estimation of nonlinear macrokinetic models*, April 26.
29. B. DE RIJK, Universiteit Leiden, Mathematisch Instituut, Leiden, Netherlands, *Factorization of the Evans function via the Riccati transformation*, May 17.
30. S. DIPIERRO, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *Chaotic orbits for systems of nonlocal equations*, January 6.
31. J. EBERT, Humboldt-Universität zu Berlin, Institut für Mathematik, *Wasserstein barycenters of random probability measures*, April 12.
32. J. FENG, University of Kansas, Department of Mathematics, Kansas, USA, *Hamilton–Jacobi PDEs in the space of probability measures, the metric nature explored*, September 14.
33. I. FRANOVIC, University of Belgrade, Institute of Physics Belgrade, Serbia, *Mean-field approach for analysis of collective dynamics and activation processes in coupled noisy excitable systems*, May 11.
34. J. GIENGER, Physikalisch-Technische Bundesanstalt, Modellierung und Simulation, Berlin, *Application of inverse light scattering by a single red blood cell*, October 11.
35. A. GOLDENSLUGER, University of Haifa, Department of Statistics, Haifa, Israel, *Statistical inference for the M/G/infinity queue*, August 23.
36. J. GRÄFE, Leibniz-Institut für Gemüse- und Zierpflanzenbau e.V. (IGZ), Großbeeren, *Plant leaf optics – Problems and some solutions*, November 29.
37. A. GRETTON, University College London, Gatsby Computational Neuroscience Unit, London, UK, *Nonparametric statistical tests using kernels*, July 6.
38. R. GRIBONVAL, Centre de Recherche INRIA Rennes, Parsimony & New Algorithms for Audio & Signal Modeling, France, *Dictionary learning: Principles, algorithms, guarantees*, May 18.
39. D. GROH, Humboldt-Universität zu Berlin, Institut für Mathematik, *Bilevel optimization method for the blind deconvolution problem with total variation regularization*, May 24.

40. S. HAJIAN, Humboldt-Universität zu Berlin, Institut für Mathematik, *Total variation diminishing RK methods for the optimal control of conservation laws*, November 22.
41. M. HALLIN, L'Université Libre de Bruxelles, Statistique Mathématique, Belgium, *Monge–Kantorovich ranks and signs*, April 20.
42. J. HEILAND, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg, *A generalized POD space-time Galerkin scheme for parameter dependent dynamical systems and optimal control*, February 25.
43. M. HEINKENSCHLOSS, Rice University, Department of Computational and Applied Mathematics, Houston, Texas, USA, *A parallel-in-time gradient-type method for optimal control problems*, July 12.
44. L. HELTAI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, *Problem solving at realistic complexities using the deal.II library*, September 21.
45. F. HILDEBRAND, Robert Bosch GmbH, Computational Materials Engineering, Renningen, *Technological challenges and chances of Li-metal solid state batteries*, November 28.
46. M. HOFFMANN, Freie Universität Berlin, Fachbereich Mathematik, *Adaptive finite element methods for Stokes–Darcy*, March 3.
47. M. HOLLER, Karl-Franzens-Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Graz, Austria, *Higher order regularization and applications to medical image processing and data decompression*, October 21.
48. W. HUANG, University of Kansas, Department of Mathematics, Lawrence, USA, *A new implementation of the MMPDE moving mesh method and applications*, June 28.
49. W. IFF, Université Jean Monnet, Laboratoire Hubert Curien UMR CNRS 5516, Saint-Etienne, France, *Rigorous and extremely fast electromagnetic methods for diffraction problems*, October 25.
50. T. JÄGER, Friedrich-Schiller-Universität Jena, Fakultät für Mathematik und Informatik, *Mode-locking phenomena in low-dimensional dynamics*, November 29.
51. M. KANITSAR, Karl-Franzens-Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, *Numerical shape optimization for an industrial application*, November 29.
52. S. KAYA MERDAN, Middle East Technical University, Department of Mathematics, Ankara, Turkey, *Numerical analysis of a fully discrete decoupled penalty-projection algorithm for MHD in Elsässer variables*, May 24.
53. ST. KAYSER, Leibniz-Institut für Kristallzüchtung, Berlin, *Lateral-Photovoltage-Scanning (LPS)- und Scanning-Photo-Lumineszenz (SPL)-Methode*, November 16.
54. T. KEIL, Humboldt-Universität zu Berlin, Institut für Mathematik, *Strong stationarity conditions for the optimal control of a Cahn–Hilliard–Navier–Stokes system*, July 21.
55. G. KITAVTSEV, University of Bristol, School of Mathematics, Bristol, UK, *Liquid crystal defects in the Landau–de Gennes theory in 2D – Beyond the one-constant approximation*, December 14.
56. M. KOHLHASE, Friedrich-Alexander-Universität Erlangen-Nürnberg, Informatik, *FrameIT: From serious games to modeling and applying mathematical models*, November 9.
57. R. KRAAIJ, Delft University of Technology, Department of Applied Probability, Netherlands, *Path-space moderate deviations for the Curie–Weiss model and Gamma convergence of path-space rate functions*, June 2.
58. M. KRAUS, Ostbayerische Technische Hochschule Regensburg, Fakultät Informatik und Mathematik, *Modeling of porous metal-electrolyte interfaces*, November 22.
59. P. KREJČÍ, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, *Contact of elastoplastic bodies*, April 13.

60. L. KUNYANSKY, The University of Arizona, Department of Mathematics, USA, *Inversion of the spherical means transform by reduction to the classical Radon transform*, June 22.
61. T. LAHMER, Bauhaus-Universität Weimar, Institut für Strukturmechanik, *Aspects of a model-based design of experiments for inverse problems*, April 19.
62. P. LEDERER, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, *An exact divergence-free reconstruction operator for the Taylor–Hood element*, August 4.
63. S. LEE, Seoul National University, Department of Economics, Korea (Republic of), *Oracle estimation of a change point in high dimensional quantile regression*, May 11.
64. M.M. MALAMUD, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Slavyansk, Ukraine, *Scattering matrix and Dirichlet-to-Neumann maps*, April 6.
65. A. MANTILE, Université de Reims, Laboratoire de Mathématiques, Reims, France, *Selfadjoint operators with boundary conditions on not closed hypersurfaces and the direct scattering problem*, July 5.
66. H.G. MATTHIES, Technische Universität Braunschweig, Institut für Wissenschaftliches Rechnen, *Probability, analysis, and numerics*, June 27.
67. Y. MAXIMOV, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, *High dimensional non-Gaussian component*, May 25.
68. L. MAZZIERI, Università di Trento, Dipartimento di Matematica, Italy, *Monotonicity formulas for electrostatic potentials and static metrics: Part II*, July 6.
69. H. MEINLSCHMIDT, Technische Universität Darmstadt, Fachbereich Mathematik, *Hölder-estimates for non-autonomous parabolic problems with rough data and applications to quasilinear problems*, January 13.
70. ———, *The Keller–Segel model is well-posed*, July 13.
71. CH. MOLLET, Universität zu Köln, Mathematisches Institut, *Existence of moments and quasi-optimality of Petrov–Galerkin discretizations of parabolic random PDEs*, March 8.
72. B. MRAMOR, Albert-Ludwigs-Universität Freiburg, Mathematisches Institut, *Minimisers of the Allen–Cahn equation on hyperbolic graphs*, April 27.
73. A. NAUMOV, Lomonosov Moscow State University, Faculty of Computational Mathematics and Cybernetics, Moscow, Russian Federation, *Distribution of linear statistics of singular values of the product of random matrices*, January 6.
74. ———, *Extreme singular values of random matrices*, June 7.
75. S. NESENEKO, Technische Universität Berlin, Institut für Mathematik, Berlin, *A Fitzpatrick function approach in the homogenization of elasto-viscoplastic models with isotropic hardening effects*, June 8.
76. J. NOVO, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Madrid, Spain, *Non inf-sup stable mixed finite element approximations to the evolutionary Stokes equations*, November 17.
77. L. PESTOV, Immanuel Kant Baltic Federal University, Kaliningrad, Russian Federation, *On determining an absorption coefficient and a speed of sound in the wave equation by the boundary control method*, July 6.
78. M. PIÑEIRO, University of Santiago de Compostela, Department of Applied Mathematics, Spain, *MaxFEM: An open source software for numerical simulations in electromagnetism*, June 28.
79. M. REITZNER, Universität Osnabrück, Institut für Mathematik, *Stochastic geometry and stochastic analysis: Poisson U-statistics*, January 6.
80. T. ROUBÍČEK, Czech Academy of Sciences, Institute of Thermomechanics, Prague, *Thermodynamics of magneto- and poro-elastic materials at large strains*, November 23.
81. A. SCHLICHTING, Universität Bonn, Hausdorff Center for Mathematics, *Macroscopic limits of the Becker–Döring equation via gradient structures*, January 20.

82. J. SCHMIDT-HIEBER, Leiden University, Mathematical Institute, Netherlands, *Asymptotic equivalence between density estimation and the Gaussian white noise model revisited*, November 9.
83. J. SCHNECK, Konrad-Zuse-Zentrum für Informationstechnik Berlin, *Goal-oriented error estimation applied to topology optimization*, May 3.
84. CH. SEIS, Universität Bonn, Institut für angewandte Mathematik, *A quantitative theory for transport equations*, January 20.
85. J. SHEWCHUK, University of California at Berkeley, Computer Science Division, USA, *Restricted constrained Delaunay triangulations*, September 15.
86. E. SIEBER, University of Exeter, College of Engineering, Mathematics and Physical Sciences, Exeter, UK, *Convergence of equation-free methods in the case of finite time scale separation*, December 20.
87. C. SINISTRARI, Università di Roma “Tor Vergata”, Dipartimento di Matematica, Italy, *Evolution of convex hypersurfaces by curvature flows*, April 27.
88. J. SÖHL, University of Cambridge, Statistical Laboratory, UK, *Nonparametric Bayesian posterior contraction rates for discretely observed scalar diffusions*, June 22.
89. J. SONNTAG, Technische Universität Berlin, Institut für Mathematik, *Feedbackcontrol of the Schlögl model*, September 27.
90. A. STEPHAN, Humboldt-Universität zu Berlin, Institut für Mathematik, *On operator-norm estimates for approximations of solutions of evolution equations using the Trotter product formula*, May 18.
91. K. STURM, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, *Shape optimisation problems with nonsmooth cost functions: From theory to numerics*, March 1.
92. K. STURM, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, *Convergence of Newton’s method in shape optimisation*, November 15.
93. A. SUVORIKOVA, Humboldt-Universität zu Berlin, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series Analysis”, *Wasserstein barycenters: Theory and application*, January 5.
94. D. TURAEV, Imperial College London, Department of Mathematics, UK, *Adiabatic acceleration in quantum mechanical systems*, July 28.
95. V. ULYANOV, Lomonosov Moscow State University, Department of Mathematical Statistics, Probability Theory, Statistics, Russian Federation, *Generalized Cornish–Fisher expansions: Achievements, problems, applications*, January 12.
96. ———, *Non-asymptotic analysis – General approach*, July 13.
97. W. VAN ACKOOIJ, Electricité de France R&D, Palaiseau, France, *Eventual convexity of feasible sets for non-linear probabilistic constraints with elliptically symmetric distributions*, December 6.
98. M. VARGA, Technische Universität Dresden, Institut für Mathematik, *Homogenization via stochastic unfolding*, August 31.
99. A. WAHAB, Korea Advanced Institute of Science & Technology, Department of Bio & Brain Engineering, Daejeon, *A non-iterative algorithm for elastography using joint sparsity*, July 21.
100. CH. WANG, Northeastern University, State Key Laboratory of Synthetical Automation for Process Industries, Shenyang, China, *Product design and engineering analysis technologies*, June 14.
101. ST. WEISSER, Universität des Saarlandes, Fachrichtung Mathematik, Saarbrücken, *Convection-adapted BEM-based finite element method on tetrahedral and polyhedral meshes*, November 17.
102. K.-M. WEITZEL, Philipps-Universität Marburg, Fachbereich Chemie, *Ionen-transport durch feste Materie – BIIT Experimente und numerische Beschreibung mittels Nernst-Planck-Poisson-Theorie*, April 14.

103. M.-TH. WOLFRAM, University of Warwick, Mathematics Institute, UK / Johann Radon Institute (RICAM), Linz, Austria, *Applied PDE in the socio-economic sciences*, December 20.
104. W. WOLLNER, Technische Universität Darmstadt, Fachbereich Mathematik, *Optimization of partial differential equations subject to pointwise constraints on the gradient of the state*, April 14.
105. B. ZWICKNAGL, Universität Bonn, Institut für Angewandte Mathematik, *Variational analysis of microstructures in low-hysteresis shape memory alloys*, December 19.



## A.14 Software

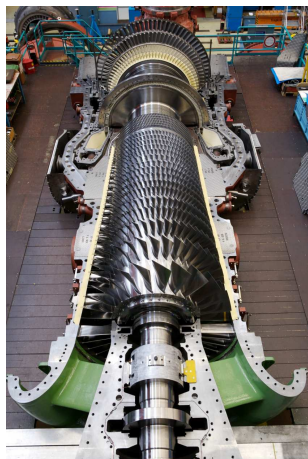
**AWS** (contact: J. Polzehl, phone: +49 30/20372-481, e-mail: joerg.polzehl@wias-berlin.de)

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>).

**BALaser** (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.radziunas@wias-berlin.de)

BALaser is the software tool used for simulations of the nonlinear dynamics in high-power edge-emitting Broad-Area semiconductor Lasers. It integrates numerically the laterally extended dynamic traveling wave model (one- and two-dimensional partial differential equations), executes different data post-processing routines, and visualizes the obtained data.

More information: <https://www.wias-berlin.de/software/balaser>



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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, which combines deterministic and stochastic numerical methods. It allows to solve dynamic as well as steady-state problems and provides capabilities for, e.g., Monte Carlo simulation, correction curve computation, optimization, Bayesian parameter calibration, regression analysis, 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 the simulation of heavy-duty gas turbines. Here, BOP covers a broad range of simulation tasks, from performance validation and optimization to the development of new process models.

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

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

The statistical software ClusCorr98<sup>®</sup> 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<sup>®</sup> runs in the host application Excel 2013.

Further information: <https://www.wias-berlin.de/software/ClusCorr98>

**DiPoG** (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: [andreas.rathsfeld@wias-berlin.de](mailto: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 <https://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: <https://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 <https://www.wias-berlin.de/software/MeFreSim>.

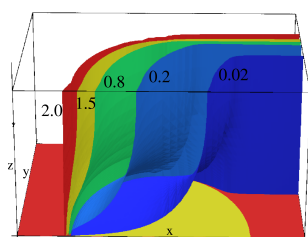
**Par Moon** (contact: U. Wilbrandt, phone: +49 30/20372-571, e-mail: [ulrich.wilbrandt@wias-berlin.de](mailto:ulrich.wilbrandt@wias-berlin.de))

**Par Moon** 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 `ParMoon` are

- the availability of more than 100 finite elements in one, two, and three space dimensions (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
- hybrid parallelization with MPI and OpenMP

`ParMoon` is a joint development with the group of Prof. S. Ganesan (IISc Bangalore) and the group of Prof. Matthies (TU Dresden).



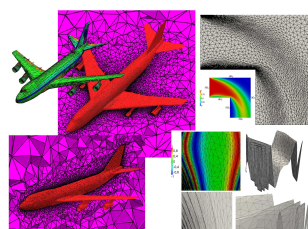
Concentration isosurfaces in a thin-layer flow cell (`pdelib`)

**`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
- 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 and pressure robust discretizations for Navier–Stokes
- 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 languages Python and 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 <https://www.wias-berlin.de/software/pdelib>.



Adapted tetrahedral meshes and anisotropic meshes for numerical methods and scientific computation

**`TetGen`** (contact: H. Si, phone: +49 30/20372-446, e-mail: [hang.si@wias-berlin.de](mailto:hang.si@wias-berlin.de))

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

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

**`WIAS-TeSCA`** (contact: H. Stephan, phone: +49 30/20372-442, e-mail: [holger.stephan@wias-berlin.de](mailto:holger.stephan@wias-berlin.de))

`WIAS-TeSCA` is a **Two-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.

WIAS is currently focusing on the development of a new generation semiconductor simulator prototype. Therefore, WIAS-TeSCA is in maintenance mode and is used for benchmarking of the new code and the support of running projects.

For more information please see <https://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 <https://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/>).

**WIAS Software Collection for Neuroscience** (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: [karsten.tabelow@wias-berlin.de](mailto:karsten.tabelow@wias-berlin.de))

`dti` is a contributed package within the R-Project for Statistical Computing. The package contains tools for the analysis of diffusion-weighted magnetic resonance imaging data (dMRI). It can be used to read dMRI data,

to estimate the diffusion tensor, for the adaptive smoothing of dMRI data, the estimation of the orientation density function or its square root, the estimation of tensor mixture models, the estimation of the diffusion kurtosis model, fiber tracking, and for the two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (<http://cran.r-project.org>). The multi-shell position-orientation adaptive smoothing (msPOAS) method for dMRI data is additionally available within the ACID toolbox for SPM (<http://www.diffusiontools.com>).

`fmri` is a contributed package within the R-Project for Statistical Computing that contains tools to analyze fMRI data with structure adaptive smoothing procedures. The package is available from the Comprehensive R Archive Network (<http://cran.r-project.org>).