



Weierstrass Institute for Applied Analysis and Stochastics

Intelligent solutions for complex problems

Annual Research Report 2015

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Cover figure: Diffraction pattern of a chromium mask illuminated by a Gaussian beam.

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Foreword

The Weierstrass Institute for Applied Analysis and Stochastics, Leibniz Institute in Forschungsverbund Berlin e.V. (WIAS, member of the Leibniz Association), presents its Annual Report 2015. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2015. 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.

Special attention was again devoted to the proper functioning of the IMU Secretariat. Its eager staff, headed by the WIAS Authorized Representative of the Director and IMU Treasurer Prof. Alexander Mielke, continued their work, serving mathematics and mathematicians all over the world. Meanwhile, only five years after its official opening in February 2011, the IMU Secretariat at WIAS has become a well-known and well-accepted meeting point of the worldwide mathematical community, which has increased the international visibility of WIAS tremendously.

In March 2015, the long and successful era of Prof. Jürgen Sprekels as the director of WIAS finally terminated, without, however, a new director having been appointed. This unfortunate situation hampered the institute's prospects to make far-reaching decisions for its future development, which was even more unfortunate since also the future of Research Group 7 needed forwardlooking decisions, because its current head, Prof. Wolfgang Dreyer, will retire in March 2016. The official tasks were taken over by two equally Authorized Representatives of the Director, Prof. Alexander Mielke and myself. As can be seen from this report, the institute was flourishing in 2015 on the accustomed high level, but nevertheless, long-range decisions had to wait until the new director would have taken office. Fortunately, this has now, at the beginning of 2016, happened, and the institute is sorting out all the promising possibilities for shaping its future.

But let me come back to the year 2015, in which many positive things happened in and to WIAS. The evaluation of mid-2017 already threw its shadow, as the audit of the Scientific Board took place in Fall 2015, which is a kind of "dress rehearsal" for the evaluation and an important test for the scientific performance. The preparations for the audit have bound a lot of resources for months, as some 500 pages had to be filled, containing programs, concepts, facts, and figures. However, it was really worth it, since the event itself made all colleagues stand together and work hard one for another, and created a kind of institute's spirit. Even better, also the Scientific Advisory Board was very positively impressed by the output of WIAS of the last years and found highly praising words in its report. The prospects for the evaluation in 2017 are very good, but a lot of additional work will have to be done on the way!

WIAS is named after the famous Berlin mathematician *Karl Theodor Wilhelm Weierstrass* (1815–1897), whose importance for the foundations of the area of Analysis cannot be overestimated. In 2015, the institute celebrated Weierstrass's 200th birthday. In order to honor him, Prof. Sprekels and myself edited a Festschrift with the Springer-Verlag containing nine original essays written by eminent mathematics historians. Moreover, precisely on the day of Weierstrass's 200th birthday, WIAS organized a festive event in the Berlin-Brandenburg Academy of Sciences, at which a number of esteemed speakers gave speeches, among them Germany's Minister for Research and Education, Prof. Johanna Wanka. In the scientific part of this event, the nine authors gave accounts on their Festschrift contributions. About 130 invitees enjoyed the event, which put a milestone in the public awareness of the institute.



Prof. Dr. Wolfgang König, Authorized Representative of the Director



Even though 2014 had been a year of records for WIAS regarding publications, preprints, promotions, and third-party funds, the results of 2015 were not far behind, if not even exceeding, the marks that were set in 2014, as one can read in detail in the facts-and-figures part of this report. All important indicators of scientific productivity and quality have been on a comparable level; the success story of WIAS continued.

From a great number of successes, let me pick out the award of the EU project *MIMESIS – Mathematics and Materials Science for Steel Production and Manufacturing*, a European Industrial Doctorate (EID) project in the programme Innovative Training Networks (ITN) and part of the Marie Skłodowska Curie Actions. This structured doctorate program will be entirely run by WIAS and will be headed by the head of Research Group 4, Prof. Dietmar Hömberg. Another WIAS-associated researcher who received high distinction in 2015 is Prof. Peter Friz, not only the head of a new DFG Research Unit, but also the new holder of an ERC consolidator grant, both in the main field of one of the 2014 Fields medalists, Martin Hairer (Warwick), a close colleague of Peter Friz. A substantial part of his research activities will be carried out at WIAS.

The Young Scientists' Group *Modeling of Damage Processes* under the leadership of Dr. Christiane Kraus, which was founded in 2012 following a recommendation of the institute's Scientific Advisory Board, continued their work with great success. This group was founded as a measure of WIAS to promote women in leadership positions. The first goal of this measure had already in 2013 been achieved, when the other head, Dr. Dorothee Knees, received a W3-professorship in Kassel, but it was in 2015 that also the second part of the goal was realized: Also Dr. Kraus received an offer for a professorship, in Würzburg. This success shows on the one hand that WIAS is a hotbed for young researchers, in particular female ones, and on the other hand that the appointment of young promising people as heads of an own group with responsibility for the education of Ph.D. students and young postdocs significantly increases their prospects. WIAS has observed this with great interest and has started intense discussions about adopting the constitution of such groups in the institute's general policy as a structuring measure.

The institute is committed to the implementation of the legally binding German policies and standards to achieve the goal of gender equality. In 2015, the institute defended for the second time the "audit berufundfamilie" (audit job and family) quality seal that it received in December 2013. But beyond that, in 2015 more actions took place, the most important being the employees attitude survey and the enactment of an employment agreement.

Besides these important events of the year 2015, WIAS continued its scientific work, further consolidating its leading position in the mathematical community as a center of excellence in the treatment of complex applied problems. Several scientific breakthroughs were achieved, some of which will be detailed later in this report, and WIAS further 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, 55 additional co-workers (+ 4 outside WIAS; Dec. 31, 2015) could be financed from grants.

Thirteen international workshops organized by WIAS evidenced the institute's reputation and its role as an attractive meeting place for international scientific exchange and collaboration. In addi-



tion, 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 2015 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.

Another continuing success story for the mathematical community of Berlin is the "Berlin Mathematical School" (BMS), which was extended until 2017 in the framework of the German "Exzellenzinitiative 2012" (competition for excellence). The BMS is a graduate school for advanced mathematical studies that brings together the capacities of all mathematical institutions in Berlin to attract excellent doctoral students from all over the world. Also 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.

Berlin, in July 2016

W. König

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1 WIAS in 2015

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

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

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

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

WIAS 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. WIAS made a number of cooperation contracts with universities and is one of the "motors" of the Berlin mathematical research center MATHEON.

1.2 Structure and Scientific Organization

1.2.1 Structure

To fulfill its mission, WIAS was in 2015 organized into the departments for technical services, the Secretariat of the International Mathematical Union (IMU, see page 52), the seven scientific research groups, the Young Scientists' Group, two Leibniz and two ERC groups¹:

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

- **RG 1. Partial Differential Equations**
- RG 2. Laser Dynamics
- **RG 3. Numerical Mathematics and Scientific Computing**
- RG 4. Nonlinear Optimization and Inverse Problems
- RG 5. Interacting Random Systems
- **RG 6. Stochastic Algorithms and Nonparametric Statistics**
- RG 7. Thermodynamic Modeling and Analysis of Phase Transitions
- **YSG. Modeling of Damage Processes**
- LG 3. Mathematical Models for Lithium-ion Batteries
- LG 4. Probabilistic Methods for Mobile Ad-hoc Networks
- ERC 1. EPSILON Elliptic Partial Differential Equations and Symmetry of Interfaces and Layers for Odd Nonlinearities

ERC 2. EntroPhase – Entropy Formulation of Evolutionary Phase Transitions

The organization chart on the following page gives an overview of the organizational structure of WIAS as of December 31, 2015.

1.2.2 Main Application Areas

The research at WIAS focused in 2015 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

- Nano- and optoelectronics
- Optimization and control of technological processes
- Phase transitions and multi-functional materials
- Flow and transport processes in continua
- Conversion, storage, and distribution of energy
- Random phenomena in nature and economy

To these areas, WIAS has made important contributions in the past years that have strongly influenced the directions of development of worldwide research. The institute has a special modeling and simulation expertise in promising modern technologies, for instance,

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



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

The seven research groups, the Young Scientists' group, the two Leibniz groups, and the two ERC groups form the institute's basis to fully bring to bear and develop the scope and depth of its 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 2015 in the interdisciplinary solution process described above.

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

In the following, special research topics are listed that were addressed in 2015 within the general framework of the main application areas.

1. Nano- and optoelectronics

- Microelectronic devices (simulation of semiconductor devices; in RG 1 and RG 3)
- Mathematical modeling of semiconductor heterostructures (in RG 1)
- Diffractive optics (simulation and optimization of diffractive devices; in RG 4)
- Quantum mechanical modeling of nanostructures and their consistent coupling to macroscopic models (in RG 1 and RG 2)
- Laser structures and their dynamics (multisection lasers, VCSELs, quantum dots; in RG 1 and RG 2)
- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in RG 2)
- Photovoltaics and OLED lighting (in RG 1)

2. Optimization and control of technological processes

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

3. Phase transitions and multi-functional materials

- Modeling of nonlinear phenomena and phase transitions in multi-functional materials (in RG 1, RG 7, and YSG)
- Stochastic modeling of phase transitions (in RG 5)
- Hysteresis effects (elastoplasticity, shape memory alloys, lithium batteries, hydrogen storage; in RG 1 and RG 7)
- Thermomechanical modeling of phase transitions in steels (in RG 4, RG 7, and ERC 2)
- Modeling of damage and crack processes (phase field systems and sharp interface problems, multiscale transitions; in YSG, RG 1, RG 7, and ERC 2)
- Modeling, analysis, and simulation of gas-solid and liquid-solid transitions, phase separation with thermomechanical diffusion (Stefan problems, phase field models, LSW theory, Becker– Döring models, in RG 7, YSG, and ERC 2; and many-body systems, in RG 5)
- Growth of semiconductor bulk single crystals, growth of quantum dots (in RG 7)

4. Flow and transport processes in continua

- Treatment of Navier–Stokes equations (in RG 1, RG 3, RG 7, LG 3, and YSG)
- Flow and mass exchange in porous media (in RG 3)
- Numerical methods for coupled electrochemical processes (fuel cells, batteries, hydrogen storage, soot; in RG 1, RG 3, RG 5, RG 7, and LG 3)
- Modeling of nanostructures of thin films on crystalline surfaces (fluid films, thin film solar cells; in RG 1 and RG 7)
- Stochastic particle systems as efficient solvers of kinetic equations (in RG 5)
- Transport in random media (in RG 5)
- Trajectories of message flow in mobile ad-hoc communication systems (in LG 4)



5. Conversion, storage and distribution of energy

- Photovoltaics (in RG 1)
- Light-emitting diodes based on organic semiconductors (OLEDs; in RG 1 and RG 3)
- Modeling of experimental electrochemical cells for the investigation of catalytic reaction kinetics (in RG 3)
- Lithium-ion batteries (in RG 3, RG 7, and LG 3)
- Modeling and analysis of coupled electrochemical processes (fuel cells, batteries, hydrogen storage, soot; in RG 1, RG 3, RG 5, RG 7, and LG 3)

6. Random phenomena in nature and economy

- Stochastic particle systems and kinetic equations (modeling and simulation of coagulation processes, chemical reaction-diffusion processes, and gas flows; in RG 1, RG 5, and RG 7)
- Modeling of stock prices, interest rates, and exchange rates (in RG 6)
- Evaluation of derivatives, portfolio management, and evaluation of risk (in RG 6)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6)
- Dynamical processes in nonhomogeneous media (in RG 6 and RG 7)
- Branching processes in random media (in RG 5)
- Connectivity problems in large telecommunication networks (in RG 5 and LG 4)
- Material models with stochastic coefficients (in RG 3, RG 4, RG 5, and RG 7)

1.3 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.

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

In 2015, the main task for WIAS's equal opportunity officer and her substitute was to conduct an employee attitude survey. The goal was to establish information concerning WIAS workers' options and needs on the topics of equal opportunities and family-friendly policies. The evaluation of the survey was carefully done by November 2015 and resulted in an assessment of measures to meet WIAS's workers' needs and wishes.



Since 2015, the topic *Equality, Work, and Family Life* has a permanent slot in the monthly WIAS director's meeting, in which a member of the institute's management reports on recent activities. A major activity in 2015 was the development and enactment of a company agreement regarding the compatibility of career and family. Significant changes were made in the fields of working time, fixed-term contracts, and flexibilization by exemption. Furthermore, an informative internal WIAS web page *Work and Family* has been established and is well maintained. Moreover, in 2015, WIAS hosted and financed for its employees a professional workshop on the burnout issue. Lively interest could be observed.

A number of measures were taken in 2015 for the support of females. Indeed, WIAS participated for the first time in April 2015 in the event "Girls' Day – Mädchen Zukunftstag"; female WIAS members delivered a carefully chosen scientific program for girls aged 12–17 and received an enthusiastic reply. A scientific international workshop on stochastic analysis with only female speakers was organized at WIAS in Fall 2015.

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 has been very successful in 2015, having raised a total of 3.5 million euros, from which 55 additional researchers (+ 4 outside WIAS; Dec. 31, 2015) have been financed. In total in 2015, 26.95 percent of the total budget of WIAS and 36.9 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 106ff.

1.5 Participation in Structured Graduation Programs

Graduate School Berlin Mathematical School (BMS)

Berlin Mathematical School

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



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

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

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

In October 2013, this International Research Training Group took up its work 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.

Graduate Research School GeoSim

The graduate research school "GeoSim" is funded by the Helmholtz Association, GeoForschungs-Zentrum Potsdam, Freie Universität Berlin, and Universität Potsdam. Its goal is to train a new generation of outstanding young scientists based on a strong collaboration, systematically linking methodological expertise from the areas of Earth and Mathematical Sciences. Thanks to the connections to Freie Universität Berlin, WIAS can participate in the scientific expertise of this graduate school. One student was supervised by RG 3, working at the simulation of mantle convection. For several other students from the Earth Science, the supervision of the mathematical aspects of their work is performed.

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 182ff. for a list of the 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.

WI AS







2 Scientific Highlights

- Towards the Optimization of On-chip Germanium Lasers
- Delay-differential Equations for Optoelectronic Systems
- Adaptive Anisotropic Grids for Numerical Simulations
- Phase Field Approach to Structural Topology Optimization
- New Approach for Optimal Control of Hydroelectricity Storage Systems
- Mathematical Models for Lithium-ion Batteries

2.1 Towards the Optimization of On-chip Germanium Lasers

Thomas Koprucki, Dirk Peschka, and Marita Thomas

Silicon photonics, combining electronics with photonics, has become a rapidly developing new field with a high potential for low-cost solutions to problems ranging from high-speed data transfer for optical on-chip communication to biosensing. The missing piece for the silicon photonics platform is an integrable active light source compatible to silicon technology. To fill this gap, various concepts based on silicon (Si) and germanium (Ge) are under consideration; cf., e.g., [1]. However, both Ge and Si are indirect semiconductors and therefore not capable of substantial light emission. But by applying mechanical strain to Ge, it is possible to improve its radiative efficiency due to a favorable shifting of the band structure under strain [1]. The pioneering work in this direction is the successful demonstration of an electrically pumped laser based on slightly tensile-strained Ge/Si heterostructures by Massachusetts Institute of Technology (MIT) researchers [2]. The extremely high lasing threshold currents observed in these devices lead to strong heating effects limiting their operation lifetime. This fact shows the strong demand for improvements, in particular, for a rigorous optimization of Ge semiconductor lasers.

A first step in this direction was made by scientists at the *Leibniz-Institut für innovative Mikroelektronik IHP*, by proposing a manufacturing technique for strained Ge microstrips, which is superior to the purely thermally strained MIT device. Motivated by these promising results of our colleagues at IHP [3], we work on the mathematical optimization of mechanical strain and optical properties with the goal of finding a design for a Ge laser with a highly reduced threshold current. Finding this design is the goal of the **⊕EC**Math funded MATHEON project D-OT1, which combines the long-standing expertise of WIAS regarding semiconductor modelling, analysis, and simulation with the expertise of *Humboldt-Universität zu Berlin* (Prof. M. Hintermüller, Prof. T. Surowiec) in nonsmooth partial differential equation optimization and algorithms. The quantity to be optimized is the stimulated emission, which depends on the doping through the carrier densities and on the band structure of Ge, which can be directly tuned by applying a mechanical strain. Our theoretical findings in simulations, e.g., with the software package WIAS-TeSCA, support the design of devices and interpretation of experiments at IHP.

Germanium as an optically active gain material

Light generation in a semiconductor is based on the radiative recombination of electrons with holes. In direct semiconductors, such as III-V materials, both electrons and holes occupy the Γ -valleys in the energy landscape possessing a similar momentum, which allows for an efficient radiative recombination. However, in unstrained Ge, the negatively charged electrons (*n*) mainly occupy the lower-lying conduction band *L*-valley, see Figure 2, thus making their momentum incompatible to that of the positively charged holes (*p*) in the valence band Γ -valley. Additional phonons are required to assist the optical transition, which makes radiative recombination much less likely.



Fig. 1: Ge microstrips with additional SiN stressor layer built at IHP provide higher biaxial strain compared to purely thermally strained Ge

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Fig. 2: Schematic Ge band structure showing the occupation of electrons and holes in the conduction and valence band. The combined effect of tensile strain and n -doping resulting in an increase of stimulated emission by reducing the direct band gap $E_c^{\Gamma} - E_v$ (strain) and by filling the Γ -band (doping)

By applying a tensile mechanical strain to Ge, the energy difference $E_c^{\Gamma} - E_c$ between the Γ -valley and the L-valley conduction band edges can be decreased. For biaxial strains beyond 1.7% Ge even becomes a direct semiconductor, where $E_c^{\Gamma} < E_c$. Moreover, by adding a suitably high n-type doping, i.e., by implanting some impurities creating an excess of negative charges, the number of electrons available for optical emission can be highly increased. With this band-filling effect, it is possible to inject additional electrons into the Γ -valley enhancing the radiative recombination. If the radiative recombination rate is sufficiently high, light is amplified by stimulated emission. This amplification is measured by the so-called *optical gain*, which depends on carrier densities of electrons and holes, on the mechanical strain, and on the n-type doping.

The *optical gain* can be described by a quantum mechanical model where the modified band structure due to the mechanical strain e is used in the calculations [4]. The gain data obtained in this way are fitted in [5] to a macroscopic expression that we use for WIAS-TeSCA simulations with the afore-mentioned semiclassical optoelectronic laser model. The expression for the optical gain $g(\psi, n, p; \omega, e)$ obtained in [5] depends on the values of electron and hole densities n, p, as well as on the frequency of light ω , on the spatially inhomogeneous strain e, and on the doping density C.

The computed material gain spectra for the transverse electric (TE) polarization [5] and different values of the biaxial tensile strain ranging linearly from 0.35% to 0.70% and different excess carrier densities $\delta n = n - C$ for the n-type doped Ge are shown in the left panel of Figure 3. The right panel shows the corresponding fit to the analytic expression for g from [5] for the wavelength $\lambda = 1620$ nm. As expected, the material gain increases with increasing strain and increasing excess density, which are our main quantities to use in the optimization.



Fig. 3: Left: Material gain for TE polarization computed for different excess densities δn and nine linearly increasing biaxial strains 0.35% - 0.7% for Ge with n-type doping $C = 5 \cdot 10^{19} \text{ cm}^{-3}$. Right: Fit to analytic expression for fixed wavelength $\lambda = 1620 \text{ nm}$; see [5].



TE 1







Fig. 4: Optical TE modes for $\lambda = 1.7 \mu m$ for an IHP geometry is concentrated in optically active Ge (dashed)

Mathematical modeling and optimization strategy

We illustrate the approach for the optimization of a strained Ge microstrip, which is pursued in the MATHEON project D-OT1. Here, the optical gain depends on the mechanical strain e and on the carrier densities n, p for electrons and holes, making it sensitive to both the doping density C and the material distribution. When suitable physical optimization goals are identified, a mathematically rigorous optimization might generate producible improved laser designs.



For a semiconductor occupying the domain $\Omega \subset \mathbb{R}^d$, charge transport is described by the *van Roosbroeck* system (1a), where, for a given doping profile *C*, one seeks the state $\xi = (\psi, \phi_n, \phi_p)$ consisting of the electric potential ψ , and the quasi-fermi potentials ϕ_n, ϕ_p for electrons and holes. With distribution function *F*, the carrier densities *n*, *p* are related to the potentials by

$$n = N_{\rm c} F\left(\frac{q(\psi - \phi_n) - E_{\rm c}}{k_{\rm B}T}\right), \qquad p = N_{\rm v} F\left(\frac{q(\phi_p - \psi) + E_{\rm v}}{k_{\rm B}T}\right),\tag{2}$$

with statistics F, where the energy levels $E_c(e)$, $E_v(e)$ of the conduction band and valence band depend on the mechanical strain e. Additionally, the recombinations R in (1a) contain a contribution from stimulated emission of the form $R_{\text{stim}} \simeq gS|\Theta|^2$. The *Helmholtz equation* (1b) for the optical mode Θ couples to the van Roosbroeck system through the dependence of the permittivity

$$\varepsilon_r(\xi;\omega,e) = \left(\mathsf{n}_r + \frac{ic}{2\omega}[g(\xi;\omega,e) - \alpha(\xi)]\right)^2 \tag{3}$$

on the state ξ and on the strain e. The complex eigenvalue β of the Helmholtz equation (1b) enters the balance of *photon numbers* (1c), where Im β is typically increasing with increasing gain, so that a large gain results into a strong amplification of photon numbers, until, finally, the losses increase and balance the gain. The main effect of the material distribution on the strain is through the material-dependent thermal strains e_0 and stresses σ_0 . Additionally, the refractive index n_r depends on the material. By creating a contrast of n_r within Ge with respect to the surrounding media, one creates confined optical modes with low losses outside the optically active Ge (Figure 4).

The main goal is to find such a doping and material distribution, so that the laser operates at a low threshold current, i.e., a sufficient amplification of $S \simeq$ "output power" at low electrical currents, i.e., with low heat production. In the following case study we explain different empirical strategies how this aim can be achieved, and how it can be translated into cost functionals.



Empirical case study

In [5], this modeling approach was used in order to identify promising starting geometries and feasible cost functionals for a doping and topology optimization. As an outcome, the case study underlined that a mathematically rigorous optimization may indeed be useful since the devices in fact show the possibility for a substantial lowering of the threshold currents. This observation is of great practical interest, because the device developed at MIT had a very short lifetime due to its high threshold currents.

As in [5], we consider two competing designs: First, the standard design shown in Figure 5 consisting of a SiN stressor on top of the optically active Ge on an insulating SiO₂ layer. The doped silicon contacts are indicated by green layers in Figure 5. Second, the empirically improved aperture design shown in Figure 6, where electric currents are injected into the optically active Ge through a narrow opening near the center of the main mode (see insets in Figure 6). Both devices consist of a layered heterostructure based on an insulating SiO₂ substrate, with a Ge block sandwiched between the Si contacts (Si-n and Si-p) and a SiN layer on top, which, as experimentally and numerically verified in [3], induces a tensile strain to the Ge layer, linearly decreasing in vertical y-direction from top to bottom.



For the standard device, which is considered a feasible and producible design by IHP, one observes significant leakage currents. They are very pronounced for the hole transport, cf. Figure 7 (left), where the carriers flow directly from the p-contact to the n-contact along the edges of the device without passing through the center of Ge, where the fundamental mode, indicated by the red isolines, is located. This observation is in contrast to the hole currents of the aperture device in Figure 7 (right), where the carriers are injected into the center of the fundamental mode, leading to a lower threshold thanks to a higher gain due to higher carrier densities and due to a more effective replenishment of carriers lost through stimulated recombination.

The quantitative improvement of the aperture design over the standard design is shown in Figure 8, where one can see that the threshold current for the aperture device is lower than the threshold current for the standard device by a factor of almost four for transverse magnetic (TM) modes. The factor is even higher for TE modes; however, because of their lower gain, their threshold remains above that of TM modes.

Towards rigorous device optimization

The major difference between the IHP device concept and the purely thermally strained devices of MIT is the spatially nonuniform strain of the first, which is experimentally verified to increase



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Fig. 5: Cross section through standard *Ge heterostructure* similar to Fig. 1



Fig. 6: Cross section through aperture Ge heterostructure

Fig. 7: Hole current for left: standard device and right: aperture device above threshold. Red lines indicate the isolevels of Θ^2 , whereas the white arrows and the colored background show the direction and magnitude of (the current) $j_p = -\mu_p p \nabla \phi_p$.



Fig. 8: Threshold currents for aperture and standard design and TE/TM modes for different wavelengths



Fig. 9: Strain in Ge along y-direction is constant or linearly increasing 0.35%–0.7% as achievable at IHP [5]



Fig. 10: Gain g (full lines) and losses α (dashed lines) for strains from Fig. 9 with optical mode Θ^2 in blue-shaded area



linearly with y as shown in Figure 9, leading to a substantial spatial variation of the band gaps and the gain shown in Figure 10. This property should be exploited in the topology optimization and in the doping optimization. The band gaps and the gain thereby depend on the y-coordinate from bottom to top, which, so far, were realized in the WIAS-TeSCA simulations by introducing nine artificial material layers in the Ge block with piecewise constant strain. The layering is indicated by regions of constant gray color in Figure 5 and by the section through the device center in Figure 9, where two different realizations of strain distributions through Ge are shown.

Figure 10 shows that, in contrast to the uniform strain, the strong *IHP strain* results in a very nonuniform gain, with the strongest enhancement in regions of highest strain. It is interesting to note that the main term responsible for photon amplification in (1c) can be approximated by lowestorder perturbation theory as

$$\mathrm{Im}\beta \approx \int_{\Omega} \left(g(\xi; \omega, e) - \alpha(\xi) \right) \Theta^2 \,\mathrm{d}x \tag{4}$$

and, therefore, is called *modal gain*. For spatially constant densities, uniform gain, and a normalized confined mode, leading to $\text{Im}\beta \approx (g - \alpha)$, with g and α constant throughout Ge. However, for spatially nonuniform gain, the optimization goal implied by (4) is to engineer a device so that the mode coincides with regions for large gain. For doping optimization, where the optical mode Θ is given, which implies optimizing the doping C so that $(g - \alpha)$ weighted with Θ^2 is maximal. In the context of topology optimization, we have to distribute the material such that the regions of large tensile strains and the shape of the optical mode overlap in an optimal way.

We refer to this concept as *overlap engineering* and, together with threshold currents, consider it a feasible cost functional for a rigorous doping and topology optimization of such an optoelectronic device.

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2.2 Delay-differential Equations for Optoelectronic Systems

Matthias Wolfrum and Serhiy Yanchuk

A fundamental principle for the modeling of dynamical processes is that the state of a system already determines a tendency in which way this state is going to change in the next moment. In simple cases, a system can be described by a finite number of quantities, which change continuously in time. One obtains in this way so-called *ordinary differential equations*. Beginning with Isaac Newton, such equations have been successfully used to model a huge variety of dynamical processes, ranging from celestial mechanics to the metabolism of cells or to monetary processes in economics.

A qualitatively new feature appears when the evolution of the system depends not only on its present state, but also on the state of the system at previous moments of time. Such a delayed interaction can be observed, for example, in coupled systems where the interaction between distant units takes place with a finite speed of signal propagation. A prominent example is the dynamics of neural systems, where a transmission delay between the individual neurons often plays an essential role for the dynamics. Other examples of delay systems arise in biology, where the delay can be induced by the life cycles of organisms, or in systems with an external control acting with a certain latency.

Also in the field of optical systems, delay effects can frequently be observed, even though the signal transmission in optics happens at the fastest possible speed, namely the speed of light. While the internal time scales in a laser are in the range of picoseconds, already a light propagation over millimeters induces a significant delay. And within larger optical cavities, the round-trip time of the light can even be large compared to the internal time scales on which an optically active material may react on the propagating signal.

Delay-differential equations with large delay

A general delay-differential equation (DDE) can be written in the form

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = f(y(t), y(t-\tau)),\tag{1}$$

where the vector $y \in \mathbb{R}^n$ contains the state variables of the system, $\tau > 0$ is the delay time, and f is some nonlinear function depending on the present state y(t) and on the delayed state $y(t - \tau)$. While for an ordinary differential equation, with f depending only on the present state y(t), a solution can be found for any initial condition $y_0 = y(0) \in \mathbb{R}^n$, a DDE can be solved uniquely only with initial data $y_0(t)$ given for a whole interval of time $t \in [-\tau, 0]$, called the *history interval*. Consequently, the phase space in which the trajectory evolves is an infinite-dimensional space of functions, even though there is only a finite number n of state variables. In this way, potentially high-dimensional and complex dynamics become possible. In particular, it turns out that the effective dimension of the resulting dynamics can become large if the delay time τ increases. Exactly this situation can be found in various models from optoelectronics, where highly complex dynamics with the interplay of processes on different time scales can be observed.



Fig. 1: Examples of pseudo-continuous and strongly unstable spectrum for the Lang–Kobayashi model

This was the starting point for the research at WIAS aiming to achieve a better understanding of the resulting physical effects by applying and further developing a mathematical singular perturbation theory and multiple time-scale methods to this problem. The basic idea is that one investigates the limit $\tau \to \infty$ and considers the case of very large τ as a small perturbation of this situation. The mathematical challenge consists of the fact that this limit exists not in a unique way and the structure of the problem changes in the limit. This is why it is called a *singular* limit. Indeed, rescaling the time variable $T = t/\tau$, the system with large delay appears in the form

$$\varepsilon \frac{\mathrm{d}y(T)}{\mathrm{d}T} = f(y(T), y(T-1)), \tag{2}$$

where $\varepsilon = 1/\tau$ is a small parameter. Here, the former limit of large delay is given by the limit $\varepsilon \rightarrow 0$, where the DDE transforms into a mapping in implicit form and the differential nature of the original equation has disappeared. Instead, this mapping describes the slow variations from one history interval to the next as a discrete process.

The two different scalings indicate that in DDEs with large delay one has to expect dynamics on different time scales and one has to figure out the interplay between these time scales.

Scaling properties of the spectrum. A first fundamental theoretical result in this direction was obtained in [1] describing the asymptotic properties of the spectrum of a DDE with large delay, linearized at an equilibrium solution. It turns out that in most cases the spectrum can be decomposed into two parts with different scaling properties with respect to τ :

(i) pseudo-continuous spectrum consisting of eigenvalues λ that scale as $\operatorname{Re}(\lambda) \sim 1/\tau$ for large τ . These eigenvalues appear in pseudo-continuous families, which are located along curves that can be calculated analytically by a corresponding scale-free limit problem. They correspond to the slow but high-dimensional dynamics described by the discrete mapping.

(*ii*) strongly unstable spectrum consisting of finitely many eigenvalues with positive real part that scale as $\text{Re}(\lambda) \sim 1$. They correspond to instabilities that develop on a fast time scale, shorter than a single history interval, and their location can be found as well from a limit problem. Examples of such spectra are shown in Figure 1 for the Lang–Kobayashi model describing the dynamics of a semiconductor laser with optical delayed feedback [5].

Furthermore, this approach was extended to a certain class of periodic solutions [3], where the Floquet spectrum, determining the stability of the periodic solutions, can again be decomposed into families of pseudo-continuous spectrum and strongly unstable spectrum with a corresponding scaling behavior. Even for chaotic solutions, one can distinguish in a similar way between strong and weak chaos, where the first one is characterized by a few positive Lyapunov exponents and the latter one is of extensive nature, reflecting the high dimensionality of the underlying processes [4]. The central example in all these cases is the classical Lang–Kobayashi model for a semiconductor laser with delayed optical feedback. Based on the new theoretical results, a comprehensive description of the stability properties of all stationary lasing states was obtained [5].

Moreover, fundamental differences in the synchronization behavior of weekly and strongly chaotic lasing regimes were discovered.



Spatio-temporal representation. Already almost twenty years ago, it was observed that there is a relationship between DDEs and spatially extended systems. Indeed, based on equation (2), one can parametrize the time within the history interval by an extra "spatial" variable. The stepwise evolution on the slow time scale from one history interval to the next one appears then like the temporal evolution of a spatial profile, which in a usual spatially extended dynamical system is described by a partial differential equation (PDE). This result can be used, for example, to visualize the various high-dimensional dynamical phenomena; see Figures 2, 3, 4.

Amplitude equations. The analogy to partial differential equations describing the evolution in a spatially extended system goes even further. Starting from the curves of the pseudo-continuous spectrum, one can classify the instabilities of DDEs in analogy to the instabilities of PDEs with a corresponding shape of the spectrum in their dispersion relation. This observation is the basis to establish a rigorous relation between the dynamics of a DDE with large delay and a PDE. In [2], we present a new result proving that for scalar delay-differential equations close to the destabilization threshold, one can explicitly find a Ginzburg–Landau equation of the form

$$\frac{\partial u}{\partial \theta} = \alpha \frac{\partial^2 u}{\partial x^2} + \beta \frac{\partial u}{\partial x} + pu + \gamma u^3$$

that recovers the dynamics of the DDE with large delay. The variable θ describes here the evolution on the slow time scale, while the "spatial" variable x parametrizes the time within the history interval; see Figure 2.



Applications. In cooperation with the Institute for Complex Systems, Florence, we investigated theoretically and experimentally the dynamics of vertical cavity lasers with long-delayed optoelectronic feedback [6]. These laser systems show characteristic spatio-temporal coarsening dynamics where regions of two different phases, corresponding to different polarization modes of the lasers, are separated by moving fronts, which are generated and annihilated in pairs as shown in Figure 3.

2 Scientific Highlights



Fig. 3: Spatio-temporal representation of experimental data of the laser intensity. Insets: (a) front generation, (b) annihilation, (c) a nucleation of the white state into the black

In a model of a semiconductor laser with two delayed optical feedbacks, a corresponding spatiotemporal representation has to include two spatial dimensions. Figure 2 shows the snapshots of two different spatial patterns. Note that the stable defects, shown in panel (a), are stationary in time, while the defect turbulence (b) displays additionally an irregular turbulent evolution in time.



Fig. 4: Semiconductor laser with two delayed feedbacks, two-dimensional representation of two different dynamical regimes; (a) stationary defects, (b) defect turbulence

> **Summary.** Delay-differential equations are used at WIAS as a versatile tool for the modeling of optoelectronic devices. They are able to capture complex high-dimensional dynamical effects caused by feedback and interaction at finite propagation speed and, at the same time, they allow for a qualitative understanding of many physical effects by applying advanced methods from the mathematical theory of dynamical systems. Triggered by specific application problems, a comprehensive mathematical theory for the singular limit of large delay times was developed, including multiscale approaches to the stability of equilibria, periodic solutions, and different types of chaotic motion. Moreover, for certain cases a mathematically rigorous justification of the Ginzburg–Landau equation as an amplitude equation for the behavior close to the destabilization threshold was obtained. This theory was successfully applied to study various optoelectronic systems, such as lasers with feedback, localized structures of light, stabilization and destabilization of cavity solitons, and mode-locked lasers.

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2.3 Adaptive Anisotropic Grids for Numerical Simulations

Lennard Kamenski

Background and motivation

Many physical processes are modeled by partial differential equations (PDEs), whose analytical solutions are unavailable and must be simulated using numerical approximations. A common numerical simulation starts with a subdivision of the physical domain into a finite number of elementary geometrical building blocks (*mesh elements*), on which the solution of the PDE is approximated using a simple set of basis functions. This process (*mesh generation*) is followed by the discretization and results in a system of linear equations, which is then solved: This is the essence of the finite element and finite volume methods.

The accuracy of a numerical simulation crucially depends on the mesh resolution, which is usually controlled by the number and size of the mesh elements. However, higher resolution leads to larger linear systems and, consequently, to a higher computational cost of the whole process, introducing a trade-off between the accuracy of the numerical method and its computational cost.

One of the obvious reasons for *anisotropic* mesh adaption, i.e., adaption of not only the size but also the shape and the orientation of mesh elements, is that the orientation of the mesh building blocks is an additional degree of freedom during the adaption process, which allows more flexibility and a better compromise in case of different, possibly contradicting, objectives of adaption.

Another, very strong, reason for exploring specifically the anisotropic adaption comes from the physical problems itself: In a simulation, particularly challenging are physical processes having *anisotropic* structure, such as *boundary layers* (thin regions of rapid change along domain boundaries), characterized by a *directional* variation of the physical quantity; for example, the concentration of a reactant dissolved in a mixture flowing over a catalyst, the concentration of charge carriers near a transistor gate contact, or the velocity of a turbulent flow. Likewise, *interior layers* occur in the interior of the domain; classic examples being shock waves and chemical reaction fronts. Boundary and interior layers are characterized by a strong *directional* variation of the solution: It is very large in one direction, but small in the other. Adapting the mesh by only adjusting the number and size of the mesh elements (which is the classic, *isotropic*, approach to mesh adaption) would lead to unnecessarily large linear systems and, thus, excessive computational costs. Consequently, near the boundary or interior layers, the optimal mesh should have a high resolution in the direction of rapid changes (in order to improve the accuracy), but the resolution should stay low in the directions of slow variation (in order to keep computational costs reasonable), meaning that the optimal mesh for resolving such layers should be *anisotropic*.

In brief, for a successful numerical simulation, *the structure of the problem should be reflected in the mesh*. To reach this goal, the major components of mesh generation have to be studied.

First, the question *"What is the best mesh for a given problem?"* needs to be answered by deriving criteria for the optimal mesh in dependence on the objectives of the simulation and restrictions imposed by the employed methods. The derived requirements on the mesh are then passed to



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the actual mesh generation stage; here, the important question is *"How to construct a mesh with given properties?"* Finally, the obtained mesh should be examined to see if it fulfills the desired properties and, if necessary, readjusted. This procedure results in a typical mesh generation cycle:

assessment of mesh requirements \Longrightarrow mesh generation

 \implies assessment of mesh quality \implies mesh generation / adaption

These stages are strongly connected to each other and require knowledge in numerical analysis, discrete geometry, and scientific computing. Thus, the ultimate goal of our research is the connection of these areas for a better understanding of anisotropic mesh adaption and its impact on the numerical methods involved, which is the key to accurate and cost-effective numerical simulations.

Numerical analysis in mesh generation

Different objectives impose different requirements on the mesh, and they can even contradict each other. For example, as noted above, a mesh that is good for minimizing the approximation error of the solution may be inappropriate from the computational efficiency point of view. Thus, an optimal grid is often a compromise between multiple objectives and requirements. Moreover, grids obtained from grid generators seldom fulfill the desired requirements exactly and it is important to know how this inaccuracy affects other stages of the numerical simulation. To resolve these questions, the development of meaningful, goal-oriented mesh quality measures is unavoidable.

Mesh quality measures. A good quality measure has to be goal- and problem-oriented and depend on the parameters of the underlying problem. Mesh quality measures can be based on quantities computed during the simulation (a posteriori information) or on information available prior to the simulation, which is often the case for the mentioned above physical problems exhibiting boundary layers.

Our objective is *goal-oriented* mesh quality measures, which are able to give a meaningful statement on how good is the mesh for a given task and how the (in practice unavoidable) non-conformity of the mesh with the posed specifications affects a given quantity of interest, e.g., solution approximation error, stability condition for time integrators [1], or conditioning of the resulting stiffness matrix [2]. Naturally, this research topic is strongly connected to both the error analysis and the actual mesh generation by defining criteria for the mesh generation and the quality assessment of the constructed mesh.

Research on mesh quality measures as well as recent advances in mesh improvement techniques, such as robust algorithms for mesh smoothing [3], are closely connected to the further development of the WIAS software package TetGen.

Obtaining directional information. For the proper element orientation and shape we need directional information, which may come from the physical properties of the problem (such as the orientation of boundary layers or diffusion directions) as well as from the solution itself. Usually, the optimal mesh orientation is obtained from a reconstruction of the Hessian of the exact solution from the numerical approximation (to minimize the interpolation error, the underlying mesh should be aligned with the major curvature directions of the solution). The proof of convergence of such an adaptive scheme relies crucially on the accuracy of the recovery. Unfortunately, a convergent Hessian recovery cannot be obtained from the linear finite element approximation on general meshes except for the special situation when the numerical solution exhibits superconvergence. However, it has been also observed that adaptive meshes obtained by means of such a non-convergent Hessian approximation still lead to the optimal error convergence of the finite element approximation. This phenomenon indicates that a convergent Hessian recovery is not necessary for the purpose of mesh adaption and explains why Hessian recovery is still widely used despite its non-convergence. Our current results provide an error bound for the linear finite element solution of a general boundary value problem under a mild assumption on the closeness of the recovered Hessian to the exact one [4]. It also shows that the finite element error changes gradually with the closeness of the recovered Hessian, providing a good theoretical explanation of why a non-convergent recovered Hessian works in mesh adaption. However, in some cases theoretical bounds are still larger than the ones observed numerically, which indicates that further investigation is needed to clarify the issue.

Conditioning of linear systems arising from discretization of PDEs. Another direction of research targets the impact of adaptive grids on the last stage of a numerical simulation: the solution of linear systems arising from the discretization of PDEs. There is a concern that the discretization based on anisotropic meshes can lead to extremely ill-conditioned linear systems, and that may outperform the accuracy and efficiency improvements gained by anisotropic adaption. The difficulty in resolving this question is that most of the available estimates consider only the special case of isotropic or locally uniform meshes and, typically, are much too pessimistic to be useful for general anisotropic grids. A new analysis was necessary to resolve this problem and, recently, we were able to achieve a significant progress: Our recent result for the example of the elliptic second-order problems shows that the conditioning of finite element equations with anisotropic adaptive meshes is much better than generally assumed, especially in one and two dimensions [2]. This is the first accurate result that has been proven for the general case, that is, *without any assumptions on the mesh regularity or topology*, which allows it to be employed in the context of anisotropic adaption and gives hope that one does not necessarily have to trade off between adaption and conditioning.

In particular, the new theoretical bounds on extremal eigenvalues of the mass matrix and the largest eigenvalue of the stiffness matrix are tight within a constant mesh-independent factor *both from below and above* for *any mesh* with *no assumptions on mesh regularity or topology*.

New results for eigenvalues of the stiffness matrix allow further research in related areas. Currently, the stability of explicit one-step methods and the conditioning of implicit one-step methods for the finite element approximation of linear diffusion equations on anisotropic meshes is under investigation; the derived theoretical bound on the largest permissible time step is surprisingly simple but still tight for any mesh and any diffusion matrix within a mesh-independent constant factor [1].

Example 1: Two-dimensional groundwater flow through an aquifer

Consider the initial boundary value problem (IBVP)

$$\begin{cases} \partial_t u = \nabla \cdot (\mathbb{D}\nabla u), & x \in \Omega, \quad t \in (0, T], \\ u(x, t) = 0, & x \in \Gamma_{\mathrm{D}}, \quad t \in (0, T], \\ \mathbb{D}\nabla u(x, t) \cdot n = 0, & x \in \Gamma_{\mathrm{N}}, \quad t \in (0, T], \\ u(x, 0) = u_0(x), & x \in \Omega \end{cases}$$

with a square domain $\Omega = (0, 100) \times (0, 100)$ and two impermeable subdomains $\Omega_1 = (0, 80) \times (64, 68)$ and $\Omega_2 = (20, 100) \times (40, 44)$; Figure 1 shows the diffusion matrix \mathbb{D} and the boundary conditions (the model problem is taken from [5]). Although \mathbb{D} is isotropic itself, it jumps between the subdomains, causing the anisotropic behavior of the solution. Figure 2 shows solution snapshots with the corresponding anisotropic adaptive meshes.



(1)

Fig. 1: Groundwater flow: domain and the diffusion \mathbb{D}



Fig. 2: Groundwater flow: solution snapshots, mesh examples and close-ups at the upper right corner at the entrance of the tunnel





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(b) At $t = 1.0 \times 10^5$, 20 334 mesh elements

Example 2: Anisotropic diffusion and the discrete maximum principle

We consider the BVP

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$$\begin{cases} \nabla \cdot (\mathbb{D} \nabla u) = f & \text{in } \Omega, \\ u = g & \text{on } \partial \Omega, \end{cases} \quad \text{with} \quad \mathbb{D} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} 1000 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}, \quad (2)$$

 $\Omega = (0, 1)^2 \setminus [4/9, 5/9]^2$, $\theta = \pi \sin x \cos y$, and boundary conditions as in Figure 3. The exact solution of (2) satisfies the maximum principle ($0 \le u \le 2$) and has sharp jumps near the inner boundary (Figure 4). Standard finite element methods are known to produce unphysical spurious

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Fig. 4: Problem (2): solution

Fig. 5: Anisotropic diffusion: meshes and contour plots of the numerical solution

oscillations for this kind of problems if applied straightforwardly. For this example, we adapt the element size to improve the accuracy of the solution and use the element orientation to satisfy the so-called *anisotropic non-obtuse angle condition*, requiring the mesh to be aligned with the major directions of the diffusion in order to satisfy the discrete maximum principle.

Figure 5(a) shows what happens if the mesh is only solution adaptive and the diffusion directions are not taken into account: unphysical negative minima occur (min $u_h \approx -0.0032$). In contrast, no unphysical minima can be observed for the solution- and diffusion-adaptive mesh in Figure 5(b). Although the solution in Figure 5(b) is not as smooth as in the purely solution-adaptive case of Figure 5(a), it still provides a good adaption to the sharp solution jump near the interior boundary, allowing a good compromise between the accuracy and the physical properties of the solution. (A more detailed discussion on this example can be found in [6].)



(a) Purely solution-adaptive mesh

(b) Solution- and diffusion-adaptive mesh

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2.4 Phase Field Approach to Structural Topology Optimization

M. Hassan Farshbaf Shaker

Introduction

Topology optimization deals with problems of finding optimal material distributions in a given design domain subject to certain criteria that are given by an objective functional. Known quantities in these problems are, e.g., the applied loads, possible support conditions, the volume of the structure, and possible restrictions as, for example, prescribed solid regions or given holes. A priori, the precise shape and the connectivity (the "topology") of the structure is not known. Often also the problem arises that several materials have to be distributed in the given design domain.

Various methods have been used to deal with shape and topology optimization problems. The classical method uses boundary variations in order to compute shape derivatives that can be used to decrease the objective functional by deforming the boundary of the shape in a descent direction. The boundary variation technique has the drawback that it needs high computational costs and does not allow for a change of topology.

Sometimes one can deal with the change of topology by using homogenization methods, see [1], and variants of it, such as the SIMP method; see [2] and the references therein. These approaches are restricted to special classes of objective functionals.

Another approach, which was very popular in the last ten years, is the *level set method* that was originally introduced by Stanley Joel Osher and James Albert Sethian. The level set method allows for a change of topology and was successfully used for topology optimization by many authors. Nevertheless, for some problems the level set method has difficulties to create new holes. To overcome this problem, the sensitivity with respect to the opening of a small hole is expressed by so-called *topological derivatives*. Then, the topological derivative can be incorporated into the level set method in order to create new holes.

The principal objective in shape and topology optimization is to find regions that should be filled by material in order to optimize an objective functional. In a parametric approach, this is done by a parametrization of the boundary of the material region, and in the optimization process, the boundary is varied. In a level set method, the boundary is described by a level set function, and in the optimization process, the level set function changes in order to optimize the objective. Since the boundary of the region filled by material is unknown, the shape optimization problem is a free boundary problem. Another way to handle free boundary problems and interface problems is the phase field method, which has been used for many different free boundary-type problems; see [5].

In structural optimization problems, the phase field approach has been used by some authors; see [3, 4] and the references therein. It is capable of handling topology changes, and also the nucleation of new holes is possible; see [3, 4]. The method is applied for domain-dependent loads,

fixed **Fig. 1:** Cantilever beam, geometry



Fig. 2: Cantilever beam, numerical simulation with two phases



Fig. 3: A cantilever beam simulation with four phases

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Fig. 4: 3D cantilever beam simulation with two phases



Fig. 5: Gibbs simplex for three phases indicated as the green area

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Fig. 6: Sketch: topology optimization problem

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multi-material structural topology optimization, minimization of the least-square error to a target displacement, topology optimization with local stress constraints, mean compliance optimization, compliant mechanism design problems, eigenfrequency maximization problems, and problems involving nonlinear elasticity.

Multi-material topology optimization and phase field approach

The goal in multi-material shape and topology optimization is to partition a given bounded Lipschitz design domain $\Omega \subset \mathbb{R}^d$ into regions that are either void or occupied by N-1 different materials, such that a given cost functional is minimized subject to given constraints. Within the phase field approach, we describe the different material distributions with the help of a phase field vector $\boldsymbol{\varphi} := (\varphi^i)_{i=1}^N$, where φ^N describes the fraction of void and $\varphi^1, \ldots, \varphi^{N-1}$ describe the fractions of the N-1 different materials. The phase field approach allows for a certain mixing between materials and between materials and void, but the mixing will be restricted to a small interfacial region. In order to ensure that the phase field vector $\boldsymbol{\varphi}$ describes fractions, we require that $\boldsymbol{\varphi}$ lies pointwise in the Gibbs simplex $\boldsymbol{G} := \{\boldsymbol{v} \in [0, \infty)^N \mid \sum_{i=1}^N v^i = 1\}$; see Figure 5 for the Gibbs simplex with only three phases. In this work, we prescribe the total spatial amount of the material fractions through $f_\Omega \boldsymbol{\varphi} = \boldsymbol{m} = (m^i)_{i=1}^N$, where it is assumed that $\sum_{i=1}^N m^i = 1$ with $m^i \in (0, 1), i = 1, \ldots, N$, and where $f_\Omega \boldsymbol{\varphi}$ denotes the mean value on Ω . We remark that, in principle, inequality constraints for $f_\Omega \boldsymbol{\varphi}$ can also be dealt with.

In the simplest situation, a working or design domain Ω , see Figure 6, with a boundary $\partial\Omega$, which is decomposed into a Dirichlet part Γ_D (where the design domain is fixed), a non-homogeneous Neumann part Γ_g (where a surface load is acting), a homogeneous Neumann part Γ_0 , and body and surface forces $\mathbf{f}: \Omega \to \mathbb{R}^d$ and $\mathbf{g}: \Gamma_g \to \mathbb{R}^d$ is given. Now, one tries to find a phase field vector $\boldsymbol{\varphi}$ (which represents the material distribution) and the displacement $\boldsymbol{u}: \Omega \to \mathbb{R}^d$, such that the mean compliance (i.e., deformation energy)

$$F(\boldsymbol{u},\boldsymbol{\varphi}) := \int_{\Omega} \left(1 - \varphi^N \right) \mathbf{f} \cdot \boldsymbol{u} + \int_{\Gamma_g} \boldsymbol{g} \cdot \boldsymbol{u}$$
(1)

or the error compared to a required target displacement u_{Ω} , i.e.,

$$J_0(\boldsymbol{u}, \boldsymbol{\varphi}) := \left(\int_{\Omega} \left(1 - \varphi^N \right) c \left| \boldsymbol{u} - \boldsymbol{u}_{\Omega} \right|^2 \right)^{\frac{1}{2}}$$
(2)

is minimized, where c is a given weighting function, and $|\cdot|$ is the Euclidean norm. Moreover, in our phase field approach as an approximation of the perimeter functional the Ginzburg–Landau functional,

$$E^{\varepsilon}(\boldsymbol{\varphi}) := \int_{\Omega} \left(\frac{\varepsilon}{2} |\nabla \boldsymbol{\varphi}|^2 + \frac{1}{\varepsilon} \Psi(\boldsymbol{\varphi}) \right)$$
(3)

is added to the above functionals (1) or (2); see [3, 4]. The small parameter ε in (3) is related to the thickness of the interfaces between the domains, which is a characteristic feature in phase field modeling; see Figure 7 for a model with three phases at the triple junction. The potential $\Psi: \mathbb{R}^N \to \mathbb{R} \cup \{\infty\}$ is assumed to have global minima at the unit vectors \mathbf{e}_i , i = 1, ..., N, which
correspond to the different materials and to the void. In (3), we have chosen an obstacle potential $\Psi(\boldsymbol{\varphi}) = \Psi_0(\boldsymbol{\varphi}) + I_{\boldsymbol{G}}(\boldsymbol{\varphi})$, where Ψ_0 is smooth and I_G is the indicator function of the Gibbs simplex \boldsymbol{G} .

In (1) and (2), the displacement \boldsymbol{u} is the solution of the linearized elasticity system

	$-\nabla \cdot [\mathbb{C}(\boldsymbol{\varphi})\mathcal{E}(\boldsymbol{u})]$	=	$\left(1-\varphi^N\right)\mathbf{f}$	in Ω ,	
Į	и	=	0	on $\Gamma_{\rm D},$	(4)
	$[\mathbb{C}(\boldsymbol{\varphi})\mathcal{E}(\boldsymbol{u})]$ n	=	8	on Γ_g ,	()
	$[\mathbb{C}(\boldsymbol{\varphi})\mathcal{E}(\boldsymbol{u})]$ n	=	0	on Γ_0 ,	

where **n** is the outer unit normal to $\partial\Omega$. As described before, the Dirichlet part of the boundary $\Gamma_{\rm D}$ is fixed, i.e., the displacement vector is $\boldsymbol{u} = \boldsymbol{0}$ there, which is given by the second equation in (4). Moreover, in case of linear elasticity, the strain tensor is given by $\mathcal{E} = \mathcal{E}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)$. The elasticity tensor \mathbb{C} is assumed to depend smoothly on $\boldsymbol{\varphi}$, \mathbb{C} has to fulfill the usual symmetry condition of linear elasticity and has to be positive definite on symmetric tensors. For the phase field approach the void is approximated by a very soft material with an elasticity tensor $\mathbb{C}^N(\varepsilon)$ depending on the interface thickness, e.g., $\mathbb{C}^N = \varepsilon^2 \tilde{\mathbb{C}}^N$ with a fixed tensor $\tilde{\mathbb{C}}^N$. Discussions on how to interpolate the elasticity tensors \mathbb{C}^i , for i = 1, ..., N, given in the pure materials onto the interface can be found in [3].

Summarizing, the multi-material structural optimization problem can be formulated as: Given $(\mathbf{f}, \boldsymbol{G}, \boldsymbol{u}_{\Omega}, c)$, we want to solve

$$(\mathcal{P}^{\varepsilon}) \qquad \min_{\substack{(\boldsymbol{u},\boldsymbol{\varphi})}} J^{\varepsilon}(\boldsymbol{u},\boldsymbol{\varphi}) := \alpha F(\boldsymbol{u},\boldsymbol{\varphi}) + \beta J_0(\boldsymbol{u},\boldsymbol{\varphi}) + \gamma E^{\varepsilon}(\boldsymbol{\varphi}) \quad \text{such that (4) is fulfilled,}$$

where $\alpha, \beta \geq 0, \gamma, \varepsilon > 0$, $f_{\Omega} \boldsymbol{\varphi} = \boldsymbol{m} \in (0, 1)^N$ with $\sum_{i=1}^N m^i = 1$.

From the application point of view, it might be desirable to fix material or void in some regions of the design domain. This fixing can be done by defining a subset $S_0 \subset \Omega$ of the design domain, which characterizes material, i.e., there is no void. Moreover, by choosing S_0 such that $|S_0 \cap \text{supp } c| \neq 0$, we can ensure that it is not possible to choose only void on the support of c, i.e., in (2), we ensure $|\text{supp } (1 - \varphi^N) \cap \text{supp } c| > 0$.

Mathematical analysis

Although many computational results on phase field approaches to topology optimization exist, there has been relatively little work on analytical aspects. In [3], we show the existence of a minimizer to $(\mathcal{P}^{\varepsilon})$ and rigorously derive first-order optimality conditions. Moreover, we consider the sharp interface limit of the first-order conditions, i.e., we take the limit $\varepsilon \to 0$ and, therefore, the thickness of the interface converges to zero. We obtain limiting equations with the help of formally matched asymptotic expansions and relate the limit, which involves classical terms from shape calculus, transmission conditions, and triple junction conditions, to the shape calculus as presented in [1].



Fig. 7: Phase field model with three phases, which are separated by a diffuse interface of thickness ε



Fig. 8: Bridge configuration



Fig. 9: Deformation of the bridge

Simulation results

After formulating the multi-material structural optimization problem in $(\mathcal{P}^{\varepsilon})$, the next step is to find its solutions or minimizers characterizing the optimal configurations. In general, it is impossible to calculate an analytic solution to $(\mathcal{P}^{\varepsilon})$. Hence, the strategy will be to compute numerical approximations. For our numerical simulations, we use finite element approximation in combination with iterative methods; see [3] for details. In the following, the superscript *h* will always indicate the corresponding finite element solutions.

Cantilever beam problem

To begin with, a minimum compliance problem for a cantilever beam is considered, i.e., we have $\beta = 0$ in $(\mathcal{P}^{\varepsilon})$; see Figure 1. It aims to construct a structure with maximal global stiffness and is a basic problem in topology optimization. Figure 2 shows a numerical simulation with two materials and Figure 3 with four materials of the optimal shape. We can also easily simulate three-dimensional problems; see, e.g., Figure 4.

Bridge construction

Next, the classical problem of the bridge configuration—depicted in Figure 8—is considered ($\beta = 0$). In Figure 10, we display only results for initial data of checkerboard structure. We point out that the connectivity of the regions occupied by material is found by the method without using information on topological derivatives. One also observes several topological changes during time (or iterations); see also [6]. Figure 9 shows the deformed optimal configuration.



fixed ◄── g



Fig. 10: Bridge simulation

checkerboard initial data, material in red and void in

with N = 2 and

blue

fixe

Fig. 11: Push configuration

Push construction

For the construction problem under pushing forces we present numerical simulations for the configuration depicted in Figure 11, where one minimizes the target displacement only. We set therefore $\alpha = 0$. In Figure 12, a simulation for the push configuration is given. The corresponding deformed optimal configuration is displayed in Figure 13.





Fig. 12: Push simulation with N = 2, material in red and void in blue

Future Work

In continuation of our work, several directions of future research can be considered. Numerical results show high stresses on domain boundaries. Therefore, it is of practical relevance to study topology optimization problems with stress constraints. We plan to investigate this subject in cooperation with a wind turbine development company. Another direction of research is to combine our phase field topology optimization problem with uncertain loading, material data, and chance state constraints. Even in the finite-dimensional case, the derivation of optimality conditions including gradient formulas is completely open. This problem is investigated in the MATHEON research project C–SE13 "Topology optimization of wind turbines under uncertainties" (ECMath). In the long run, including an appropriate damage model as additional state equation will be a further task of great practical importance.



Fig. 13: Deformed optimal configuration

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2.5 New Approach for Optimal Control of Hydroelectricity Storage Systems

Roland Hildebrand and John G. M. Schoenmakers

The Energiewende has boosted the share of renewable energies in Germany's total energy production from a meager 3% in 1990 to over 25% last year. This change is accompanied by a massive and ongoing restructurization of the energy sector. The geographic locations of energy production and energy consumption have become more and more disconnected, and as a result, the interdependencies of the players and the complexity of their behavior have increased dramatically. Unlike energy production from fossil fuels, the input in the grid from renewable sources such as wind and solar energy comes along with a high uncertainty and is difficult to predict, resulting in an increased volatility of the energy prices and in the emergence of energy markets to facilitate matching offer and demand. These new energy markets have some points in common with classical financial markets such as the stock exchange or the bond market. Modeling the dynamics of processes in the energy sector and developing strategies for its actors then makes the application of statistical methods inevitable.

Like the actors on the classical markets, both producers and large-scale consumers of energy face risks and seek protection from these risks by structured contracts, so-called *energy derivatives*. In the gas and energy markets, for example, so-called *swing options* have become very popular. An example swing option gives the holder the right to buy or sell a certain amount of gas, electricity, or storage capacity at a certain prescribed number of trading dates. A key issue in the energy markets is the fact that some forms of energy (in particular, oil, gas, and hydro-electric power) can be stored physically. Corresponding storage facilities allow for anticipating and exploiting market fluctuations of energy prices according to the principle "sell high and buy low". Initially, storage facilities were only accessible by major players in the respective industries, who had sufficient capital to build and maintain them. Meanwhile, due to the emerging liberalization of the energy markets, all participants have the possibility to trade storage services via storage exchange platforms. As a consequence, on the one hand, optimal strategies involving buying, storing, and selling energy over time are called for. On the other hand, this development results in a high demand of proper statistical prediction algorithms based on an adequate statistical modeling of energy prices and storage markets.

These distinctive properties of energy markets make the existent repertoire of statistical methods and algorithms developed in the framework of classical financial mathematics insufficient and call for the development of new tailored methods. For example, finding correct prices for energy derivatives is typically difficult due to their complex-structured exercise features and their highly path-dependent structure. When developing strategies for energy producers and/or traders, both the particularities of the energy market and the constraints posed by the limited storage and production resources of the actor have to be adequately modeled.

As a general consequence, the rising complexity of the markets poses challenging mathematical issues that may be categorized into the following main streams:



- New numerical methods and algorithms for solving multidimensional problems in optimal (multiple) stopping and optimal control
- Adequate modeling of various energy price processes including modern statistical forecast techniques

Particularly in electricity markets, the evaluation of (swing) options requires efficient algorithms for multiple stopping and more complicated control optimization problems.





In our work, we consider a combined model of a hydro-electric storage and production facility and of the day-by-day electricity bid market. This coupled model has been introduced in [2]. The production facility consists of a number of interconnected water reservoirs. Electricity can be produced from these reservoirs by releasing water from a reservoir situated at higher elevation to one at lower elevation. It can also be stored in the form of potential energy by pumping water from a reservoir at lower elevation to one at higher elevation. The energy conversion efficiency of these processes is lower than 100%, however, and running the water in a cycle leads to a certain loss. The reservoirs are filled by rain and other natural processes, which are modeled as a stochastic process. When exploiting the reservoirs, the operator has to meet certain constraints such as not exceeding the capacity of any turbine and not emptying a reservoir completely. Currently, the reservoirs are assumed to be ordered linearly, a schematic depiction is given in Figure 1.





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This model of the storage and production facility is coupled to a model of the electricity market. At the end of each day, the company operating the production facility submits a bid curve to the market operator. This bid curve specifies how much electricity the company is ready to buy or sell, in dependence on the price of the electricity. The curve will be monotonically increasing, since the company is ready to sell more if the price is higher. It is modeled as a piecewise linear curve determined by its values on a fixed grid in the price dimension. An example of such a bid curve is given in Figure 2.

The operator then calculates the equilibrium price from all submissions and makes it available. The next day, the company has to sell or buy the amount of electricity it specified the day before. This electricity is then produced or stored by means of operating the water reservoirs. The price set by the market operator is modeled as a stochastic process, which is dependent on the process modeling the water inflow.

Each day the company is then faced with the problem to decide on the bid curve to be submitted and on the modus operandi of the reservoirs. These quantities constitute the decision variables that in the end determine the value of the problem, which is the total profit generated over the considered time horizon.

Instead of solving this problem directly, we choose a dual martingale approach, where a dual problem is solved by a Monte Carlo simulation. This class of methods was initially developed in [5] and [3]. John Schoenmakers then first adapted it to multiple stopping problems occurring in option pricing [1]. This representation was extended to much more general pay-off profiles in [4]. In this extended setting, it is possible to treat more realistic energy derivatives. Such derivatives may involve several volume and exercise refraction constraints, as well as processes driving several underlying energy titles. In the current work, we apply our extended setting to the optimal control of stochastic processes.

Optimal control of stochastic processes

We shall now describe the general class of stochastic optimal control problems to which the dual martingale method is applicable. The problem is defined in a discrete-time setup over a finite time horizon, i.e., the time *t* takes values $0, \ldots, T$. At each time instant *t*, we observe the realization ω_t of a stochastic process and have to choose a control action $a_t \in A_t$ from some control space. At the end of the time horizon, we obtain a reward $U(a, \omega)$, which is the objective value of the control problem.

Our goal is to design an optimal control strategy, i.e., an adapted function

$$\alpha: \omega \mapsto \alpha(\omega) = (\alpha_0(\omega), \dots, \alpha_T(\omega))$$

that puts a control action in correspondence to every realization ω , such that the action to be taken at time instant t depends only on the values ω_s for $s \le t$, and that maximizes the expectation of the reward map.

In other words, we have to find the value and the maximizer of the problem

$$V_0^* = \sup_{\alpha \in \mathfrak{P}} \mathbb{E}_0 U(\alpha)$$

where \mathfrak{P} is the set of all admissible control strategies. At time instant t, certain control actions a_0, \ldots, a_{t-1} have already been taken, and we have to solve the problem

$$V_t^*(a_0,\ldots,a_{t-1}) = \sup_{\alpha^{(t)}\in\mathfrak{P}_t} \mathbb{E}_t U(a_0,\ldots,a_{t-1},\alpha^{(t)}),$$

where \mathfrak{P}_t is the set of admissible control strategies $\alpha^{(t)} = (\alpha_t, \ldots, \alpha_T)$ from time t on. According to the Bellman principle, we then have to solve the problem

$$V_t^*(a_0,\ldots,a_{t-1}) = \sup_{a_t \in A_t} \mathbb{E}_t V_{t+1}^*(a_0,\ldots,a_{t-1},a_t), \quad t = 0, ..., T - 1.$$

Duality then states that the martingales defined by

$$\xi_t^*(\mathbf{a}) = \xi_t^*(a_0, \dots, a_{t-1}) = V_t^*(a_0, \dots, a_{t-1}) - \mathbb{E}_{t-1} V_t^*(a_0, \dots, a_{t-1})$$

satisfy

$$V_0^* = \sup_{\mathbf{a} \in \mathbf{A}} \left(U(\mathbf{a}) - \sum_{t=1}^T \xi_t^*(\mathbf{a}) \right)$$

almost surely, where $a = (a_0, ..., a_T)$ lies in the set $\mathbf{A} = A_0 \times \cdots \times A_T$. Moreover, every general adapted martingale $\xi_t(\mathbf{a}) = \xi_t(a_0, ..., a_{t-1})$ yields an upper bound on the value of the problem, i.e.,

$$V_0^* \leq \mathbb{E}_0 \sup_{\mathbf{a}\in \mathbf{A}} \left(U(\mathbf{a}) - \sum_{t=1}^T \zeta_t(\mathbf{a}) \right) \,.$$

The *dual martingale approach* pursued in this work solves the above dual problem for an almost surely optimal martingale ζ^* by a Monte Carlo simulation. Namely, a number of realizations of the stochastic process is simulated, and a martingale ζ is fitted in the form of a linear combination of basis martingales whose values are constructed from the realizations. The obtained suboptimal martingale yields an upper bound on the value of the problem and is subsequently used as a penalty term in the solution of the original problem on the control strategy.

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Fig. 1: Illustration of structure and functionality of a lithium-ion battery with a many-particle electrode and a metallic lithium electrode



Fig. 2: Voltage-capacity diagram of a LiFePO₄ electrode vs. metallic lithium

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2.6 Mathematical Models for Lithium-ion Batteries

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

A model-based understanding of the fundamental processes occurring in lithium-ion batteries is a key feature to improve charging times, storage capabilities, safety, and lifetime. In addition, a rigorous modeling should be adoptable to the several types of lithium-based batteries that are promising for electromobility applications, namely LiFePO₄ -based batteries, lithium-air or -sulfur batteries, or redox-flow type cells. Common to all lithium-ion batteries is the setup of two electrodes, which are connected by a Li⁺ -conducting electrolyte. Since the electrodes are electronic conductors, electrons flow through an outer circuit to the counter-electrode and drive an electric consumer. During discharging, the lithium ions adsorb at the electrode surface and react with the electrons to lithium. Then, the lithium is stored within the electrode, which is generally made of $10^9 - 10^{17}$ storage particles. Figure 1 illustrates the principal structure and functionality of a lithium-ion battery.

One very promising electrode material for lithium-ion batteries is LiFePO₄, which is cheap, nontoxic, and electrochemically stable. The charging/discharging characteristic of such a many-particle electrode, i.e., the voltage-capacity diagram, is shown in Figure 2. The graph shows broad horizontal branches indicating a phase transition in the many-particle electrode. Moreover, we observe hysteresis, i.e., charging and discharging evolve along different paths.

In the battery, all charges are balanced immediately, except for the thin regions at the electrodeelectrolyte interface, where charge layers are formed. These charge layers are characteristic for almost all electrochemical systems.

The functionality of a battery relies on a complex and subtle interplay of quite different electrochemical processes. A mathematical battery model must be able to represent and predict

- ion transport within the electrolyte,
- surface reactions on the particle surfaces,
- formation of the charge layers at the electrolyte-electrode interface,
- phase transition within the many-particle electrode.

During the last three years, WIAS's Leibniz Group LG 3 *Mathematical Models for Lithium-ion Batteries* made substantial contributions to the modeling of all these processes, thereby changing some fundamental doctrines of electrochemistry as detailed in the following.

Electrolyte model

Our starting point for the modeling of electrolytes was a revision of the Nernst–Planck model [4]. It is well known that the standard Poisson–Nernst–Planck (PNP) model leads to unphysically high mole densities n_{α} of the ionic species A_{α} , $\alpha = 1, ..., N$, with molar mass m_{α} and electric charge $z_{\alpha}e_{0}$. Several attempts have been made in the literature to overcome this problem. The crucial ingredient of our new approach is the formulation of a free energy density, which explicitly accounts

for entropical and mechanical interactions among the ionic species and the solvent A_0 . Based on this free energy, the constitutive equations for the remaining constitutive quantities, such as the chemical potentials μ_{α} , the pressure p, or the mass fluxes J_{α} , are derived. For an incompressible electrolyte the chemical potentials are

$$\mu_{\alpha} = g_{\alpha}(T) + \frac{k_B T}{m_{\alpha}} \ln\left(\frac{n_{\alpha}}{n}\right) + \frac{v_{\alpha}^R}{m_{\alpha}} \left(p - p^R\right) \quad \text{with } n = \sum_{\alpha=0}^N n_{\alpha} . \tag{1}$$

The first term is a reference contribution depending on the temperature T. In the entropic part, k_B denotes the Boltzmann constant. The third term is missing in the electrochemical literature. It accounts for the mechanical interaction of the different constituents. Here, p^R is a reference pressure, and v_{α}^R represents the specific volume of the constituent A_{α} .

The pressure p is a local quantity that cannot be neglected or assumed to be constant. We emphasize that, however, this assumption is commonly made in the textbook literature for liquid electrolytes. Due to the rigorous thermodynamic derivation, we have knowledge of the missing equation in electrochemistry that accounts for the interaction between matter and the electric field: the momentum balance. The stationary momentum balance reads

$$abla p = -n^F \nabla \phi$$
 with $n^F = \sum_{\alpha=0}^N z_\alpha e_0 n_\alpha$ (2)

and states that the electric force $-n^F \nabla \phi$ is balanced by a pressure gradient. In the charge layers, where the electric potential varies strongly, a non-constant pressure p is generated; cf. Figure 3. This interaction has also a strong impact on the chemical potentials due to the pressure contribution.

Quite similar to the assumption of constant or negligible pressure p, a common additional textbook assumption is that the solvent A_0 can be ignored. This is not possible due to mass conservation, which implies that only N independent mass fluxes exist and the (N + 1)-st mass flux is given by the constraint $J_0 = -\sum_{\alpha=1}^N J_\alpha$. The generalized Nernst–Planck fluxes for the ionic species A_{α} , $\alpha = 1, ..., N$ are

$$J_{\alpha} = -M_{\alpha} \bigg(k_B T \,\nabla n_{\alpha} + n_{\alpha} \, z_{\alpha} e_0 \nabla \phi - k_B T \, \frac{n_{\alpha} m_{\alpha}}{n_0 m_0} \nabla n_0 + v_{\alpha}^R n_{\alpha} \bigg(1 - \frac{v_0^R m_{\alpha}}{v_{\alpha}^R m_0} \bigg) \nabla p + \frac{k_B T}{n} \bigg(\frac{m_{\alpha}}{m_0} - 1 \bigg) n_{\alpha} \nabla n \bigg).$$
(3)

In contrast to the standard Nernst–Planck model, there are three additional terms, highlighted in blue. These terms represent the ion-solvent interaction and the pressure contribution. These three contributions lead to physically meaningful bounds on the ion concentration and correct the deficiencies of the standard Nernst–Planck theory (cf. Figure 4).

The contribution of the pressure to the mass fluxes J_{α} increases with the partial molar volume v_{α}^{R} of the constituents A_{α} . Since most solvent molecules have a microscopic dipole, there is an additional microscopic electrostatic interaction between solvent and ionic species. This interaction leads to a clustering of κ_{α} solvent molecules around a central ion of constituent A_{α} , which is known as solvation effect (cf. Figure 5). These bound solvent molecules do not participate in the entropic interaction anymore; however, they increase the partial molar volume v_{α}^{R} of the ionic

Fig. 3: Comparison of material pressure in

material pressure in boundary layer standard Nernst–Planck (dashed line) vs. generalized Nernst–Planck (solid line)



Fig. 4: Comparison of the standard and generalized Nernst–Planck theory. The standard theory (blue dotted line) leads to an unphysically high anion mole density at a metal-electrolyte interface. The generalized theory (blue solid line) predicts a bounded ion mole density. The red line represents the number density of pure water.



Fig. 5: Sketch of a solvated cation and a solvent constituent. Due to the solvation effect, we have for the specific volumes of the ionic species $v_a^R \gg v_a^R$.

species.

The pressure correction together with the solvation effect yield for the first time a physically meaningful boundary layer charge $Q_{BL} = -\int_{\Omega_{BL}} n^F dx$ for liquid electrolytes. Figure 6 illustrates the influence of the pressure correction and the solvation effect on the boundary layer charge Q_{BL} .

Electrode surface model

Modeling the interface between an electrode and some electrolyte is a central aspect for a proper description of batteries and electrochemical systems in general. For this purpose we developed a thermodynamic surface theory that accounts for all aspects occurring on an electrode surface [2, 5]. Similar to the volume phase, the central quantity is the surface free energy density. All constitutive functions, e.g., the surface chemical potentials $\mu_{s,\alpha}$ and the surface tension γ , are derived from the surface free energy density.

Exemplarily, we studied a metal in contact with a liquid electrolyte. The surface is built by some metal ions M and electrons e, on which electrolytic constituents and their reaction products $(A_{\alpha})_{\alpha=0,1,\dots,N_s}$ can be present. In contrast to the electrolyte, the metal ions form a lattice with adsorption sites. Not every adsorption site is necessarily occupied, which makes it necessary to introduce the surface vacancies V.

We derived a surface free energy that accounts for the entropical interactions of the adsorbates on the lattice and for the elastic properties of the metallic surface. From this free energy we derived the surface chemical potentials

$$\mu_{s,\alpha} = g_{s,\alpha}(T_s) + \frac{k_B T_s}{m_\alpha} \ln\left(\frac{n_{s,\alpha}}{n_\ell}\right) - \omega_\alpha \frac{k_B T_s}{m_\alpha} \ln\left(\frac{n_{s,V}}{n_\ell}\right), \quad \text{with } n_\ell = \sum_{\alpha=0}^{N_s} n_{s,\alpha} + n_{s,V}, \quad (4)$$

for the adsorbates $(A_{\alpha})_{\alpha=0,1,\ldots,N_s}$ as well as the surface chemical potentials

$$u_{s,M} = g_{s,M}(T_s) + \omega_M \frac{k_B T_s}{m_M} \ln\left(\frac{n_{s,V}}{n_\ell}\right) - \frac{a_M^K}{m_M}(\gamma - \gamma^R) \quad \text{and} \quad \mu_{s,e} = const.$$
(5)

for the metal ions and the electrons. Here, $n_{s,lpha}$ denote the surface mole density and ω_lpha the number of adsorption sites of constituent $A_{s, \alpha}$, a_M^R is the partial molar area of the metal surface, and $g_{s,\alpha}(T_s)$ is some reference contribution.

If the adsorption processes are in thermodynamic equilibrium, we have at the surface S

$$\mu_{s,\alpha} = \mu_{\alpha} \big|_{S}, \qquad \alpha = 0, 1, \dots, N_{s}, M, e ,$$
(6)

which actually couples the metallic and electrolytic volume phases to the surface. In particular, this coupling leads to an interaction between pressure and surface tension.

Similar to the volume, an adsorbed ion covers $\kappa_{s,\alpha}$ solvent molecules in its partial solvation shell, which affects the number of adsorption sites ω_{α} (cf. Figure 7). The solvation shell in turn strongly affects the electric charge, which is stored at the surface $Q_S = -e_0 \sum_{\alpha=0}^{N_s} z_{s,\alpha} n_{s,\alpha}$, where $z_{s,\alpha} e_0$ is the electric charge of the constituent A_{α} , $\alpha = 0, ..., N_s$.



Reaction Boun products Fig. 7: Sketch of the constituents on the surface.

Adsorbed ions form a

solvation shell.

Solvent



-0.25

-0.06 0 0.06

Charge Q_{BL} [µC/cm²]

100

100

-0.5



Double layer

At an electrode-electrolyte interface, ionic as well as electronic species are accumulated, forming layers of opposite charge. This structure is commonly known as electric *double layer*, which is a major subject of electrochemistry. Its understanding is of fundamental importance to comprehend the behavior of colloids, dispersion, larger biomolecules, corrosion, electrolysis, electrocatalysis, as well as fuel cells and batteries. Our electrode-electrolyte interface model [2] made substantial contributions to the understanding of the double layer.

In order to validate our theoretical model, we consider a planar interface between a metallic single crystal and an electrolytic solution. Precise measurements of such systems are a standard tool for the characterization of new electrodes and electrolytes, as well as of their interaction. One characteristic property of a specific metal-electrolyte interface is the differential capacity *C* as function of the cell voltage *E*. Figure 8 displays the measured capacity of a silver (110) electrode in contact with aqueous NaClO₄ solutions of various salt concentrations. In contrast to a plate condenser, where the capacity is a constant, the capacity *C* of an electric double layer is a highly nonlinear function of the voltage *E*. Thus, the capacity is a unique fingerprint of the interface.

The capacity *C* is the derivative of the double layer charge *Q* with respect to the applied potential *E*, i.e., C = dQ/dE. In the thermodynamic equilibrium, we obtain *Q* as a function of potential drop $\phi_s - \phi^E$ between the metal surface and the electrolyte. Based on balance equations for the electrode charge, we showed that the total charge *Q* consists of the boundary layer charge Q_{BL} and the surface charge Q_s , i.e., $Q = Q_{BL} + Q_s$. Further, we derived a relationship between the measurable cell potential *E* and $\phi_s - \phi^E$, namely $E = \phi_s - \phi^E + U^R$, where U^R depends on $\mu_{s,e}$ as well as on the reference electrode. Since $\mu_{s,e}$ is dependent on the surface orientation, e.g., of silver (110), our derivation explains naturally the dependence of the reference potential on the specific metal surface. We showed that there exist fundamental relations between the charge contributions Q_{BL} and Q_s to the pressure $p_s = p|_s$ at the surface and to the surface tension γ :

$$Q_{BL}(E) = -\operatorname{sgn}(E - U_R)\sqrt{2\varepsilon_r(p_s(E) - p^E)} \quad \text{and} \quad Q_S(E) = -\frac{d\gamma}{dE}.$$
 (7)

Many previous and recent approaches to understand the behavior of electrochemical interfaces rely essentially on an a priori conception of the double layer structure. The translation into a mathematical model, however, never lead to a satisfactory agreement between measured and computed capacity data. In Figure 9, we display computed capacity curves for an Ag (110) |NaClO₄ (aq) interface. We find a remarkable agreement between the experimental data and our model, both in the potential range of 1 V and the salt concentration c = [0.005 - 0.1] M. Our new model is the first continuum model that is capable to describe the capacity curve over a broad voltage range and for various salt concentrations.

After validating our model on measured capacity data, we can analyze the structure of the space charge layers that are predicted by the model.



Fig. 8: Measured capacity (Fig 2.b from G. Valette, J. Electroanal. Chem., 122 (1981), pp. 285–297, reprinted with permission from Elsevier)



Fig. 9: Computed capacity of an Ag (110) *INaClO*₄ (aq) interface





We find the formation of several layers in front of the metal surface, which can be reinterpreted in terms of the classical conception of the double layer; see Figure 10. However, we find also some crucial deviations from the doctrine of the classical literature, e.g., the Stern layer width is not constant, but grows with the applied potential [1].

Many-particle electrode model

LiFePO₄ (LFP) is a promising material for the lithium-ion battery market. An LFP electrode consists of many LFP particles of nanometer size on a metallic substrate. The particle ensemble exists as a size distribution in the range of 25 – 500 nm. During the discharging process of the battery, lithium atoms are reversibly stored on interstitial lattice sites of the iron phosphate lattices. This storage process is accompanied by a phase transition from a lithium-poor to a lithium-rich phase. In 2010, a new model was proposed at WIAS that demonstrated that the phase transition occurs within the many-particle system and not within the individual storage particles on the time scale of charging/discharging [3]. The many-particle effect is the crucial process that controls the behavior of the LFP electrode. Recently, this new idea was experimentally confirmed by W.C. Chueh et al. (Adv. Mater., **27** (2015) , pp. 6591–6597) on the characteristic time scale of battery charging/discharging.

The LFP particles are not all of equal size, but follow a particle size distribution function; see Figure 11. In order to investigate the effect of various distribution functions, e.g., arising from different synthesis and production methods, the Leibniz Group developed a new model that describes the charging process by a system of stochastic differential equations. For each of the N_P LFP particles $(P^i)_{i=1,...,N_P}$ there is a relation

$$dy^{i} = \frac{1}{\tau^{i}} \left(\mu_{s,Li} - \mu_{Li}^{i} \right) dt + \frac{\sqrt{2}\nu^{i}}{\sqrt{\tau^{i}}} dW^{i} \quad \text{with} \quad \tau^{i} = \tau_{0} \frac{V^{i}}{A^{i}} \quad \text{and} \quad \nu^{i} = \nu_{0} \frac{1}{\sqrt{V^{i}}} , \quad (8)$$

where $y^i = n_{Li}^i / n_{FePO_4}$ denotes the lithium mole fraction, V^i the volume, and A^i the surface area of particle P^i . Since LFP is a phase-separating material, μ_{Li} represents the non-monotone



Fig. 11: Typical particle size distribution of a many-particle electrode

chemical potential of intercalated lithium. Micro fluctuations on the particle surface are modeled with a Wiener process W^i , where v_0 controls the strength of the fluctuations. The rate of the intercalation process is controlled by $\tau_0 > 0$, where $\tau_0 \rightarrow 0$ corresponds to fast intercalation, while $\tau \rightarrow +\infty$ corresponds to slow intercalation.

Due to the assumed fast surface diffusion, the surface chemical potential $\mu_{s,Li}$ is the same for all particles. It is controlled by a relation between the lithium mole fractions y^i and the electric current I,

$$Idt = -e_0 n_{FePO_4} \sum_{i=1}^{N_P} V^i dy^i .$$
⁽⁹⁾

Typically, the distance between the electrodes in a battery is smaller than $100 \,\mu$ m. Due to the high mobilities of the species in the electrode and electrolyte, the time-depending behavior of the battery is exclusively controlled by surface phenomena. Based on our general electrode-electrolyte interface theory, we are able to derive a relation for the voltage between the many-particle electrode and metallic lithium,

$$U = U_0 - \frac{1}{e_0} \mu_{s,Li} + (R_{ad} + R_{re})I.$$
(10)

Here, R_{ad} and R_{re} are resistances, which take into account the lithium adsorption from the electrolyte to the electrode surface and the electron transfer reaction Li⁺ + e⁻ = Li at the surface. The new model is capable to simulate the voltage-capacity diagram for an LFP electrode shown in Figure 12 with the particle size distribution of Figure 11. The simulation shows all features of the experimental data given in Figure 2, where only two parameters τ_0 and ν_0 have to be adjusted.

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Fig. 12: Computed voltage-capacity diagram for an LFP many-particle electrode with 7000 particles

3 IMU@WIAS



3.1 The IMU Secretariat

Lena Koch and Sylwia Markwardt

Since January 2011, the Secretariat of the International Mathematical Union (IMU) has been permanently based in Berlin, Germany, at the Weierstrass Institute. Under the supervision of the IMU Executive Committee, the Secretariat runs IMU's day-to-day business and provides support for many IMU operations, including administrative assistance for the International Commission on Mathematical Instruction (ICMI) and the Commission for Developing Countries (CDC) 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. The General Assembly 2014 in Gyeongju, Republic of Korea, appreciated the performance of the staff of the IMU Secretariat and thanked them for their dedicated work and for all their multiple contributions to the IMU.



Fig. 1: The team of the IMU Secretariat

Staff members (Figure 1):

- Alexander Mielke, *Head of the Secretariat and IMU Treasurer*. A. Mielke is a professor at Humboldt-Universität zu Berlin, Deputy Director of WIAS, and head of Research Group 1 at WIAS. In his function as the head of the secretariat he assumes the personnel responsibility for the staff. 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.
- Sylwia Markwardt, *Manager of the Secretariat*. S. Markwardt's responsibilities involve heading and supervising all administrative operations of the secretariat and actively participating 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.
- Pragnya Challapalli, *Student Assistant*. P. Challapalli's task is to assist various programs of the Commission for Developing Countries (CDC) and the International Commission on Mathematical Instruction (ICMI). (She is not in the group photo of the Secretariat.)

Helge Holden (he is not in the group photo) is the IMU Secretary. H. Holden holds a professorship at the Norwegian University of Science and Technology, Trondheim, and at the Center of Mathematics for Applications, University of Oslo, Norway. He 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 The IMU and its Role in Fostering Mathematics in the Developing World

Major challenges such as disease, hunger, climate change, environmental remediation, and energy development require strong mathematical, computational, statistical, and other quantitative skills. It has become increasingly clear that the developing world is home to a significant but largely untapped mathematical talent. This latent talent may have the potential to transform both local and international mathematical communities. A mathematically educated population is a powerful tool to spur economic development in all nations, but especially in countries that are economically disadvantaged.







Given such challenges and the opportunities for development, more support is needed for those who wish to become educators and researchers in mathematics. For the IMU, raising international mathematical literacy has been one of its major long-term goals. The IMU has maintained programs of cooperation in support of mathematical institutions and individual mathematicians, including sponsoring research travel and conference grants as well as volunteer lectures, joint research projects and capacity building projects, to take a more active role in supporting mathematics in developing countries.

During the last years, IMU has intensified its efforts to foster mathematics in the developing and economically disadvantaged countries. To improve efficiency, the IMU decided to merge its two bodies working in the field, the Commission on Development and Exchanges (CDE) and the Developing Countries Strategy Group (DCSG), into one commission, the Commission for Developing Countries (CDC) as of 2011. A considerable rate of the IMU budget is allocated for activities in developing countries. Additional grants programs have been launched, existing programs have considerably been extended. The CDC is in charge of managing all IMU initiatives in support of mathematics research and advanced mathematical teaching in developing countries; primary activities include conference support, project support, the Volunteer Lecturer Program, the Library Assistant Scheme, individual research travel grants, and public outreach activities.



Fig. 1: Photos: L. Koch, W. Dalitz, A. Pineda

Since 2011, the CDC has regularly been supporting graduate student projects in Africa, Latin America, and Asia. Supported projects include the Africa Mathematics Millennium Science Initiative (AMMSI) and the Mentoring African Research in Mathematics (MARM) program. Also the first Central American PhD program in mathematics, which was launched by the Superior Council of Central American Universities (CSUCA) in collaboration with the International Centre for Theoretical Physics (ICTP) and its member universities, is receiving support.

Mathematics teachers and teacher educator training has been supported through the Capacity and Network Project (CANP) that fosters mathematics teacher training and capacity building in developing countries. The CANP program is organized under the responsibility of the International Commission on Mathematical Instruction (ICMI). Since 2011, two-week long CANP workshops addressing teacher educators and secondary schoolteachers have been held in Mali, Costa Rica, Cambodia,



and Tanzania. Support is also provided to a project in Cambodia that will help schoolteachers use technology to enhance interactive learning among their students as well as to a teacher-training project in the Philippines, which holds intensive 10-day training programs on curriculum content and the teaching of calculus.

The CDC has partnered with the Simons Foundation (USA) and the Niels Henrik Abel Board (Norway). The IMU-Simons Travel Fellowship Program and the Abel Visiting Scholar Program support individual research visits of mathematicians professionally based in the developing world to a center of excellence in any part of the world for collaborative research in mathematics. The IMU-Simons Travel Fellowship Program covers travel and insurance cost and has no age limit. The Abel Visiting Scholar Program supports annually three early stage postdoctoral mathematicians in their professional careers. It is designed to offer the opportunity for a *research sabbatical*, a necessary complement to teaching and other academic duties for mathematicians desiring to sustain a viable research program.

The Volunteer Lecturer Program (VLP) as well as the Conference Support Program are two other successful CDC programs. The VLP offers universities in the developing world lecturers for intensive three- to four-week courses in mathematics at the advanced undergraduate or master's level. The Conference Support Program gives partial support to conferences organized in developing and economically disadvantaged countries.

The MENAO (Mathematics in Emerging Nations: Achievements and Opportunities) symposium was a milestone in IMU's activities. Organized by CDC, the symposium took place one day before the opening of the International Congress of Mathematicians 2014 in Seoul, Republic of Korea. Approximately 260 participants from around the world attended the symposium, including representatives of embassies, scientific institutions, private business, and foundations. Attendees heard inspiring stories of individual mathematicians and specific developing nations, and they were presented three regional reports about challenges and opportunities in Africa, Latin America and the Caribbean, and Southeast Asia. The reports described the status of international partnerships to support mathematical development and the current state of mathematics in these regions and pointed up new initiatives and projects in need of financial support. The MENAO event was a substantial initiative to raise awareness and build partnerships between mathematical communities, governments, international agencies, private business, and foundations.

The CDC continues to drive for funding and support from both the public and the private sector to allow the IMU to take a strong and active role in supporting mathematics in developing countries.

The IMU Web site provides more information about IMU's activities for developing countries; see http://www.mathunion.org/cdc.



3 IMU@WIAS

3.3 Events of Major Significance in 2015



Organizational structure of the Union

Committee for Women in Mathematics (CWM) established. At its meeting in March 2015, the IMU Executive Committee decided to establish a committee on women in mathematics with the official name *Committee for Women in Mathematics (CWM)*. The CWM has a chair, a vice-chair, and 6–8 members-at-large. The committee's work is governed by Terms of Reference. CWM aims at promoting international contacts between national and regional organizations for women and mathematics and to undertake other related activities. The central goal until the next ICM will be to help to establish networks of women mathematicians especially in Asia, Latin America, and Africa. CWM's Web site is at http://www.mathunion.org/cwm.

Grants

IMU won ICSU grant 2015. IMU's application to the International Council for Science (ICSU) for a €30,000 grant was successful. The grant project was entitled "Global Change Impact on Diseases and Alien Species Expansion". Supporting applicants were the International Union of Biological Sciences (IUBS), the International Union of Immunological Societies (IUIS), the International Council for Industrial and Applied Mathematics (ICIAM), the International Social Science Council (ISSC), the ICSU Regional Office for Africa (ICSU ROA), the ecoHEALTH from Future Earth, and the International Society for Biometeorology (ISB); associate partners were the African Institute for Mathematical Sciences (AIMS), the South African Mathematical Society (SAMS), the DST-NRF Centre of Excellence for Invasion Biology (CIB), and the Mathematics of Planet Earth (MPE) initiative.



Fig. 1: Meetings snapshots

Meetings

CDC meeting. The newly elected Commission for Developing Countries held its meeting at the IMU Secretariat in Berlin from March 12–13, 2015.

Joint IMU-EC and CDC meeting. The Executive Committee of the IMU and the Commission for Developing Countries held a joint meeting at the IMU Secretariat in Berlin on March 13, 2015. Main topics were the follow-up of the MENAO event and past, present, and future collaboration of

IMU/CDC. The meeting was concluded by a gathering of the members of the IMU Executive Committee, the Commission for Developing Countries, and several guests.

IMU Executive Committee meeting. The newly elected Executive Committee of the IMU held its annual meeting at the IMU Secretariat in Berlin from March 14–15, 2015.

CEIC meeting. The Committee on Electronic Information and Communication (CEIC) held its annual meeting at the IMU Secretariat in Berlin from March 21–22, 2015. The CEIC is a standing committee of the IMU Executive Committee (EC). CEIC's mandate is to advise the EC on matters concerning information and communication; see http://www.mathunion.org/ceic/.

Events

IMU Office Committee. The IMU Office Committee visited the IMU Secretariat from October 22–23, 2015. This was the Committee's first visit of the office in the period 2015–2018. The purpose of the Office Committee, which is not part of the Secretariat, is to monitor the performance of the IMU Secretariat on behalf of the IMU Executive Committee and the Adhering Organizations.

Heidelberg Laureate Forum. The third Heidelberg Laureate Forum (HLF) took place from August 23–28, 2015 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 2015 who had been awardees of the Fields Medal (FM) or the Nevanlinna Prize (NP) were: Sir Michael Francis Atiyah (FM), Shigefumi Mori (FM), Andrei Okounkov (FM), Robert Endre Tarjan (NP), Leslie G. Valiant (NP), Vladimir Voevodsky (FM), Efim Zelmanov (FM).

Guests of the IMU Secretariat. The table on the next page gives an overview of guests who visited the IMU Secretariat in 2015.

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

- IMU ICME 2020 site visits, Sydney, Australia; Honolulu, USA; Shanghai, China (L. Koch)
- ICMI IPC meeting, Hamburg, Germany (L. Koch)
- ICMI Executive Committee meeting, Macau, China (L. Koch)
- Heidelberg Laureate Forum, Heidelberg, Germany (S. Markwardt)





Fig. 2: Korean guests visiting the IMU Secretariat



Date	Guests	Event
Jan 9	Victor Buchstaber, Russia; Annalisa Buffa, Italy;	7ECM Program
	Étienne Ghys, France; Timothy Gowers, UK; Ben	Committee
	Green, UK; Peter Littelmann, Germany; Jaroslav Ne-	
	setril, Czech Republic; Walter Schachermayer, Aus-	
	tria; Kristian Seip, Norway; Sylvia Serfaty, France;	
	Saharon Shelah, Israel; Stanislav Smirnov, Switzer-	
	land; Juan S. Soler, Spain	
Jan 20	Martin Grötschel, Germany	Individual
		visit
Feb 2	Martin Grötschel, Germany	Individual
		visit
Feb 10	Martin Grötschel, Germany	Individual
		visit
March 12 – 15	Herbert Clemens, USA; Alicia Dickenstein, Ar-	CDC meeting,
	gentina; Mama Foupouagnigni, Cameroon; Bene-	joint EC-CDC
	dict H. Gross, USA; Helge Holden, Norway; Vaughan	meeting,
	Jones, New Zealand/USA; Srinivasan Kesavan, In-	IMU EC
	dia; János Kollár, USA; Shigefumi Mori, Japan;	meeting
	Wandera Ogana, Kenya; Alf Onshuus, Colombia;	
	Hyungju Park, Korea; Angel Pineda, USA/Honduras;	
	Christiane Rousseau, Canada; Budi Nurani Ruch-	
	jana, Indonesia; Angel Ruiz, Costa Rica; Vasudevan	
	Srinivas, India; Polly Sy, Philippines; John Toland;	
	UK; Wendelin Werner, Switzerland	
March 21 – 22	Thierry Bouche, France; Olga Caprotti, Sweden; Tim	CEIC meeting
	Cole, USA; James Davenport, UK; Carol Hutchins,	
	USA; Patrick Ion, USA; Masakazu Suzuki, Japan;	
	Wendelin Werner, Switzerland	
April 28	Marie-Francoise Roy, France	CWM
June 21 – 25	Guillermo Curbera, Spain	IMU Archive
July 9	Levis Eneya, Malawi	Individual
		visit
Sep 3	Dosang Joe, Republic of Korea; Sue Seungyeon Lee,	Individual
	Republic of Korea; Youngho Woo, Republic of Korea	visit
	(Figure 2)	
Oct 22 – 23	Bernard Hodgson, Canada; Ragni Piene, Norway;	IMU Office
	John Toland, UK; Wendelin Werner, Switzerland	Committee
Oct 29	Stefan Eichler, Germany; Andreas Greven, Ger-	WIAS Scien-
	many; Barbara Kaltenbacher, Austria; Barbara Niet-	tific
	hammer, Germany; Felix Otto, Germany; Markus	Advisory
	Reiß, Germany; Barbara Wohlmuth, Germany	Board
Nov 12 – 13	Caroline Series, UK	IMU working
		group

4 Research Groups' Essentials



- RG 2 Laser Dynamics
- RG 3 Numerical Mathematics and Scientific Computing
- RG 4 Nonlinear Optimization and Inverse Problems
- RG 5 Interacting Random Systems
- RG 6 Stochastic Algorithms and Nonparametric Statistics
- RG 7 Thermodyn. Modeling & Analysis of Phase Transitions
- YSG Modeling of Damage Processes
- 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 suitable coupled systems
- Multiscale methods for deriving effective large-scale models from models on smaller scales, including models derived from stochastic particle systems
- Existence, uniqueness, and regularity theory for initial and boundary value problems in nonsmooth 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 gives a considerable impact on the construction of efficient numerical algorithms. In cooperation with other research groups, corresponding software tools are under development that will enable parameter studies or the optimization of technological devices.

Semiconductors

In the field of the mathematical treatment of semiconductor device problems, the group is involved in several third-party-founded projects. The physical Collaborative Research Center SFB 787 *Semiconductor Nanophotonics: Materials, Models, Devices* was under review in June 2015 and received a very positive recommendation. In particular, the subproject B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters", jointly with RG 2 Laser Dynam*ics* and the Zuse Institute Berlin, will continue for another four years starting from January 1, 2016.

Two MATHEON projects funded by ECMath (Einstein Center for Mathematics Berlin) are currently in the middle of their three-year term. For the subproject D-OT1 "Mathematical modeling, analysis, and optimization of strained germanium microbridges", which is a joint project with the Humboldt-Universität zu Berlin, see the Scientific Highlights article on page 20.

OLEDS. The MATHEON subproject D-SE2 "Electrothermal modeling of large-area organic lightemitting diodes" is carried out in close cooperation with the Institut für Angewandte Photophysik (TU Dresden). The aim is to study new device concepts based on organic semiconductors from a mathematical viewpoint; see [3]. In particular, new mathematical models for these devices were derived and investigated concerning their analytical properties. Moreover, the fundamental operation mechanisms as well as limiting factors for the performance of organic permeable base and



Fig. 1: Electron density in organic permeable base transistor for different applied base potentials



Fig. 2: Characteristics of an organic permeable base transistor for variations of base-opening radius r



vertical field-effect transistors were discovered by simulating the charge carrier transport; see Figures 1 and 2.



Fig. 3: Numerical solutions of p(x) Laplace equation in 2D for a discontinuous exponent p

New lighting concepts using large area-emitting organic LEDs are nowadays introduced as an alternative to conventional solid-state lighting. However, the higher brightness that is important in this application is accompanied by substantial self-heating due to high currents and unpleasant inhomogeneities in the luminance. In MATHEON subproject D-SE2, the interplay between current flow and heat conduction is described on a phenomenological level by a partial differential equation (PDE)-based thermistor model consisting of a current-flow equation and the heat equation with Joule heating. Motivated by a discrete equivalent circuit model, the PDE system in [3] is based on a p(x) Laplacian structure of the current-flow equation with an in general discontinuous exponent p, which takes into account different current-voltage (power) laws in subregions of the device.

The model was discretized using a finite volume scheme (see [3]) and implemented in the WIAS toolbox pdelib in close cooperation with RG 3 *Numerical Mathematics and Scientific Computing*. The two main difficulties are the intrinsic instability due to regions of negative differential resistance and voltage turnover points in the characteristics (see Figure 4) and the derivation of suitable discretization schemes for the p(x) Laplace operator. The former can be resolved by using numerical path-following methods, and the latter is based on a hybrid finite element / finite volume approach. Figure 3 shows solutions of the p(x) Laplace equation $-\nabla \cdot (|\nabla u|^{p(x)-2}\nabla u) = f$ with constant right-hand side, homogeneous Dirichlet boundary conditions, and different piecewise constant exponents p(x).

Methods in mathematical physics. One of the aims of RG 1 *Partial Differential Equations* and in the ERC project "Analysis of Multiscale Systems Driven by Functionals" (AnaMultiScale) is to further develop mathematical methods inspired by applications from nano- or optoelectronics. From the physical point of view, many of these methods are motivated by quantum mechanics, while from the mathematical point of view they are closely related to operator theory on Hilbert spaces. Several aspects of this theory were addressed in a series of publications this year. A model of a light-emitting diode was considered in [1]. Moreover, the point spectrum of a Hamiltonian describing photon-electron interaction with any coupling constant was studied, and mathematical methods for the point spectrum of point interactions were developed. These results have application to the Landauer–Büttiker formula, which is widely used in quantum transport.

A second topic in this area is the derivation of GENERIC and damped Hamiltonian systems from microscopic Hamiltonian systems. For the quantum case, the focus lies on effective evolution



Fig. 4: Simulation of current-voltage characteristics for OLEDs for varying conductivities



European Research Council Established by the European Commission



Fig. 5: Simulation of temperature distribution in current-induced steel hardening

equations for the reduced density operator that fulfill the basic principles of thermodynamics. For special cases, nonlinear equations can be derived, which do not belong to the class of Lindblad equations that are frequently used to model dissipative quantum systems.

Applications of regularity theory in optimization. The investigation of the van Roosbroeck system in three space dimensions as well as of the three-dimensional thermistor problem has been a challenge for many years; this investigation concerns questions of existence, uniqueness, and regularity, including realistic geometries, discontinuous dielectric permittivity functions, and mixed boundary conditions. Based on equivalent reformulations of these two problems as quasilinear parabolic equations, recent results on maximal parabolic regularity and on optimal elliptic regularity [2] were used to solve these systems. The research on the thermistor problem is carried out in collaboration with Christian Meyer (TU Dortmund) and Hannes Meinlschmidt (TU Darmstadt) and includes optimal control via adjusted voltage as well as numerical simulations for steel hardening in cooperation with RG 4 *Nonlinear Optimization and Inverse Problems*.

Delay and networks

Networks of coupled dynamical systems form an important class of spatially extended systems that are used in many applications. In neural networks, neurons are considered as nodes, and synaptic connections form the links between the nodes. One of the fundamental adaptation mechanisms of the nervous system is spike-time-dependent plasticity (STDP); depending on the spiking behavior, plasticity regulates the coupling between individual cells and controls the network connectivity. Jointly with the Institute of Neuroscience and Medicine (Research Center Jülich), ensembles of synchronized spiking neurons with adaptive coupling were studied, which are perturbed by random inputs; cf. [4]. For such networks, the phenomenon of self-organized resistance to noise has been reported that is characterized by an increase of the overall coupling and preservation of synchrony in the neural populations with STDP in response to the external noise growth.





The influence of noise on the microscopic level was studied by considering only two coupled neurons; cf. [4]. Adopting a phase description for the neurons and using the Fokker–Planck formalism, the problem was reduced to a two-dimensional system, which describes the averaged dynamics of the coupling strengths. It could be shown that a multistability of several coupling configurations is possible, some of which are not found in systems without noise, such as a strong bidirectional

coupling; see Figure 6. This result backs the finding that increased noise can be the reason for an antagonistic response of the system and the increase of the average coupling. This mechanism, as well as a high potential for multistability, is also demonstrated numerically for a coupled pair of Hodgkin–Huxley neurons.

In this area, two Ph.D. theses have been successfully defended: Jan Philipp Pade "Synchrony and bifurcations in coupled dynamical systems and effects of time delay" and Leonhard Lücken "Patterns of activity in coupled systems with applications to neuronal dynamics".

Material modeling

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*.

Homogenization of Cahn–Hilliard-type equations. Within the subproject "Pattern formation in systems with multiple scales" of the Collaborative Research Center SFB 910 *Control of Self-Organizing Nonlinear Systems*, Sina Reichelt successfully defended her Ph.D. thesis "Two-scale homogenization of systems of nonlinear parabolic equations" in November 2015. Besides other homogenization results, this thesis treats Cahn–Hilliard-type equations with coefficient functions, which oscillate on the microscopic level, to derive effective macroscopic systems via two different methods from evolutionary Γ -convergence. These two abstract approaches were developed in the ERC project "AnaMultiScale", namely (i) the more general, but less precise, energy dissipation principle and (ii) the more restrictive method involving evolutionary variational inequalities. The comparison of the two methods is highlighted by illuminating the different assumptions needed and the different results obtained.

Diffuse interface models for complex fluids. A very effective approach describing the interaction of two fluids is based on the use of *diffuse-interface models* in which the sharp interface separating the two fluids is replaced by a region where a partial mixing is admitted, leading, from the analytical viewpoint, to the introduction of a suitable order parameter, the dynamics of which is described by a nonlinear evolution equation (e.g., of Cahn–Hilliard type). These models, which are based on Ginzburg–Landau theory of phase transitions, simplify the mathematical treatment of the interaction with respect to the sharp-interface models and lead to major advantages for numerical analysis. Moreover, these models are successfully employed in many applications, e.g., from phase separation of fluids to liquid crystals and to tumor dynamics. In collaboration with ERC Group 2 *Entropy Formulation of Evolutionary Phase Transitions*, the following subjects were studied:

(i) Nonlocal models for flow and phase separation of binary mixtures of incompressible fluids. In

particular, the case where the two fluids have different densities was addressed, and existence of dissipative global-in-time weak solutions was established for the case of singular double-well potentials and nondegenerate mobilities; cf. [5]. Moreover, for the "matched-densities case", the analysis from the point of view of regularity and optimal control was performed in the physically relevant situation of singular potentials and degenerate mobilities.

(ii) Models for tumor growth. An optimal control analysis was developed for the model due to Hawkins-Daarud, van der Zee, and Oden, where the control is taken in the nutrient source on the boundary of the domain where tumor and healthy cells coexist.

Free-boundary problems for thin film flows. Another topic studied is the gradient structure of free-boundary problems, in particular of degenerate fourth-order parabolic problems of the form

$$\partial_t u = \nabla \cdot \left(u^\alpha \nabla \left(\frac{\delta E}{\delta u} \right) \right), \quad \text{where } E(u) = \int_{\mathbb{R}^d} \frac{1}{2} \| \nabla u \|^2 + \chi_{\{u > 0\}} \, \mathrm{d}x. \tag{1}$$

The resulting PDEs are relevant in thin film flows over a substrate, where u has the interpretation of a film thickness. This equation is a free-boundary problem because it is natural to consider the set $\omega = \{x \in \mathbb{R}^d : u > 0\}$ as parts of the unknowns in (1). A novel algorithm for problems of this type was developed in [6], and an exemplary solution is shown in Figure 7. The main problem here is to properly resolve the singularity in $\nabla(\delta E/\delta u)$ as $u \to 0$ at the boundary of ω .

Further highlights of 2015

Since April 2015, the former WIAS Director Professor Jürgen Sprekels has been an External Member of WIAS and affiliated with this research group.

In November 2015, the book *Rate-Independent Systems: Theory and Application* was published by Springer Verlag, New York. It is the result of a long-term collaboration of Alexander Mielke and Tomáš Roubíček, which was started in late 2007 and which profited from regular one-month visits of the second author to WIAS. On its 660 pages, this monograph provides a comprehensive and systematic treatment of rate-independent systems for the first time. The focus is mostly on fully rate-independent systems, first on an abstract level and then on the level of various applications in continuum mechanics of solids. Selected applications are accompanied by numerical simulations illustrating both, the models and the efficiency of computational algorithms.



Three minisymposia at ICIAM 2015 organized by members of RG 1. The International Congress of Industrial and Applied Mathematics took place in Beijing on August 10–14, 2015. Three researchers contributed to the ICIAM 2015 in Beijing with the organization of minisymposia in three different research fields.

The motivation for the ICIAM 2015 minisymposium "Recent Progress in Modeling and Simulation of Multiphase Thin-film-type Problems" organized by Dirk Peschka and Li Wang (UCLA) was to discuss new developments in applications and in the mathematics of thin-film-type problems of multiphase systems. The four talks were devoted to problems with surfactant transport, suspension



Fig. 7: Solution of (1) with

 $\alpha = 2$ close to a pinch-off

 $(u \equiv 0 \text{ in the blue region})$

flows, or flows over liquid substrate, focusing on the thermodynamically consistent statement of such problems via gradient flows and the correct modeling of the underlying microscopic physics.

The minisymposium "Analysis of Nonsmooth PDE Systems with Applications to Material Failure" was organized by Dorothee Knees (Kassel) and Marita Thomas and consisted of eight talks. It brought together scientists from the fields of modeling, analysis, and numerics to discuss analytical methods and numerical strategies, both for (quasi-)static and rate-dependent, non-smooth failure models.

The minisymposium "Numerical and Analytical Aspects in Semiconductor Theory" organized by Nella Rotundo and Wil Schilders (TU Eindhoven) aimed at providing insights on recent mathematical advances on semiconductor theory. The four talks covered analytical results as well as numerical methods and approaches to optimization for edge-emitting heterostructures.

Gesellschaft für Angewandte Mathematik und Mechanik. In the period 2013–2015 Marita Thomas was a member of the GAMM Juniors, and in 2015, she was their elected speaker. The GAMM Juniors are representatives of young scientists in Applied Mathematics and Mechanics, who foster their scientific fields within the academic research and the society. Their activities include the contribution to the Committee "Future of GAMM" to support young researchers' activities, the organization of interdisciplinary workshops and summer schools (SAMM) for young scientists, and the establishment of networking among young researchers in the GAMM. In this context, Marita Thomas and Jan Giesselmann (Stuttgart) organized the summer school "SAMM 2015 – Materials with Discontinuities", see page 115. Since October 2015, Marita Thomas has also been an officer in the board of the GAMM activity group "Analysis of Partial Differential Equations".

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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 2015 within the Research Center MATHEON (subproject D-OT2 "Turbulence and extreme events in nonlinear optics"), the DFG individual grant "Ab-initio description of optical nonlinearities in femtosecond filaments", the Marie Curie Initial Training Network PROPHET, the BMBF-supported project MANUMIEL between the Technical University of Moldova, the Ferdinand Braun Institute for High Frequency Technology (FBH), Berlin, and WIAS, as well as the 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". A particular highlight was the excellent evaluation of the DFG Collaborative Research Center SFB 787 *Semiconductor Nanophotonics: Materials, Models, Devices*. Based on the positive decision of the DFG, the group will be able to continue its research within the subprojects B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters" (jointly with the 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".

Dynamics of semiconductor lasers

On the basis of a hierarchy of models that range from nonlinearly coupled systems of wave and diffusion equations, delay-differential equations (DDEs), and ordinary differential equations (ODEs), dynamical phenomena of a variety of semiconductor-based emitters were investigated. A selection is presented below.

Mode-locked semiconductor lasers (MLL) are attractive for many applications, because they are compact sources for trains of short optical pulses with a high repetition rate. A semi-analytical method of calculating the timing fluctuations in MLL was developed and applied to study the effect of delayed coherent optical feedback on pulse timing jitter in these lasers [1]. The proposed method greatly reduces computation times and therefore allows for the investigation of the dependence of timing fluctuations over greater parameter domains. It was shown that resonant feedback can reduce the timing jitter and that a frequency-pulling region forms about the main resonances where a timing jitter reduction is observed. The width of these frequency-pulling regions increases linearly with feedback delay times. An analytic expression for the timing jitter was derived that predicts a monotonic jitter decrease for resonant feedback of increasing delay lengths.

Furthermore, using a DDE model, the dynamics of a semiconductor laser with one active cavity coupled to an external passive cavity was investigated; see Figure 1. Numerical simulations indicated



Fig. 1: Schematic of a laser with one active cavity coupled to an external passive cavity, R.M. ARKHIPOV, A. AMANN, A.G. VLADIMIROV, Pulse repetition-frequency multiplication in a passively mode-locked semiconductor laser coupled to an external passive cavity, *Appl. Phys. B*, **118** (2015), pp. 539–548.

that, when the coupling between the two cavities is strong enough and the round-trip time of the active cavity is an integer multiple of the round-trip time of the passive cavity, the pulse repetition frequency of the laser can be increased as a result of synchronization with the inverse round-trip time of the external passive cavity. The electric field amplitude sensitively depends on the relative phase between the electric fields in both cavities, giving rise to this resonance behavior.

High-power semiconductor lasers with spatio- and temporal modulated electrical injection, see Figure 2, were studied jointly with Kestutis Staliunas (UPC Barcelona), with special attention to the improvement of the lateral beam shaping. For this, a (2+1)-dimensional traveling wave (TW) model and its reduction to a (1+1)-dimensional linear Schrödinger equation with a periodic potential and a coupled-mode system describing the evolution of the most important Bloch-mode components of the optical field were studied. In particular, in [2], the stabilization of vertical external cavity surface-emitting semiconductor lasers (VECSEL) by spatio-temporal modulation of the injection was investigated, by performing a Floquet stability analysis of the (1+1)-dimensional system of coupled paraxial equations for optical field and carrier density, including periodic modulation. Thereby, conditions were identified that allow to suppress the modulation instability, which is a common origin of the irregular behavior in high-power semiconductor lasers.

External-cavity diode lasers (ECDLs) are compact sources with potential narrow linewidth emission, the control and stabilization of which received considerable attention. The coexistence of multiple stable steady states in such lasers was investigated in [3] (joint work with Vasile Tronciu (TU Moldova), Hans Wenzel (FBH Berlin), and Andreas Wicht (Humboldt-Universität zu Berlin) in the frame of the MANUMIEL project), where the concept of longitudinal modes of the (1+1)-dimensional TW system was extensively exploited. An algorithm was presented allowing to calculate instantaneous longitudinal optical modes in nearly arbitrary coupled laser configurations.

Single-photon sources based on semiconductor quantum dots enable many interesting applications in the fields of quantum cryptography, quantum computing, and quantum metrology. In colaboration with RG 1, mathematical models to describe the complex physical processes from charge transport to radiative carrier recombination are in the center of interest for this novel type of optoelectronic devices. The group's approach involves the coupling of the van Roosbroeck system to dissipative open quantum systems and elements of quantum-mechanical many-body theory. Within the SFB 787, the group collaborates with research groups from TU Berlin (Dieter Bimberg, Stephan Reitzenstein, Andreas Knorr). In this framework, significant contributions towards the performance enhancement of particular devices based on the group's simulation results were already made; see Figure 3.

Pulses in nonlinear optical media

An important event in 2015 was the workshop "Waves, Solitons and Turbulence in Optical Systems" (WASTOS 2015), organized with the support of the Einstein Center for Mathematics Berlin, Research Center MATHEON, which aimed at bringing together applied mathematicians, theoretical



Fig. 2: Schematic of a broad-area amplifier with spatially modulated contact, from M. RADZIUNAS, R. HERRERO, M. BOTEY, K. STALIUNAS, Far-field narrowing in spatially modulated broad-area edge-emitting semiconductor amplifiers, J. Opt. Soc. Am. B, **32**:5 (2015), pp. 993–1000.



Fig. 3: Schematic cross section of a single-photon emitter, from M. KANTNER, U. BANDELOW, TH. KOPRUCKI, J.-H. SCHULZE, A. STRITT-MATTER, H.-J. WÜNSCHE, Efficient current injection into single quantum dots through oxide-confined pn-diodes, WIAS Preprint no. 2169, 2015.

and experimental physicists to discuss recent advances concerning experimental findings and theoretical investigation of such dynamical phenomena as optical wave turbulence, optical solitons and rogue waves, supercontinuum generation, spatio-temporal dynamics in active and passive optical cavities, and effects related to the control of optical systems by delayed feedback.



Fig. 4: Participants of the workshop WASTOS 2015

Rogue waves, which have long been considered a seafarer's yarn, now appear to be a generic dynamical behavior observed in nonlinear hydrodynamical, optical, or quantum-mechanical systems. A wave qualifies as rogue if it appears out of nowhere and vanishes without a trace, and if it exceeds the system's significant wave height at least twice. While the first criterium seems to indicate that rogue waves are completely stochastic and unpredictable, the group found evidence for deterministic chaotic behavior in the dynamics of rogue waves, both in the ocean and in optical multifilaments. This could allow to estimate the limits of predictability of these potentially harmful events.



Fig. 5: Recorded time series of different rogue wave supporting systems: optical multifilaments (a), oceanic Draupner event (b), nonlinear optical fiber (c), cf. S. BIRKHOLZ, C. BRÉE, A. DEMIRCAN, G. STEINMEYER, Predictability of rogue events, Phys. Rev. Lett., **114** (2015), pp. 213901/1–213901/5.

Solitons are attractive long-living objects that naturally appear in nonlinear systems. On the basis of a Hamiltonian framework for short optical pulses [4], an adiabatic theory for solitons interacting with dispersive waves was formulated. The theory uses a wide spectrum of methods borrowed from quantum mechanics, optics, and nonlinear dynamics, and made it possible to control solitons in a predictable way using the so-called *optical event horizons*.

The formation of planar solitons (strong confinement) in microcavity polaritonic waveguides was also studied. In particular, the conditions for the existence of solitons in the presence of modulational instability and multistability originating from co-existence of different transverse modes were investigated. Finally, soliton propagation in tilted waveguides could be demonstrated, where a critical tilt angle for the soliton propagation was found.

Dynamical systems

The research in the mathematical field of dynamical systems is devoted to mathematical theory and methods that are related to the applied research on nonlinear optics and optoelectronics . In 2015, the main focus was on delay-differential equations and systems of coupled oscillators.

In collaboration with RG 1, a rigorous derivation of the Ginzburg–Landau equation as an amplitude equation for delay-differential equations with large delay was obtained. This result represents another cornerstone in the mathematical theory of delay-differential equations with large delay, which is an essential tool for various problems in optoelectronics; see the Scientific Highlights article on page 25..

In the field of coupled oscillators, the research was continued on self-organized patterns of coherence and incoherence in systems of coupled oscillators, so-called *chimera states*. It was shown that, in addition to the well-elaborated approach of studying chimera states in the framework of the continuum limit $N \to \infty$, there is also a way to study their emergence for small N by methods of classical dynamical systems theory. Slightly modifying the nonlocal coupling scheme with a global feedback on the phase-lag parameter drastically enhances the stability of chimera states without otherwise significantly changing them, and thus they can be traced down to a very small system size [5].



Fig. 6: Regular and irregular excitation patterns in a system of nonlocally coupled oscillators

Pursuing this approach, it can be shown that chimera states, which have been described in large

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systems as a single, statistically stationary regime, in small systems transform into a huge variety of regular or irregular self-localized patterns; see Figure 6. The variety of different patterns is organized in a complex bifurcation scenario including transitions between regular dynamics and chaos by period-doubling cascades, torus breakup, and intermittency.

Moreover, the transition to synchrony in a one-dimensional array of oscillators with nonlocal coupling was studied. 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. Then, a collective macroscopic chaos appears as an intermediate stage between complete incoherence and stable partially coherent plane waves. The emerging chaos exhibits a transition from phase turbulence to amplitude turbulence.

Also mathematical problems related to ecological systems were studied. In particular, the existence of multiple stable equilibrium states, which are possible in real-life ecological systems (e.g., the so-called *predator pit* phenomenon), was investigated. In order to verify the hypothesis that such a multitude of equilibrium states can be caused by the adaptation of animal behavior to changes of environmental conditions, a simple predator-prey model was considered where the prey changes its behavior in response to the pressure of predation. This model exhibits two stable coexisting equilibrium states with basins of attraction separated by a separatrix of a saddle point [6].

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

RG 3 studies the development of numerical methods and their numerical analysis. Software for the numerical solution of partial differential equations and differential-algebraic systems is implemented. Many of the research topics have been inspired by problems from applications. Below, a selection of research topics of the group will be described briefly. Further topics include the numerical analysis of convection-dominated problems, the simulation of gas turbines (in collaboration with Research Group RG 6 *Stochastic Algorithms and Nonparametric Statistics*), of problems from hemodynamics, of population balance systems, uncertainty quantification (in collaboration with Research Group RG 4 *Nonlinear Optimization and Inverse Problems*), reduced-order modeling, and the development of algorithms for anisotropic mesh generation.

Mixed-element mesh generation for complex geometrical models

The objective of this research topic is to develop a mixed-element (tetrahedrons, prisms, pyramids) mesh generation method for complex geometrical models, such as those encountered in geological modeling. Depending on the method used to build a three-dimensional geological model, and on the exact purpose of this model, its mesh must be adapted so that it satisfies criteria on element types, maximum number of elements, and mesh quality. Meshing methods developed for other applications than geomodeling forbid any modification of the input model. These modifications are desirable in geomodeling to better locally control the type of element built and their quality, and globally control the number of elements. Geological models indeed contain small features such as very thin layers, tangential angle contacts that can very efficiently be meshed with quadrilaterals and prisms instead with over-refined triangles or tetrahedrons.

The group's approach is based on the surface remeshing method proposed in [6], which was granted the Computers & Geosciences Best Paper Award of 2014. The method relies on two key ideas: (1) the use of a well-shaped Voronoi diagram to subdivide the model and (2) combinatorial considerations to build mesh elements from the connected components of the intersections of the Voronoi diagram with the geological model entities. This approach allows modifications of the input model, a crucial point for meshing geological models whose level of detail is very different from the level of detail desired for the mesh.

One point of focus is the formalization of the rules to build the mesh elements, allowing to determine the area in which prisms, pyramids, and tetrahedrons can be built with this method and the area where using another mesh generator, such as Tetgen would be more appropriate. Future work will be devoted to validating the generated meshes with real application cases and evaluating their quality for geomechanical finite element computations. Since the implementation of that method is a key step on which the applicability of the method to real data sets depends, an important part of the work consists in implementing the C++ RINGMesh open-source programming library to load, checking the validity, and saving three-dimensional geological structural models built by geomodeling software [5]. This research project is a collaboration with the RING team in



Nancy (https://www.ring-team.org/) and it is funded in the framework of a cooperation with TOTAL E&P, France.

Fig. 1: Synthetic geological model remeshing at several resolutions, i.e., with varying Voronoi seed number, from [6]



Fig. 2: Comparison of accuracy between the 1973 Crouzeix–Raviart (CR) mixed finite element method versus the new pressure-robust Crouzeix-Raviart element (CR^+) [3] for an incompressible Stokes problem with $v = 10^{-3}$. Comparison of H^1 error. *The new pressure-robust* Crouzeix-Raviart element is about ten refinement levels more accurate, which is a computational speedup by roughly a factor of 10^6 .

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Towards pressure-robust solvers for the incompressible Navier–Stokes equations

The simulation of flow problems is daily routine in meteorology, engineering, and science. Mathematically, a major breakthrough was the construction of mixed finite element methods for the incompressible Navier–Stokes equations in the early 1970s, which enabled the construction of provably convergent discretizations for incompressible flow problems. Flow solvers based on mixed finite element methods compute approximations of the flow field and the pressure in a fluid.

Despite this indisputable success, mixed finite element methods for the incompressible Navier– Stokes equations do not behave in a really robust manner [3]. For typical flow problems at medium or high Reynolds numbers, i.e., when the inertial forces in the fluid are large with respect to friction forces, the error between the correct and the simulated flow field can be arbitrarily large—even if the velocity field could be very well approximated in the given finite element space.

Recent research at the Weierstrass Institute [3, 4] allows now to fix an important issue of many classical mixed discretizations, which have been proposed in the last forty years. Classical discretizations compute inaccurate velocity fields whenever the pressure gradient is large compared with the friction forces. In effect, these discretizations are not pressure-robust at medium or high Reynolds numbers. They provide accurate approximations of the velocity field only if simultaneously the pressure is very well approximated. In contrast, pressure-robust mixed finite element methods computed accurate velocity fields independently of the resolution of the pressure! In terms of the finite element error analysis, the velocity error of pressure-robust mixed methods is independent of the pressure. Interestingly, for more than thirty years the construction of pressure-robust discretizations based on mixed finite element methods for the incompressible Navier–Stokes equations was considered to be practically impossible.


Fig. 3: Comparison of accuracy between the 1973 Crouzeix–Raviart (CR) mixed finite element method versus the new pressure-robust Crouzeix–Raviart element (CR⁺) [3] for an incompressible Stokes problem with $v = 10^{-3}$. Comparison of velocity isolines.

The key observation made at the Weierstrass Institute is that discretizations that are not pressurerobust do not strictly comply with a fundamental principle of vector analysis: divergence-free forces in the Navier–Stokes equations balance only with divergence-free forces, and irrotational forces balance only with irrotational forces [3]. Choosing the velocity test functions in a more sophisticated manner than usual allows to transform all known mixed finite element methods with discontinuous pressure spaces for the incompressible Stokes and Navier–Stokes equations to pressure-robust discretizations [4], provided the underlying grids are built of triangles in two or tetrahedra in three space dimensions. Moreover, current research indicates that this novel approach seems to allow the construction of pressure-robust counterparts for all inf-sup stable mixed finite element methods. The traditional belief that pressure-robust mixed methods are nearly impossible to construct is proved to be wrong. Since the robustness properties of flow solvers based on mixed finite element methods are greatly improved with this new approach, an important impact on computational fluid dynamics seems to be in reach in the near future. Potential applications comprise, e.g., coupled flow processes and meteorology.

Numerical methods for transport and reaction in semiconductors and electrochemical systems

Detailed macroscopic 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 homogeneus reactions. The densities of the charged particles influence the electric field via the Poisson equation for the electrostatic potential. Classical models and their numerical realization mostly assume Boltzmann statistics for the dependency of particle densities on the chemical potential, leading to unphysically high densities in electrolytes, organic semiconductors, and other systems. In the field of semiconductors, different variants of Fermi and Gauss–Fermi statistics and their approximations are known to give correct answers. For electrolytes, the WIAS Research Group RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* and Leibniz Group LG 3 *Mathematical Models for Lithium-ion Batteries* recently developed a model that includes finite particle volumes, solvation shells, and the contribution of the solvent.

Classically, the Scharfetter–Gummel upwind finite volume method has been used successfully as a space discretization that in the case of thermodynamic equilibrium allows to obtain stationary

solutions for the time-dependent drift-diffusion system that are identical to those of the reduced nonlinear Poisson system describing the equilibrium case. The necessary generalizations of this scheme for the described more general dependencies between chemical potential and densities are under investigation. In this context, based on an averaging of activity coefficients, a method was proposed that allows to obtain simulation results for the newly developed models of LG3 [1], at the same time 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 as part of its research initiative on energy storage systems. This approach, along with other methods is being investigated in an assessment of different possibilities for the generalization of the Scharfetter–Gummel scheme for general carrier statistics [2] (see also Figure 4), as part of a joint effort of the research groups RG 1 *Partial Differential Equations*, RG 2 *Laser Dynamics*, and RG 3 to develop the next generation of semiconductor simulation codes of WIAS.



Fig. 4: Electron (left) and hole (right) density in an oxide-confined pn-diode in low-injection regime

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4.4 Research Group 4 "Nonlinear Optimization and Inverse Problems"

The research group 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 non-smooth 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 the research groups RG 3 *Numerical Mathematics and Scientific Computing* and RG 6 *Stochastic Algorithms and Nonparametric Statistics*, the group investigates direct and inverse problems for partial differential equations (PDEs) with uncertain coefficients. A special highlight of these activities was the organization of the workshop "Direct and Inverse Problems for PDEs with Random Coefficients", November 9 – 13, 2015, together with RG 3. Sixty-eight participants from ten countries discussed various topics related to the analysis and numerical treatment of PDEs with stochastic data: efficient numerical methods for the direct problem, control problems with uncertainties, sparse and low-rank tensor representations, and inverse problems with random data.

Last but not least, the group succeeded in acquiring a grant in the European Industrial Doctorate (EID) programme in the Marie Skłodowska-Curie actions of the EU. With its research funding of 2.1 million euros, the project "MIMESIS – Mathematics and Materials Science for Steel Production and Manufacturing" is an interdisciplinary and intersectoral Ph.D. program between applied mathematics and materials science for eight Ph.D. students. Further partners in the project are the University of Oulu, the Berlin Mathematical School, and three industrial companies from Norway and Finland.

In the following, selected scientific achievements of the research group in 2015 are detailed.

Inverse problems

Scattering phenomena arise in many fields of application, e.g., in acoustics, for electromagnetic fields in nano- and micro-optical elements, and in seismology. They can be employed, e.g., for the design of diffractive devices, for the testing of materials, measurements, and for the exploration of natural sources. Though the uniqueness of inverse scattering solutions is tacitly used in many applications, a proof or disproof is quite complicated and is possible, in general, only under simplifying assumptions. In [3], it has been proved, e.g., that acoustically penetrable obstacles with corners or edges scatter every incident wave nontrivially. Moreover, the shape of a convex penetrable scatterer of polyhedral or polygonal type can be uniquely determined by the far-field pattern over all observation directions incited by a single incident plane or point source wave.

To simulate diffractive gratings and other nano- and micro-optical elements, scalar methods like, e.g., ray-tracing are increasingly replaced by electromagnetic approaches. Such a field-tracing requires the electromagnetic simulation of the scattering of general time-harmonic electromagnetic fields (cf. Figure 1) by micro-optical devices. The approach for diffractive gratings is based on the approximation of the incidence field by plane waves, the numerical solution of the corresponding **Fig. 1:** Diffraction pattern of a chromium mask illuminated by a plane wave (left), a Gaussian beam (middle), and a beam through a circular hole (right) diffraction problems, and the superposition of the obtained plane wave solutions. But the methods for plane wave approximations described in the engineering literature are not efficient. Here, mainly uniformly distributed incidence angles are used as approximating nodes, leading to inefficient algorithms and rather inaccurate solutions.



A new adaptive algorithm was developed and implemented, which allows the computation of diffracted fields up to a prescribed accuracy. It is based on the application of Floquet–Fourier techniques to transform the Maxwell equations for the grating problem with general three-dimensional incidence fields to systems of Helmholtz equations with quasi-periodic incidence, which depend on two parameters. Those problems can be solved efficiently by a modification of the existing integral solver for conical diffraction. Then, the approximation of the diffracted fields can be obtained from the solution of general conical diffraction problems for suitably chosen parameters. An optimal choice of these parameters is unknown, it depends on the illumination, the non-smooth behavior of the diffracted fields, and the underlying grating structure. Therefore, an adaptive strategy was developed that applies and extends ideas from cubature methods for two-dimensional integrals.

For the simulation and reconstruction of complex periodic and doubly periodic surface structures, a fast and storage-saving numerical method is needed. In particular, the treatment of aperiodic rough surfaces or of geometries including stochastic details can be realized by periodic computations over large periods. Another application of such a method is to provide the computational basis for the in-situ measurement to control semiconductor processing in modern factories. To this end, a scattering matrix algorithm (SMA) was implemented, which, purging through the geometry sliced in the direction orthogonal to the surface, avoids the solution and storage of huge global matrices. The purging is organized by a stable recursion, and the integration of the differential equation inside the slices w.r.t. the purge direction is realized by a predictor-corrector scheme. Altogether, the approach is efficient for deep surface structures. In order to prepare the solution of inverse problems, a new variant of the SMA was considered, based on the computation of shape derivatives. The most time-consuming parts, eigenvector decomposition and inversion of fully populated matrix blocks, are the same as for the SMA without shape derivative.

Optimization and optimal control

The research group continued its intensive work in the domains of stochastic and non-differentiable optimization. The focus of 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* was laid on the efficient computation of the probability of demand satisfaction in stationary gas networks [5]; see also Figure 2.

Connected with this work, the supervision of a Ph.D. project – financed for one year by a young researchers grant of TRR 154 – was initiated. At the same time, a research project within the *Gaspard Monge Program for Optimization and Operations Research* funded by the *Jacques Hadamard Mathematical Foundation* (Paris) could be acquired for one year (with possible extension to three years). Here, the research topic is the derivation of (sub-) gradient formulae for possibly non-smooth probability functions with potential applications to hydro-power management. Apart from intensifying the existing collaboration with Electricité de France, this project is accompanied by the cosupervision of a Ph.D. project with the Center of Mathematical Modeling (CMM) at the University of Santiago de Chile. On the algorithmic side, the implementation of SQP-based solution approaches for probabilistic programming was extended to bilinear probabilistic constraints and estimates for the optimal value were provided.

In the area of non-differentiable optimization, substantial progress was made in the characterization of the calmness property for solution maps to linear programs. This progress is reflected by two recent publications (e.g., [2]), which are the output of an ongoing collaboration with partners from the Universities of Elche and Alicante (Spain).

In collaboration with the Young Scientists' Group *Modeling of Damage Processes*, a phase field model for damage processes in two-dimensional viscoelastic media with non-homogeneous Neumann data describing external boundary forces was investigated [4]. The main difficulty is caused by the irreversibility of the phase field variable, which results in a constrained PDE system. The global-in-time existence is established by a taylored time discretization procedure. Moreover, an optimal control problem is considered where a cost functional penalizes maximal deviations from prescribed damage profiles. The goal is to minimize the cost functional with respect to exterior forces acting on the boundary, which play the role of the control variable in the considered model.

The analysis and development of efficient numerical methods for high-dimensional stochastic (or in general parametric) problems was continued. A central achievement was the combination of low-rank hierarchical tensor representations with complete a posteriori adaptivity based on a residual error estimator. By these modern model reduction techniques, previous results obtained with an adaptive Galerkin scheme for stochastic PDEs could be improved and very large discretizations in the order of 10⁷⁰ became tractable. This approach paved the way for the consideration of even more involved (so-called) *lognormal* problems, which are of particular interest for real-world applications.

A new numerical scheme for the solution of stochastic PDEs based on global regression with respect to the solution of many stochastic differential equations (SDEs) was developed (cf. Figure 3 and [1]). This collaboration project with RG 3 and RG 6 underlines the possible benefits of combining expertise from stochastic and numerical analysis. The method allows for complete parallelization and the adaptive choice of all discretization parameters, in particular (and opposite to all standard methods such as Monte Carlo), the number of samples pointwise.

The work on the MATHEON subproject C-SE13 "Topology optimization of wind turbines under uncertainties" was continued. The aim is the topology optimization of the main frame of a wind tur-

Fig. 2: German H-gas and L-gas network system of the German network operator OGE (Open Grid Europe)



Fig. 3: Global regression of pointwise stochastic equations as approximation of stochastic PDE solution



bine accounting for stochastic uncertainties in the material data and the loads. In 2015, numerical methods for the deterministic shape optimization problem were implemented, and first results were obtained. A related sharp-interface model was studied in [6]. Furthermore, stochastic collocation methods to solve the state equation, taking the discretization of the probability space into account, were implemented and tested for first examples. The next step is to tackle the stochastic optimal control problem.

Within the framework of the joint project with RG 3 "Efficient mathematical methods for model calibration and uncertainty quantification in environmental simulations", funded by Investitionsbank Berlin, a stochastic geometric inverse problem was studied to determine the permeability of the subsurface from hydraulic head measurements within the framework of a steady Darcy model of groundwater flow. The parametrization leads to a parameter identification problem for a finite number of unknown parameters determining the geometry, together with either a finite number of permeability values (in the constant case) or a finite number of fields (in the continuous function case). To solve this parameter identification problem, a Bayesian framework was applied. The results of the parameter identification procedure with the Markov chain Monte Carlo (MCMC) method are presented in Figure 4.

Fig. 4: Posterior probability density function of geometric parameter c and physical parameters $\kappa_1, \kappa_2, \kappa_3$ calculated by MCMC method



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4.5 Research Group 5 "Interacting Random Systems"

In 2015, the group comprised the largest number of members in its history, as a great number of research programs were running on various topics like interacting particle systems, concentration properties of spectra of random operators, biological evolution models, and, in particular, in the Leibniz Group LG 4 *Probabilistic Methods for Mobile Ad-hoc Networks*, which started in July 2014, whose main scientific partner is the IHP – Innovations for High Performance Microelectronics (Frankfurt/Oder). The research spectrum of the group is complemented by some particular topics that were recently brought in by new colleagues, like a large deviations approach to physically interesting models for the polaron, and connections between large-deviation analysis of large interacting stochastic particle systems and gradient flows with respect to interesting functionals. In the latter subject, the group organized in December an international workshop with embedded minicourses by well-known experts. This subject belongs to the prominent ones at WIAS, since it combines the interests of a number of partners from other groups, notably from the Research Group RG 1 *Partial Differential Equations*.

A particular highlight in the activities of the head of the group was the organization of a festive event on the occasion of the 200th birthday of the eminent mathematician Karl Weierstrass, whose name the institute bears, and the edition (jointly with Prof. Jürgen Sprekels) of a collection of nine essays on historical aspects of him, written by international historians. The event took place in an appropriate setting in the premises of the Berlin-Brandenburg Academy of the Sciences and Humanities, and WIAS was honored by the visit and speech of Germany's Minister of Education and Research, Prof. Johanna Wanka.

Further notable organizational activities of the group concern a workshop for young females in probability: only females were invited to give talks. Moreover, on several occasions, members of the group gave a number of talks for the public, and the head of the group continued his engagement as head of the *Inspirata*, the Leipzig Institute for Education in Mathematics and the Sciences, and he continued to supervise an enormous number of bachelor theses at the Technische Universität Berlin on various subjects in the research spectrum of the RG 5.

A closer description of some of the group's achievements in 2015 follows.

Large Deviations for wireless networks

The goal of the LG *Probabilistic Methods for Mobile Ad-hoc Networks* is to develop and investigate probabilistic models for mobile ad-hoc networks as random interacting systems. These models seek to capture the most important characteristics of real-world wireless networks with randomly positioned users, and provide useful estimates on quantities like connectivity based on the signal-to-interference-and-noise ratio.

In two papers [4], [5], the group obtained results for networks of users given by planar point processes. In [4], a device-to-device setting is considered in the limit of a large number of transmitters and receivers. As a main result, it is shown that the probability that an unexpectedly large proportion of transmitters is unable to connect decreases at an exponential rate. This approach is used to develop an importance sampling algorithm that substantially reduces the variance for the numerical estimation of the rare-event probabilities. In [5], a model of relay-augmented wireless networks is considered where mobile users try to connect to a central base station. The problem of an atypically high number of users X^{λ} experiencing bad quality of service over a certain amount of time is analyzed in a high-density scenario where $\lambda > 0$, the intensity of users in a finite spatial domain, tends to infinity. The probability that the proportion of users with bad quality of service is larger than *b* decays at an exponential rate I(b)

$$\mathbb{P}(\#X^{\lambda} > \lambda b) \approx \mathrm{e}^{-\lambda I(b)}.$$

The formula that was derived for I(b) contains information about the most likely spatial distribution of the users in this unwanted event. Techniques of large deviations allow for a characterization of I(b) as a solution of a constrained entropy minimization problem. By using simulations, it is shown that solutions of this problem are potentially non-unique due to symmetry breaking; see Figure 1.



From large deviations to Wasserstein gradient flows in multiple dimensions

This work connects two—at first sight seemingly unrelated—topics: large deviations and gradient flows. The first topic concerns the stochastic concentration of independent Brownian particles in a force field Ψ . By the law of large numbers, the random concentration of particles converges to the solution of the corresponding Fokker–Planck equation $\dot{\rho}_t = \Delta \rho_t + \operatorname{div}(\rho_t \nabla \Psi)$. The exponentially small probability that the concentration of a large number *n* of particles X_1, \ldots, X_n at time τ does not follow this expected behavior is an example of a *large deviation principle*:

$$\operatorname{Prob}\left(\frac{1}{n}\sum_{i=1}^{n}\delta_{X_{i}(\tau)}\approx\rho\right)\simeq\exp\left(-nI_{\tau}(\rho\mid\rho_{0})\right)\qquad\qquad\text{for large }n.\tag{1}$$

It turns out that an asymptotic development of this functional I_{τ} for small time lags $\tau > 0$ yields

Fig. 1: Configuration in the special case of users without movement in a typical realization and in a typical realization conditioned on a frustration event. Points in green, blue, and red represent directly connected, relay-connected, and unconnected users, respectively. The rotational symmetry is broken.



a connection to the second topic:

$$I_{\tau}(\rho \mid \rho_0) \approx \frac{1}{4\tau} W^2(\rho_0, \rho) + \frac{1}{2} \mathcal{F}(\rho) - \frac{1}{2} \mathcal{F}(\rho_0) \qquad \text{for small } \tau.$$
 (2)

The right-hand side is a well-known discrete-time variational scheme for the so-called *gradient* flow of the free energy $\mathcal{F}(\rho) := \int \rho \log \rho + \int \Psi \rho$ in the Wasserstein metric *W*. A gradient flow is a mathematically rigorous formulation of the thermodynamic principle that "systems are driven by their free energy". The Wasserstein metric is closely related to the Schrödinger problem: "What is the least costly way to transport a given cloud of particles into another cloud?"

The result (2) shows that the gradient flow is strongly connected to an underlying stochastic particle system, just like the free energy itself is, via the Boltzmann formula. The proof in [3] strengthens an earlier result of this type in [1] to multiple dimensions.

The key idea behind the proof is to take the Wasserstein geodesic between ρ_0 and ρ , perturb it by running the Fokker–Planck flow P_{ϵ} for a short time, and carefully choosing $\epsilon(\tau)$ as a function of the time step τ ; see Figure 2.



Fig. 2: Construction of the curve between ρ_0 and ρ

The polaron problem in quantum mechanics

A well-known problem in statistical mechanics is the classical *polaron problem*. The physical question arises from the discussion of the slow movement of a charged particle, e.g., an electron, in a crystal whose lattice sites are polarized by this motion, influencing the behavior of the electron. In particular, as the electron moves in the crystal, it drags along a cloud of *polarized masses*, which determines its *effective behavior*. The mathematical layout of this problem was founded already in the early 1970s by Feynman, who introduced a path integral formulation and pointed out that the aforementioned effective behavior can be studied via the asymptotic behavior of a certain *Gibbs measure* for a three-dimensional Brownian motion $(B_t)_{t \in [0,T]}$ interacting with itself. This measure weights the path's probability exponentially with the energy term

$$H_{\lambda}(t) = \lambda \int_0^T \int_0^T dt ds \; \frac{e^{-\lambda |t-s|}}{|B_t - B_s|},$$

with some positive coupling parameter λ . This term induces a self-attraction on short time scales, i.e., large weight is given to Brownian paths that tend to return to a place where they have just been.

Although certain results are known for the free energy of this system by the classical Donsker-

Varadhan large deviation theory (which, roughly speaking, deals with probabilities of events that are untypical), a description of this system on the level of path measures is not easy. As a first crucial step, one has to understand a certain approximation of this problem: its mean-field version, which is also described by a self-attractive Gibbs measure, but where the aforementioned short time scale restriction is absent. The energy term used here is $H(T) = \frac{1}{T} \int_0^T \int_0^T dt ds 1/|B_t - B_s|$. The mean-field version is believed to approximate the original model for small values of the coupling parameter λ .

A detailed analysis of the mean-field version was carried out recently in a series of works by the group. Indeed, a robust theory of compact large deviations was developed in [7], its extension to the uniform strong metric for the singular Coulomb interaction was carried out in [6], and, as a culmination, in [2], the full description of the path measures was accomplished.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

The group focuses on the research topics *Statistical data analysis* and *Stochastic modeling, optimization, and algorithms*. Applications are mainly in economics, financial engineering, medical imaging, life sciences, and mathematical physics. Special interest is in the modeling of complex systems using methods from nonparametric statistics, statistical learning, risk assessment, and valuation in financial markets using efficient stochastic algorithms and various tools from classical, stochastic, and rough path analysis.

The group has a leading position with important mathematical contributions and the development of statistical software.

Members of the research group participate in the DFG Collaborative Research Center SFB 649 *Economic Risk*, DFG Research Unit FOR 1735 *Structural Inference in Statistics: Adaptation and Efficiency*, and DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*.

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

Scientific highlights achieved by the group in 2015 are provided below.

Statistical data analysis

The focus within the project area *Statistical data analysis* is on methods that automatically adapt to unknown structures using some weak qualitative assumptions. This includes, e.g., methods for regularization and estimation in inverse problems, dimension reduction, multiple testing, signal and change-point detection, feature identification, and adaptive smoothing in various applications.

Highlights 2015:

Outstanding publications:

VLADIMIR SPOKOINY, MAYYA ZHILOVA, Bootstrap confidence sets under model misspecification, Ann. Statist., **43**:6 (2015), pp. 2653–2675.

ANDREAS ANDRESEN, VLADIMIR SPOKOINY, Convergence of an alternating maximization procedure, J. Mach. Learn. Res., **17**:63 (2016), pp. 1–53.

MAXIM PANOV, <u>VLADIMIR SPOKOINY</u>, *Critical dimension in semiparametric Bernstein–von Mises theorem*, Bayesian Anal., **10**:3 (2015), pp. 665–710.

KARSTEN TABELOW, HENNING U. VOSS, JÖRG POLZEHL, Local estimation of the noise level in MRI using structural adaptation, Med. Image Anal., **20** (2015), pp. 76–86.

Ph.D. defenses of <u>Mayya Zhilova</u> and Andreas Andresen with mark "summa cum laude", and Niklas Willrich with mark "magna cum laude" at Humboldt-Universität zu Berlin.

The research of the group covers both theoretical and applied statistical problems. The convergence of general alternating algorithms was studied in Andresen and Spokoiny, a rigorous analysis of posterior distribution in semiparametric setup for finite samples was provided in Panov and Spokoiny, and the use of a multiplier bootstrap procedure for uncertainty quantification under nonclassical assumptions and the so-called *modeling bias* effect were investigated in Spokoiny and Zhilova.

Model selection for regression models with unknown heterogeneous noise with the use of bootstrap tuning is offered and studied in [1].

The research group has established strong connections to the neuroscience/neuroimaging community. Current joint research interests include the characterization of the signal distribution and noise quantification (see Tabelow et al.) and the effects of low signal-to-noise-ratios in statistical modeling of magnetic resonance imaging (MRI) experiments [2]. The problem is crucial in highresolution MRI experiments that aim for in-vivo diagnostics and diffusion-weighted MRI experiments employing high b-values. In-vivo-dignostics by multi-parameter-mapping is a recent method that uses multiple quantitative multi-parameter mapping, which is designed to provide standardized information about tissue microstructure. It relates measurements with different MR contrasts and at multiple echo times within a model derived from MR physics. The model parameters are supposed to be comparable across time points and imaging sites enabling the search for diagnostic markers for neuronal diseases in group studies. Novel ideas in the modeling of such data are pursued with the group's partners from the Wellcome Trust Institute for Neuroimaging London and Universitäts-Klinikum Hamburg-Eppendorf. An approach to automated lesion detection and classification in multiple sclerosis (MS) based on multimodal MR imaging is under development in its collaboration with neuroscientists from the Universitätsklinikum Münster. A collaboration with neurobiologists from the Leibniz Institute for Neurobiology concerns the dynamics of learning. Modeling data from learning experiments needs to combine behavioral data with functional MRI (humans) and local field potential measurements (rodents) in group studies. Statistical problems include the warping of individual subject-specific time scales and the identification of functional connectivity networks characterized by sparse precision matrices and inference procedures to test for changes in the structure of estimated networks. The group participates in efforts of the statistics community to provide solutions in analyzing neuroscience experiments. This research includes active participation in the 2015–16 Program on Challenges in Computational Neuroscience (CCNS) at the Statistical and Applied Mathematical Sciences Institute SAMSI, North Carolina, the development of prototypical neuro-statistical software (R-packages dti and fMRI), and the integration of statistical approaches into neuroscience software (ACID toolbox for SPM, Brainvoyager).

Within the BMBF-funded project EPILYZE, a new method was developed to control the *false discovery rate* in hierarchically structured systems of hypotheses. The method was successfully applied to the problem of signal detection in functional magnetic resonance imaging.

The work within the Alstom (Switzerland) Ltd. project on "Gas turbine process simulation" (joint project with RG 3 *Numerical Mathematics and Scientific Computing*) recently required to understand and implement Bayesian procedures for parameter calibration for models in WIAS's BOP

solver; see also page 182.

Aside from deterministic optimization routines, this approach makes it possible to quantify model uncertainties. Therefore, both a nonlinear Bayes approach for the complete solver, using Metropolis–Hastings Markov chains, as well as a linear Bayes approach, applied to a local linear model, are implemented. In combination, this approach allows for an efficient parameter fit and resulting performance predictions. It was presented at the ASME Turbo Expo, Montreal, and is published in the conference proceedings as M. ARIAS CHAO, P. MATHÉ, V. SCHLOSSHAUER, D.S. LILEY, *Calibration and uncertainty quantification of gas turbines performance models*, 2015. This contribution received the best paper award in the section on probabilistic models.

Stochastic modeling, optimization, and algorithms

The project 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. The development and rigorous mathematical analysis of innovative methods and algorithms based on fundamental stochastic principles are of primary interest. In particular, there is an increasing demand for effective solutions to optimal control problems for real-world high-dimensional problems appearing in energy and storage markets, for instance. Also, there is a strong expertise in financial (interest rate and equity) modeling, volatility modeling, effective calibration, and the modeling of financial derivatives, such as complex structured interest rate, energy, and volatility derivatives.

Further, the group has expertise in the highly active field of rough path analysis and regularity structures, which led, in particular, in the preceding year to the joint text book by Peter Friz and the Fields medallist Martin Hairer, and in the present year to the approval of the DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics.*

Highlights 2015:

- Acquisition of industry collaboration project with Deloitte & Touche on "Multi-curve LIBOR modeling, calibration, and pricing of related products"
- Granting of the DFG Research Unit FOR 2402 for 2016–2019, principal investigators: Christian Bayer and John Schoenmakers
- Successful Ph.D. defense by Marcel Ladkau

After the financial crisis around 2007, it became necessary to incorporate credit risk into LIBOR rates and, as a result, multi-curve LIBOR models were called for. In this context, an affine multi-curve LIBOR model was developed and finalized in [3]. This model has the advantage that, unlike in some other recent approaches, forward LIBORs and spreads with respect to overnight index swap rates can be modeled simultaneously over arbitrary periods in a mathematically consistent way. While the latter model may be considered quite nice from a mathematical point of view, its calibration requires the identification of parameters that are not directly linked to certain economic quantities, such as volatility and correlation. As a consequence, the development of the most effective calibration method for this model is still in progress. Meanwhile, WIAS has acquired an industry collaboration with Deloitte & Touche on this topic. For this collaboration, the WIAS group

effectuates a more pragmatic solution that comes down to a multi-curve version of the stochastic volatility LIBOR model developed earlier by Ladkau, Schoenmakers, and Zhang (2013).

An important contribution to the modeling of stock indices was the development of the so-called *rough Bergomi* (rBergomi) model [5]. This model is a stochastic volatility model where the stochastic volatility component is essentially given by the exponential of a fractional Brownian motion. An important difference to earlier models is that the rBergomi model allows for a Hurst index H < 1/2 and, in fact, calibration leads to choices of $H \approx 0.1$. Amazingly, this very simple, parsimonious model—based on only three free parameters—yields excellent fits of model prices to observed market prices of options on the stock or index, as extensively tested for the S&P 500 index (SPX), much better than fits obtainable from conventional stochastic volatility models. Thus, this new model is very promising both from an applied perspective, allowing option pricing fully consistent with market prices, and from a more academic point of view, as there are still many open problems in the context of the rBergomi model, such as constructing hedging strategies in the rBergomi model to the development of efficient numerical algorithms.

A perennial problem in the simulation of stochastic volatility LIBOR models and stochastic volatility asset models such as the Heston model is the effective simulation of the square-root process involved, also called the *Cox–Ingersoll–Ross (CIR) diffusion process*,

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

with *W* being a standard Brownian motion. Simulation of the CIR process is particularly difficult when the Feller condition $\sigma^2 \le 2k\lambda$ is violated. After a successful treatment of the case $4k\lambda > \sigma^2 > 2k\lambda$ based on the Doss–Sussmann approach in the preceding year by Milstein and Schoenmakers (2015), a novel method was developed in the present report period (WIAS Preprint no. 2113, to appear in Adv. Appl. Probab., 2016). The new method applies regardless whether the Feller condition is violated or not and provides trajectories that are exact at random times and uniformly close to the exact ones at all times in between. Moreover, the method is developed such that it is even applicable to rather general (one-dimensional) diffusions and is based on spectral series expansions connected with Sturm–Liouville problems.

In the field of optimization in energy markets, a combined model of a hydroelectric storage and production facility and of the day-by-day electricity bid market is considered. The water inflow to the facility and the electricity price are modeled by dependent stochastic processes. The operator is faced with the problem of deciding daily on the control of the facility and on the amount of electricity for the next day's bid to the market. The cost function, which is maximized, is the gross profit from selling the electricity. Instead of solving this problem directly, a dual martingale approach was chosen where a dual problem is solved by a Monte Carlo simulation; see also Bender, Schoenmakers, Zhang (2015, list of WIAS references in the appendix on pages 122ff).

For more details see the Scientific Highlights article on page 40.

In the area of modeling and interference of economic processes, a new procedure for the identification of the time change in a time-changed Brownian motion was developed in Belomestny and Schoenmakers (2015). Further, a new estimator for variance-mean mixture models was constructed on the basis of a generalization of the Post–Widder formula to the complex domain in WIAS Preprint no. 2186, 2015. These results were obtained in interaction with the topic *Statistical data analysis*.

Jointly with the research groups RG 3 *Numerical Mathematics and Scientific Computing* and RG 4 *Nonlinear Optimization and Inverse Problems*, stochastic differential equation-based regression methods for partial differential equations with random coefficients were developed and resulted in WIAS Preprint no. 2192, 2015. These methods provide a valuable alternative to the more usual, but computationally intensive, finite element approaches.

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

The research group is working on the thermodynamically consistent modeling, analysis, and simulation of processes in materials. Often, desirable and undesirable phase transitions occur, and their prediction is mandatory in modern key technologies.

Currently, the group is involved in three core areas:

- 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 represented by systems of nonlinear partial differential equations. Moreover, systems of stochastic ordinary differential equations are studied 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

LG 3 *Mathematical Models for Lithium-ion Batteries.* The foundations of the battery research were established within the Leibniz group *Mathematical Models for Lithium-ion Batteries*. It was externally funded between July 2012 and June 2015. The funding resulted from a successful proposal by Wolfgang Dreyer within the competition procedure of the Leibniz Association in the Pact for Research and Innovation.

The group is working on modeling, analysis, scientific computing, and simulations of various components of lithium-ion batteries, particularly

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

The research on these core items is still going on within RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*. An overview of some outstanding results is given in the Scientific Highlights article "Mathematical Models for Lithium-ion Batteries" on page 44 of this report. There is a collaboration with the research group RG 3 *Numerical Mathematics and Scientific Computing* concerning the numerical analysis of the new electrolyte models and the implementation into the WIAS numerical code pdelib. Moreover, there is a collaboration with RG 6 *Stochastic Algorithms and Nonparametric Statistics* on an interdisciplinary MATHEON subproject on "Stochastic analysis of many-particle electrodes". Particularly the new electrolyte models have motivated further developments that were started in the second part of 2015 and are described in the following. **Numerical analysis of coupled bulk-surface equations.** Many areas of modern applications concern coupled phenomena happening at the interface and within the adjacent bulk phases. The corresponding surface equation systems are quite intricate because they couple bulk fluxes across the interface to intrinsic interfacial fluxes, which were extensively treated by Clemens Guhlke in his Ph.D. thesis "Theorie der elektrochemischen Grenzfläche". The existing analysis mainly restricts itself to uncoupled equations, i.e., either normal fluxes or only tangential fluxes are taken into account. A step towards the full coupling of both phenomena was carried out by Rüdiger Müller jointly with Martin Eigel from RG 4 *Nonlinear Optimization and Inverse Problems*. In [2], they consider a system of two coupled elliptic equations defined on a bulk domain and its boundary surface domain.



Fig. 1: Solution of the coupled system for a non-smooth domain Ω with a reentrant corner. The domain consists of a ball where one octant has been removed. Left: Bulk solution, Right: Surface solution.

The discretization with conforming finite elements employs a polyhedral approximation of the surface. For the a posteriori error control of the equation system, a residual error estimator is derived, which takes into account the approximation errors due to the finite element method discretization in space as well as the polyhedral approximation of the surface. An adaptive refinement algorithm controls the overall error. Numerical experiments illustrate the reliability of the a posteriori error estimator and the ability of the proposed adaptive algorithm to efficiently solve the coupled problem on non-smooth domains with reentrant corners as shown in Figure 1.

New interpretation of the Lippmann equation. In the existing literature, the Lippmann equation is considered as a universal relationship between interfacial tension, double-layer charge, and cell potential. Based on the framework of continuum thermo-electrodynamics, some crucial new insights to this relation are provided in [4]. The new electrode-electrolyte model is applied to a curved liquid metal electrode. If the electrode radius is large compared to the Debye length, asymptotic analysis methods yield the Lippmann equation with precise definitions of the involved quantities. It turns out that the interfacial tension of the Lippmann equation is composed of the surface tension of the general model and contributions arising from the adjacent space charge layers. This finding is confirmed by a comparison of the group's model to experimental data of several mercury-electrolyte interfaces.

Analysis of partial differential equations in the context of electrochemistry. The coupling of the reaction-diffusion equations to the Navier-Stokes equation via both the pressure and the electric field is essential for proper electrochemical modeling. Particularly, the appearance of the pressure in the diffusion fluxes represents the distinctiveness of the new reaction-diffusion Navier-Stokes system, developed in LG 3. Moreover, the effective mobility matrix is represented as M = $P^T M_{emp} P$, where P is a constant projector, and M_{emp} is the empirical mobility matrix. The research to establish first rigorous mathematical results for the new coupled model is headed by Pierre-Étienne Druet. A proof of existence results suffers from multiple elliptic degeneration of the diffusion fluxes. The eigenvalues of $M_{\rm emp}$ are not bounded away from 0 and 1. Moreover, the matrix P has the eigenvalue zero. These difficulties may be removed by elliptic regularization. In order to achieve compactness, the ellipticity of the diffusion matrix on the N-1 -dimensional image (subspace) of the projector P is used, combined with an extension of the Lions method for the Navier–Stokes operator. The latter guaranties that the total mass density ρ is in a compact subset of L^1 . Thanks to a priori bounds that result from the thermodynamical consistency of the system, it is finally possible to pass to the limit with the approximation scheme. In particular, it is possible to show that the numerous nonlinearities converge to their expected limit. The current open topics are, firstly, the existence of a weak solution in the context of vanishing constituents and, secondly, an existence proof for the incompressible limit of the system.



Stochastic methods for the analysis of lithium-ion batteries. The subproject C-SE8 "Stochastic methods for the analysis of lithium-ion batteries" is a part of the application area Mathematics for Sustainable Energies of the Research Center MATHEON funded by the Einstein Center for Mathematics Berlin (ECMath). The project is headed by Wolfgang Dreyer and Peter Karl Friz from RG 6 Stochastic Algorithms and Nonparametric Statistics. The challenging topic needs mathematical techniques from both analysis and stochastics. The project aims to improve the properties of many-particle storage systems that are used as intercalation electrodes in lithium-ion batteries. The first many-particle model was introduced a few years ago by Wolfgang Dreyer and Clemens Guhlke jointly with Michael Herrmann from Westfälische Wilhelms-Unversität Münster. This model relies on the assumption that the storage particles are of equal size and describes the evolution of the many-particle electrode during a charging/discharging process by a single Fokker-Planck equation. However, there is a size distribution with particle radii between 25 and 500 nanometers. The particle size distribution has a large impact on the dynamics of the many-particle electrode, which opens the possibility for optimization. The size distribution can easily be modeled within a system of stochastic differential equations for each of the storage particles; see the Scientific Highlights article on page 44.

Figure 2 on the next page shows the loading-unloading process for N = 100 storage particles, k = 1, 2, ..., N, of different size with radii $r_1 < r_2 < ... < r_{100}$. There are two small parameters τ and ν depending on the particle size.



Fig. 2: Evolution of lithium concentrations y^k during a loading-unloading process. Red: small particles, blue: large particles. Small particles undergo the phase transition first.

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

Gradient flow perspective of thin-film bilayer flows. Barbara Wagner participates in the DFG Priority Program SPP 1506 "Transport Processes at Fluidic Interfaces" with the funded project "Dynamics of viscous multi-layer systems with free boundaries".

Barbara Wagner and Sebastian Jachalski jointly with Andreas Münch (University of Oxford) worked on the mathematical modeling, analysis, and numerical simulation of thin liquid bilayer films. In 2015, the dewetting of viscoelastic liquids of corotational Jeffreys' type from Newtonian liquid substrates as well as from solid substrates was studied. For the first time, the asymptotically consistent reduction of the free-boundary problem for the two-layer system to a system of coupled thin-film equations that incorporate the full nonlinear viscoelastic rheology could be derived. For this system the relevant asymptotic regimes that relate the viscosity ratio to a corresponding apparent slip could be identified; see [5].

In the context of thin-film analysis the doctoral student of Barbara Wagner, Tobias Ahnert, defended his Ph.D. thesis "Mathematical modeling of concentrated suspensions: Multiscale analysis and numerical solutions" at Technische Universität Berlin with *summa cum laude*.

In this thesis, the stability of two-dimensional Poiseuille flow and plane Couette flow for concentrated suspensions is investigated. If the particle volume fraction of the suspension increases, both flow geometries exhibit the existence of a convectively driven instability with increasing growth rates of the unstable modes. In addition, it is shown that there exists a bound for the particle phase viscosity below which the two-phase flow model may become ill-posed as the particle phase approaches its maximum packing fraction; see [6].

Liquid-phase crystallization (LPC). Modeling of laser-controlled LPC from atomistic to the continuum phase-field description was carried out by Barbara Wagner in collaboration with the group of





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Prof. Karsten Albe (Technische Universität Darmstadt) and with the Competence Centre Thin-Filmand Nanotechnology for Photovoltaics Berlin (PVcomB) "Microstructure Control for Thin Film Solar Cells".

Using the interatomic potential by Stillinger–Weber, an expression for the bulk free energy was derived and, moreover, an expression for the interfacial width of the liquid-crystal interface and the crystallization velocity and, hence, the corresponding anisotropic mobility for the different orientations in silicon as a function of temperature. To properly capture the behavior of the temperaturedependent viscosity near the glass transition, a Vogel–Fulcher-type model was used for the first time. These results were proven to be essential to obtain an accurate temperature dependence of the anisotropic mobility in the corresponding phase-field model for liquid-phase crystallization. The three-dimensional setting of these results with atomistically based well potentials and parameters was then implemented into the general numerical model in collaboration with the group of Prof. Ralf Kornhuber (Freie Universität Berlin) for large-scale numerical studies.

Mathematical modeling, analysis and novel numerical concepts for anisotropic nanostructured materials. The subproject C-SE4 "Mathematical modeling, analysis and novel numerical concepts for anisotropic nanostructured materials" is a part of the application area *Mathematics for Sustainable Energies* of the Research Center MATHEON funded by the Einstein Center for Mathematics Berlin (ECMath). The project is headed by Barbara Wagner, jointly with Christiane Kraus (Young Scientists' Group *Modeling of Damage Processes*), and Gitta Kutyniok (Technische Universität Berlin). One of the subproblems focused on the mechanical behavior of silicon, which could be used as alternative electrode material for lithium-ion batteries. Silicon can host ten times more lithium than the current graphite anode. Nevertheless, silicon electrodes are plagued by a number of problems. Most of them are related with the fact that, when fully lithiated, silicon electrodes increase their volume by 300–400%. This increase causes enormous stresses within the electrode that eventually cause its mechanical failure and its pulverization. Nevertheless, strategies such as the patterning of electrodes with nanowires have proved to be very promising. During this year, a simple Larché–Cahn model was used to interprete the experiments, whereupon stress-assisted phase separation was observed.

Hysteresis of electromagnetic-mechanical components and of biological systems

Hysteresis and uncertainty quantification. Actuators, sensors, or energy-harvesting devices often contain electromagnetic-mechanical components showing piezoelectricity or magnetostriction, where these phenomena are accompanied by hysteretic phenomena. Usually, the corresponding models are influenced by uncertainties in the measurements. Moreover, the observable macroscopic state may be generated by many unobservable microscopic states. Olaf Klein studies these uncertainties by applying the methods of uncertainty quantification. For illustration, the *play operator* $\mathcal{P}_{r}[w, \cdot]$ is used to show the influence of uncertainty in the *yield limit* $r \ge 0$ on the output function. To this end, the yield limit r is interpreted as a value of a random variable R. The corresponding probability density function p is shown in Figure 4. Combining this random variable with an appropriate input function u then yields that $X := \mathcal{P}_{R}[0, u](T)$ is a random variable such





Fig. 3: Lithiation process: Stress versus concentration with marked phase transition point



Fig. 4: Probability density function p for random variable R defining the yield limit r

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that the corresponding probability measure is the sum of a measure with a density function d and of a Dirac measure; see Figure 5.

Representation result for rate-independent systems. Olaf Klein extended the representation result for hysteresis operators acting on piecewise monotaffine inputs to an representation result for rate-independent systems as defined by Alexander Mielke in "Evolution of rate-independent systems in evolutionary equations", vol. II of Handb. Differ. Equ., Elsevier/North-Holland, Amsterdam, 2005, pp. 461–559. To this end, a special type of monotaffine functions was introduced: the *strictly monotaffine functions*, generated as the composition of a strictly **monot**one with an **affine** function such that the monotone functions are applied first; see [1].

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Fig. 5: Density function *d* and Dirac measure (red) leading to the probability measure generated by *X*



Fig. 1: Snapshots from a numerical simulation of phase separation and damage with horizontal loading

4.8 Young Scientists' Group "Modeling of Damage Processes"

Within the competitive procedure of the Leibniz Association in the Pact for Research and Innovation, Dorothee Knees and Christiane Kraus successfully applied for a grant that provided the basis for the Young Scientists' Group in 2009. Collaborations exist 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*.

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 works 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 develops multi-scale damage models that reflect the evolution of microdefects in effective models on the macroscopic level in a mathematically justified way.

In general, the resulting models consist of strongly coupled, nonlinear, and nonsmooth time-dependent systems of 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.

An important research topic in the group is the analysis of damage processes in elastic, heatconducting, and multi-phase materials. These physical phenomena were subject to intensive research in the last few years, but have been investigated in the mathematical literature mostly separately. The mathematical modeling of the corresponding PDEs and differential inclusion systems is important for applications in engineering and features a high degree of non-smoothness. For instance, the damage evolution law involves two subdifferentials in order to account for unidirectionality and boundedness of the associated phase field variable [1]. In addition, the heat conduction equation contains highly nonlinear dissipative terms rendering the system thermodynamically consistent. In collaboration with internal and external partners, the Young Scientists' Group achieved the outstanding result that weak solutions exist for the fully coupled system [3]. Several recent mathematical techniques, which were developed in the Young Scientists' Group, came into play. These techniques include partial convex-concave splittings in time-discretization schemes, convergence methods for variational inequalities, several enhanced a priori estimates, and nested approximation schemes. The carefully chosen time-discretization method also point out a way to conduct numerical simulations.

Based on previous works in the group, a unified model was investigated that describes damage in electrodes of lithium-ion batteries focusing on two particular physical and chemical effects: Firstly, the phase separation into a lithium-rich and a lithium-poor phase with the corresponding strains and stresses; secondly, the propagation of damage of the involved material. The latter is motivated



since the development of small cracks is often observed in experiments during the charging or discharging process of lithium-ion batteries.





Fig. 2: From left to right: First two figures: Formation of a FePO ₄ layer during delithiation of a LiFePO4 crystal. Third figure: Cracks in a single partially delithiated LiFePO ₄ crystal.

To model these effects, the group proposed a system of Cahn–Larché type coupled with a differential inclusion for the damage evolution. The novelty of the model is the chemical active boundary condition describing lithium intercalation effects at the electroyte-electrode interface. These effects are modeled by a nonlinear Newton boundary condition for the chemical potential. Such boundary conditions were proposed recently for chemical active boundaries but not yet studied theoretically. From the analytical point of view, this additional boundary condition is already difficult to handle for the Cahn–Larché system itself since the system is not mass conserving anymore, and thus it cannot be written as a linear H^{-1} -gradient flow. Nevertheless, the Young Scientists' Group was able to prove existence of weak solutions for the whole system by establishing a nonlinear gradient flow, which respects the nonlinear boundary condition. To this end, several tools were used from the field of convex analysis.

Another topic in the Young Scientists' Group is the study of optimal control problems for damage processes in linear elastic media. In a recent contribution [2], it provided the analytical basis for this endeavor. More precisely, in collaboration with RG 4, a global-in-time well-posedness result and enhanced a priori estimates were established for certain classes of rate-dependent damage/elasticity systems. In view of possible applications, time-dependent Neumann boundary conditions were included to model external forces. Novel a priori estimation and discretization techniques were introduced to achieve solvability in a strong sense. For the optimization problems, cost functionals were considered where given damage phase field patterns are approximated by the damage evolution of the system and by controlling the boundary forces. By using a penalization approach for the state system and weak convergence properties of the solution operators, existence of optimal controls was proven. This approach in combination with the enhanced a priori estimates also indicate possibilities to establish first-order optimality systems.

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

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the rate-independent case, the software allows for backtracking to ensure compliance with the energy inequality. To gain physical realistic solutions, an obstacle potential for the concentration phase field was considered to ensure that this order parameter is in the interval [-1,1]. In addition, many routines were added to the existing code. Among them are routines for an additional type of boundary conditions (Robin boundary conditions, to avoid cracking at the domain bounds), the use of anisotropic elastic moduli, and mesh creation.







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".

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4.9 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 Stefania Patrizi (until July 2015) and Eleonora Cinti (from January 2015) were/are members of his group, and more partners visited the institute to establish scientific collaborations.

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

In 2015, Enrico Valdinoci held several research courses and many invited seminars and talks. In the context of the ERC project, he organized and sponsored several events, such as the workshop "PDE2015 – Theory and Applications of Partial Differential Equations", held in Berlin in December.

Jointly with Eleonora Cinti, Stefania Patrizi, and many other international collaborators, several research projects were carried out, leading to a large number of papers on topics like crystal dislocations, partial differential equations in anisotropic media, nonlocal diffusion equations, partial differential equations in spaces of infinite dimensions, and density estimates for some nonlocal phase transition equations.



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Fig. 1: Enrico Valdinoci



Fig. 2: Stefania Patrizi



Fig. 3: Eleonora Cinti during a talk

In particular, in [1], the problem of minimization of competing nonlocal perimeter functionals is taken into account, in the light of nonlocal isoperimetric inequalities.

In [2], a nonlocal version of the Schrödinger equation is examined, proving the first concentration results with Dirichlet data in bounded domains.

In [4], a free boundary problem is considered. The problem arises from the superposition of the nonlocal perimeter functional and a Dirichlet energy and several regularity results are obtained.

The papers [6] and [5] study a model for atomic crystal dislocations. At a mesoscopic scale, the problem is driven by a nonlocal integro-differential equation of parabolic type. The equation possesses a dynamical system that moves the dislocation according to a singular potential, which can be either attractive or repulsive, depending to the orientation of the dislocation. In this sense, also the possibility of collisions between dislocations with opposite orientations are taken into account, by combining maximum principle methods with dynamical systems techniques.

Furthermore, Enrico Valdinoci acted as an editor for the special issue in [3] and as an advisor for the Ph.D. students Nicola Abatangelo, Claudia Bucur, Matteo Cozzi, and Luca Lombardini.

References

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- [3] E. VALDINOCI, ed., *Special Issue on Contemporary PDES Between Theory and Applications*, no. 12 of vol. 35 in Discrete Contin. Dyn. Syst. Ser. A, American Institute of Mathematical Sciences, Springfield, 2015, 625 pages.
- [4] L. CAFFARELLI, O. SAVIN, E. VALDINOCI, *Minimization of a fractional perimeter-Dirichlet integral functional*, Ann. Inst. H. Poincaré Anal. Non Linéaire, **32**:4 (2015), pp. 901–924.
- [5] ST. PATRIZI, E. VALDINOCI, Crystal dislocations with different orientations and collisions, Arch. Ration. Mech. Anal., 217:1 (2015), pp. 231–261.
- [6] S. DIPIERRO, G. PALATUCCI, E. VALDINOCI, *Dislocation dynamics in crystals: A macroscopic theory in a fractional Laplace setting*, Comm. Math. Phys., **333**:2 (2015), pp. 1061–1105.

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4.10 ERC Group 2 "Entropy Formulation of Evolutionary Phase Transitions"

The group is meant to collect the results obtained in the ERC-Starting Grant EntroPhase "Entropy Formulation of Evolutionary Phase Transitions" funded by the European Union in April 2011 and lasting six years. The group members are currently Elisabetta Rocca (principal investigator) and Riccardo Scala (postdoc), while Sergio Frigeri finished his postdoc in the group at the end of September 2015.

The group mainly focused in 2015 on the objective to find relevant mathematical results in order to get further insight into new models for phase transitions and special materials and the corresponding evolutionary partial differential equation (PDE) systems, in particular:

- Developing a weak notion of solution capturing the most important phenomena characteristics
- 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

The importance of the topic lies in the fact that the above phenomena arise in a variety of applied problems like:

- Control problems related to
 - nonlocal phase separations in incompressible fluids (jointly with RG 1 Partial Differential Equations; see [6])
 - Penrose-Fife- and Caginalp-type models of phase transitions (see [1])
- Entropic formulations for models of
 - phase transitions and damage in viscoelastic materials (jointly with the Young Scientists' Group *Modeling of Damage Processes* and RG 1; see [4, 5])
- Long-time behavior of liquid crystal flows and two-phase flows (jointly with RG 1; see [2])
- Diffuse interface models for tumor growth (jointly with RG 1; see [3])

The key idea

The key idea consists in building up new notions of solution, the so-called *entropic* solutions, reinterpreting the concept of weak solution satisfying a suitable energy conservation and entropy inequality—recently introduced by Eduard Feireisl (Prague) for a problem of heat conduction in fluids. These ideas turn out to be particularly useful in the analysis of highly nonlinear PDE systems arising from different applications and were already successfully applied in [2], in [5], and in [4], where liquid crystal dynamics and phase transitions in thermoviscoelastic materials were studied, respectively.



Fig. 1: Binary fluids



Fig. 2: Damage



Fig. 3: Nematic liquid crystals



Fig. 4: Tumor growth

Further activities

The knowledge transfer was developed via the organization of international workshops and the participation of group members in international conferences and workshop, but also by collaborating with international experts visiting WIAS in 2015, like Maria Schonbek (California) on March 30 – April 4; Arghir Zarnescu (Sussex) on March 16–21; Eduard Feireisl (Prague) on March 30 – April 3; Mimi Dai (Chicago) on March 29 – April 7; Pavel Krejčí (Prague) on May 25–28; Michel Frémond (Rome) on June 2–5, and Hao Wu (Shanghai) on September 30 – October 14.

Main international meetings and sessions organized in 2015

- Special Session "Applied Analysis" of the International Association of Applied Mathematics and Mechanics (GAMM) 86th Annual Scientific Conference, Lecce, Italy, March 23–27, 2015, jointly organized with Maurizio Grasselli (Milan) and Dorothee Knees (Kassel).
- INdAM-ERC Workshop "Special Materials in Complex Systems", Istituto Nazionale di Alta Matematica "Francesco Severi" (INdAM), Rome, Italy, May 18–22, 2015, jointly organized with Elena Bonetti (Pavia), Cecilia Cavaterra (Milan), and Ricarda Rossi (Brescia).
- CIME Course on "Mathematical Thermodynamics of Complex Fluids", Cetraro (CS), Italy, June 29 July 3, 2015. Main speakers: John Ball (Oxford), Constantine M. Dafermos (Providence), Eduard Feireisl (Prague), Felix Otto (Leipzig), jointly organized with Eduard Feireisl.
- Workshop "PDE2015 Theory and Applications of Partial Differential Equations", WIAS, November 30 December 4, 2015, jointly organized with Hans-Christoph Kaiser, Dorothee Knees (Kassel), Alexander Mielke, Joachim Rehberg, Marita Thomas, and Enrico Valdinoci (all WIAS).

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- [3] S. FRIGERI, M. GRASSELLI, E. ROCCA, *On a diffuse interface model of tumor growth*, Nonlinearity, **28** (2015), pp. 1257–1293.
- [4] C. HEINEMANN, C. KRAUS, E. ROCCA, R. ROSSI, *A temperature-dependent phase-field model for phase separation and damage*, WIAS Preprint no. 2164, 2015.
- [5] E. ROCCA, R. ROSSI, "Entropic" solutions to a thermodynamically consistent PDE system for phase transitions and damage, SIAM J. Math. Anal., 47 (2015), pp. 2519–2586.
- [6] E. ROCCA, J. SPREKELS, *Optimal distributed control of a nonlocal convective Cahn–Hilliard equation by the velocity in 3D*, SIAM J. Control Optim., **53** (2015), pp. 1654–1680.



Fig. 5: Course of the Centro Internazionale Matematico Estivo (CIME)

A Facts and Figures

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

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

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

A.1.1 Calls

- 1. <u>CH. KRAUS</u>, W2 professorship, June 26, Hochschule für angewandte Wissenschaften Würzburg-Schweinfurt, Abteilung Würzburg, Fakultät für angewandte Naturwissenschaften.
- 2. E. ROCCA, W2 professorship, October 22, Università di Pavia, Dipartimento di Matematica.

A.1.2 Awards and Distinctions

- 1. <u>F. FLEGEL</u>, "Physik-Studienpreis 2015" of Physikalische Gesellschaft zu Berlin, sponsored by Siemens AG, for her master's thesis, July 9.
- 2. <u>D. HÖMBERG</u>, Member of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization.
- 3. ____, Vice Chair of Cost Action TD1409 (Mi-NET).
- 4. ——, Vice President of the European Consortium for Mathematics in Industry (ECMI).
- 5. <u>A. MIELKE</u>, Head of the Secretariat of the International Mathematical Union (IMU).
- 6. ——, Member of MATHEON'S Executive Board.
- 7. _____, Member of the IMU Berlin Einstein Foundation Program Committee.
- 8. —, Treasurer of IMU.
- 9. _____, Member of the "Galileo Galilei Prize for Science" Committee, 2015.
- 10. J. PELLERIN, C&G Best Paper Award 2014, July 23.
- 11. <u>M. THOMAS</u>, Speaker of the GAMM Junior Group, Gesellschaft für Angewandte Mathematik und Mechanik, 2015.

A.1.3 Ph.D. Theses

- 1. A. ANDRESEN, *Finite sample analysis of profile M-estimators*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, August 19.
- 2. R.M. ARKHIPOV, *Modeling of mode-locking regimes in lasers*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: <u>Priv.-Doz. Dr. U. Bandelow</u>, March 3.
- 3. M. LADKAU, *Stochastic volatility Libor modeling and efficient algorithms for optimal stopping problems*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Priv.-Doz. Dr. J.G.M. Schoenmakers, July 23.
- J.P. PADE, Synchrony and bifurcations in coupled dynamical systems and effects of time delay, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: <u>Priv.-Doz. Dr. S. Yanchuk</u>, July 22.
- 5. A. SHEKHAR, *Rough paths probability and related topics*, Technische Universität Berlin, Fakultät 2 Mathematik und Naturwissenschaften, supervisor: <u>Prof. Dr. P. Friz</u>, December 9.
- 6. N. WILLRICH, *Resampling-based tuning of ordered model selection*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, November 20.



- 7. <u>A. GONZÁLEZ CASANOVA SOBERÓN</u>, *The effect of latency in population genetics*, Technische Universität Berlin, Fakultät 2 – Mathematik und Naturwissenschaften, supervisors: Prof. Dr. J. Blath, Dr. N. Kurt, October 9.
- 8. <u>L. LÜCKEN</u>, Patterns of activity in coupled systems with applications to neuronal dynamics, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: <u>Priv.-Doz. Dr. S. Yanchuk</u>, December 14.
- 9. <u>S. REICHELT</u>, *Two-scale homogenization of systems of nonlinear parabolic equations*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: <u>Prof. Dr. A. Mielke</u>, November 27.
- 10. <u>M. ZHILOVA</u>, Bootstrap confidence sets under model misspecification, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, November 2.

A.1.4 Undergraduate-degree Supervision

- 1. N. ABDI, *Turbulence modelling of the Navier–Stokes equations using the NS-* α *approach* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, April 29.
- L. ALBERTSEN, Localisation in the heavy-tailed random conductance model (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 29.
- W. BENDER, Anwendungen von DIRECT auf ausgewählte Probleme in der Nichtlinearen Optimierung (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, October 25.
- A. BOJE, Convergence of stochastic coagulating particle systems (master's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisors: Prof.Dr. W. König, Dr. R.I.A. Patterson, August 18.
- 5. J. BRASSEUR, *Nonlocal equations and slicing properties of fractional spaces* (master's thesis), Université Lyon 1, Institut Camille Jordan, supervisors: <u>Prof. Dr. E. Valdinoci</u>, Prof. Dr. P. Mironescu, September 10.
- G.J. BULLING, Isogeometrische Analysis f
 ür die inkompressiblen Navier-Stokes-Gleichungen (master's thesis), Freie Universit
 ät Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, September 22.
- 7. A. BURKARTH, Bose-Einstein-Kondensation bei positiver Temperatur (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 3.
- 8. F. CAFORIO, Assessment of Kalman filtering for parameter estimation in zero- and one-dimensional blood flow models (master's thesis), Università degli Studi di Trento, Dipartimento di Matematica, supervisor: Dr. A. Caiazzo, July 22.
- F. CEVIK, Asymptotische Verteilungen von Ordnungsstatistiken (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 5.
- 10. S. DAMES, *Struktur-adaptive Glättung in fMRI-Gruppenstudien* (master's thesis), Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Dr. J. Polzehl, March 17.
- A. DOLL, A non-intrusive Galerkin method for PDEs with random data based on adaptive sparce grids (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, November 2.
- R. DUAN, Große Abweichungen für Irrfahrten mit zufälligen Leitfähigkeiten (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 2.

A Facts and Figures

- 13. M. EBELING-RUMP, *Modellierung und Simulation von Wirbelstromproblemen mit Hysteresis* (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 17.
- 14. F. GROSCH, *Perkolation in SINR-Graphen* (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 22.
- 15. C. HINSEN, *Quantile für unabhängige Gauß'sche Prozesse* (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 5.
- S. KNELL, A review of regularity and sparse approximation and quadrature results for stochastics PDEs (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 29.
- F. KRELLNER, Gesamtmasse der Lösung des parabolischen Anderson-Modells mit Pareto-verteilten Potentialen (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 24.
- P.R. KUNZE, Optimales Routing auf einem Poisson-Delaunay-Graphen (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 22.
- 19. L. LOMBARDINI, *Fractional perimeter and nonlocal minimal surfaces* (master's thesis), Università di Milano, Dipartimento di Matematica, supervisor: <u>Prof. Dr. E. Valdinoci</u>, July 16.
- F. PETERS, Divergierende Ordnungsstatistiken der Eigenwerte zufälliger heavy-tailed Matrizen (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 30.
- 21. N. RAASCH, *Fluktuationen im Random Energy Model* (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 17.
- S. REHBERG, Stochastische Optimierungsprobleme mit Inhomogenitäten (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: <u>Prof. Dr. W. König</u>, August 18.
- S. REUKAUF, Schadensprozesse mit heavy-tailed Risiken bei Rückversicherungsverträgen (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 17.
- 24. P. SALOW, *Optimales Stoppen und das Parkplatzproblem* (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 26.
- M. SANDER, Galton-Watson-Bäume mit verschwindendem Martingallimes (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 8.
- 26. F. SATTLER, Verfahren zur numerischen Lösung nichtglatter Optimierungsprobleme (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, September 1.
- 27. N. SCHÖNKNECHT, On solvers for saddle point problems arising in finite element discretizations of incompressible flow problems (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 1.
- D. SURC, An electro-thermomechanical ansatz to identify phase transitions from dilatometer curves (master's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 3.



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

- 29. TH.P. THAN, *Grenzverteilungen des Durchmessers einer Menge von unabhängigen Vektoren* (bachelor's thesis), Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 6.
- A. TSIMBALYUK, Efficient estimation of linear functionals under one-sided erros (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 28.
- K. UHLIG, Ordnungsstatistiken für unabhängige Gauβprozesse (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 3.
- 32. A. WAPENHANS, *Konzentrationseigenschaft des parabolischen Anderson-Modells* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 29.
- Y. ZHANG, Simulation der Wärmeübertragung in instationären laminaren Rohrströmungen (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: <u>Prof. Dr. V. John</u>, August 11.

A Facts and Figures

A.2 Grants¹

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 Starting Independent Researcher Grant "Rough Path Theory, Differential Equations and Stochastic Analysis" (Prof. P. Friz in RG 6)

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

ERC Starting Grant "EPSILON – Elliptic Partial Differential Equations and Symmetry of Interfaces and Layers for Odd Nonlinearities" (Prof. E. Valdinoci in ERC 1)

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

ERC Starting Grant "EntroPhase – Entropy Formulation of Evolutionary Phase Transitions" (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 Curie Actions Initial Training Network PROPHET (Postgraduate Research on Photonics as an Enabling Technology), Project 1.4 "Modelling of mode-locked QD lasers" (in RG 2). The Initial Training Network PROPHET aims to train young researchers in the field of photonics. This network started in the beginning of 2011 and has been funded for four years by the EU 7th Framework Programme. The Weierstrass Institute (RG 2) is participating in the 1st work package of the network "Photonics Enabling Communications Applications", which is mainly focused on the investigation of quantum dot mode-locked lasers.

EU Marie Skłodowska-Curie Innovative Training Networks – European Industrial Doctorate ITN-EID "MIME-SIS – Mathematics and Materials Science for Steel Production and Manufacturing" (in RG 3 and RG 4)

In October, the Weierstrass Institute saw the launch of the EID project MIMESIS. Driven by the five partners— EFD Induction in Norway; SSAB, Outokumpu, and the University of Oulu in 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



Postgraduate Revearch on hotonics as an Enabling Technolog A Marie Curle Initial Taining Network





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

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.

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

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

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

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

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

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

The Research Initiative *Energy Storage Systems* intends to accelerate the development of energy storage technologies in Germany. The Federal government funds the development of new energy storage technologies and concepts, as well as the improvement of existing techniques. This will create an important precondition for a successful extension of renewable energies. The initiative is supported by the Ministry of Education and Research (BMBF), the Ministry for the Environment, Nature Conservation and Nuclear Safety (BMU), and the Ministry of Economics and Technology (BMWi). In this framework, WIAS (RG 3) runs from 2013 to 2017 the subproject "Makroskopische Modellierung von Transport- und Reaktionsprozessen in Magnesium-Luft-Batterien" (Macroscopic modeling of transport and reaction processes in magnesium-air 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.

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

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

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 Entreprises: 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) ENERGIESPEICHER Forschungsinitiative der Bundesregierung















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 Subproject "Nichtlineare Wahrscheinlichkeitsrestriktionen in Gastransportproblemen" (Nonlinear chance constraints in problems of gas transportation; in RG 4).

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

This research center, which has been funded by the DFG since 2005, focuses on studying economic risk. It was again positively evaluated and prolonged for a third period until the end of 2016. The Weierstrass Institute participates in the Subproject B5 "Structural methods in risk modeling" (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, and finished its second funding period at the end of 2015. The proposal for the third funding period (2016–2019) was successfully defended in July 2015. WIAS participates in the subprojects B4: "Multi-dimensionale Modellierung und Simulation von VCSELn" (Multidimensional modeling and simulation of VCSEL devices; in RG 1, RG 2, and RG 3) 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 and RG 7).

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

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. The review process in 2014 for the second four-year period 2015–2018 was successful. Since then, also the Subproject A3: "Aktivitätsmuster in Systemen mit zeitverzögerten Kopplungen" (Activity patterns in delay-coupled systems; in RG 1 and RG 2) has been treated by WIAS staff members.

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 Universität 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 for the first funding period (Oct. 2010 – Sept. 2013, principal investigators: Prof. B. Wagner and Dr. D. Peschka) and participates now for the second funding period (Oct. 2013 – Sept. 2016, principal investigator: Prof. B.


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Wagner) in the Subproject "Mathematical modeling, analysis, numerical simulation of thin liquid bilayers and validation experiments" (in RG 7)

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. WIAS participates for the first funding period (2012–2015, principal investigator: Prof. W. König) in the Subproject "Branching random walks in random enviroment with a special focus on the intermittent behavior of the particle flow" (in RG 5). In 2015, a second funding for another three years was granted.

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 funding period Oct. 2013 – Sept. 2015) 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. In 2015, a second funding period was granted (Oct. 2015 – Sept. 2017). So far, direct discretizations and operator-splitting methods for uni-variate systems were studied. The assessment of the methods is based on data from experiments that are conducted by one of the project's partners. Numerical methods for solving the population balance equation, which is an integro-partial differential equation, are developed together with two other collaborators.

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 BV functions that lead to sharp approximations of discontinuities on coarse grids and rigorous convergence proofs.

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

WIAS participated in this research unit in the Subproject P5 "Regularisierung und Relaxierung zeitkontinuierlicher Probleme in der Plastizität" (Regularizations and relaxations of time-continuous problems in plasticity"; in RG 1; second funding period: until June 2015).

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 usem it for estimation. RG 6 at WIAS is studying the convergence and efficiency of such algorithms (second funding period until March 2018) in the subprojects "Multiple testing under unspecified dependency structure" and "Semiparametric approach to structural adaptive estimation" (since April 2015 "Semiparametric structural analysis in regression estimation").

Normalverfahren (Individual Grants)

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

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













"Raue 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)

Eigene Stelle (Temporary Positions for Principal Investigators)

"Inverse Fluid-Solid-Kopplungsprobleme" (Inverse fluid-solid interaction problems; G. Hu)

Leibniz-Gemeinschaft (Leibniz Association), Berlin

Leibniz-Wettbewerb (Leibniz Competition)

"Mathematische Modelle für Lithium-Ionen-Batterien" (Mathematical models for Lithium-ion batteries; July 2012 – June 2015, in LG 3)

"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)

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 2015, WIAS again dedicated considerable financial and personal resources to the Center: Its deputy director, Prof. A. Mielke (RG 1) was member of MATHEON'S Executive Board; Prof. B. Wagner (RG 7), Deputy Chairperson of its Council; Prof. D. Hömberg (RG 4), Scientist in Charge of the Application Area C "Energy and Materials", Priv.-Doz. Dr. U. Bandelow (RG 2), Scientist in Charge of the Application Area D "Electronic and Photonic Devices"; 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)

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 Leibniz-DAAD Research Fellowship holder (in RG 3); see page 174
- A DAAD-Michail Lomonosov Programme Fellowship holder (in RG 2); see page 174
- German-Norwegian Collaborative Research Support Scheme (PPP): "Modelle und Numerik f
 ür nanofluidische elektrochemische Systeme" (Models and numerics for nanofluidic electrochemical systems; in RG 3)



Research Center MATHEON Mathematics for Key Technologies

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 is a cooperation between WIAS and the DHI-WASY GmbH Berlin. It is funded by the Investitionsbank Berlin in the framework of its "*Pro* FIT" funding program. The main purpose of the project is knowledge transfer on modern methods for partial differential equations with stochastic coefficients from research to industry. It focuses on the assessment of efficient methods for partial differential equations with stochastic coefficients and the selection of preferred methods to be implemented in the software of the project partner DHI-WASY. In addition, the investigation of stochastic methods for inverse problems will be started.

International projects

- Grant of the Russian Government to establish a Research Group "Predictive Modeling" at the University of Physics and Technology in Moscow for the head of RG 6, V. Spokoiny.
- 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)

- Alstom (Switzerland) Ltd., Baden: "Prozesssimulation bei industriellen Gasturbinen" (Process simulation for industrial gas turbines; in RG 3 and RG 6)
- Deloitte & Touche GmbH Wirtschaftsprüfungsgesellschaftung: Development, implementation, and calibration of multiple-curve interest rate models and evaluation of corresponding interest rate products (in RG 6)
- Mathshop Limited, Salisbury, Wiltshire, UK: Consulting contract (in RG 5)
- Max Planck Institute for Physics, Munich, and Max Planck Institute for Extraterrestrial Physics, Garching: Simulation of semiconductor devices for radiation detectors (in RG 3)
- PAR Medizintechnik GmbH: Consulting on the modeling of pulse waves (in RG 6)
- 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 R&D cooperation is the development of improved algorithms and software for hybrid volumetric meshing based on Voronoi diagrams for geological models.



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A.3 Membership in Editorial Boards

- 1. TH. DICKHAUS, Editorial Board, Statistics, Taylor & Francis, Berlin.
- 2. _____, Editorial Board, Annals of the Institute of Statistical Mathematics, Springer-Verlag, Heidelberg.
- 3. P. FRIZ, Editorial Board, Monatshefte der Mathematik, Springer-Verlag, Berlin.
- 4. _____, Editorial Board, Stochastic Processes and Applications, Elsevier, Oxford, UK.
- Editorial Board, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
- <u>R. HENRION</u>, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
- 7. ——, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
- 8. _____, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
- 9. ——, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
- 10. _____, Editorial Board, Optimization A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
- 11. <u>D. HÖMBERG</u>, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
- 12. ——, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
- 13. W. KÖNIG, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
- 14. P. MATHÉ, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
- 15. _____, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, Netherlands.
- 16. <u>A. MIELKE</u>, (Editor-in-Chief), GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
- 17. _____, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
- 18. _____, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
- 19. , Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
- 20. <u>H. NEIDHARDT</u>, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russian Federation.
- 21. _____, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
- 22. _____, Editorial Board, Journal of Operators, Hindawi Publishing Corporation, New York, USA.
- 23. J. POLZEHL, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
- 24. _____, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, Netherlands.
- 25. J.G.M. SCHOENMAKERS, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.



- 26. ——, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
- 27. _____, Editorial Board, Applied Mathematical Finance, Taylor & Francis, Oxford, UK.
- 28. _____, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
- 29. V. SPOKOINY, Editor, Theory of Probability and its Applications, SIAM, Philadelphia, Pennsylvania, USA.
- 30. J. SPREKELS, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
- 31. ——, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
- 32. _____, Editorial Board, Applied Mathematics and Optimization, Springer-Verlag, New York, USA.
- 33. _____, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
- 34. <u>B. WAGNER</u>, Editorial Board, Journal of Engineering Mathematics, Springer-Verlag, Dordrecht, Netherlands.
- 35. <u>W. WAGNER</u>, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
- 36. S. YANCHUK, Editorial Board, Scientific Reports, Nature Publishing Group, London, UK.

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

3RD ANNUAL ERC BERLIN-OXFORD YOUNG RESEARCHERS MEETING ON APPLIED STOCHASTIC ANALYSIS Berlin, January 27–29 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 contribute to significant progress in the following broad variety of fields: nonlinear stochastic partial differential equations driven by space-time white noise; partial differential equations driven by rough paths; regularity structures and paracontrolled distributions; scaling limits and discrete approximation for stochastic partial differential equations; expected signatures; stochastic Loewner evolution; statistics and machine learning; Gaussian rough path analysis; numerical analysis for stochastic and rough differential equations; financial mathematics.

The three-day workshop attracted around 35 participants and featured 25 invited speakers, mostly early career researchers from Berlin, Oxford, and Warwick, on topics related to the afore-mentioned fields. A fourth Berlin-Oxford meeting was originally scheduled to take place in July in Oxford, close to the 38th Conference on Stochastic Processes and their Applications (SPA2015). Stochastic Processes and their Applications is generally considered the leading conference in probability. However, in view of the large number of invited and (accepted) contributed talks of our community at SPA2015, it was decided to have the next official Berlin-Oxford meeting again in Berlin, in December (see below).

The workshop was jointly organized by the WIAS research group *Stochastic Algorithms and Nonparametric Statistics* (Peter Friz, ERC funded; Mario Maurelli), TU Berlin (Khalil Chouk), and Oxford University (Terry Lyons, ERC funded; Horatio Boedihardjo, Harald Oberhauser).

DYNAMICS AND STABILITY OF INTERACTING NONLINEAR OSCILLATORS AND THEIR APPLICATIONS Berlin, February 13 Organized by: WIAS (RG 1 and RG 2), Humboldt-Universität (HU) zu Berlin Supported by: IRTG 1740, WIAS

The one-day workshop was organized by Serhiy Yanchuk (RG 1), Matthias Wolfrum (RG 2), and Jürgen Kurths (Potsdam Institute for Climate Impact Research (PIK), HU Berlin) and was supported by the International Research Training Group (IRTG) 1740 "Dynamical Phenomena in Complex Networks: Fundamentals and Applications". The main goal of this event was to give the Ph.D. students from the IRTG the opportunity to present their results and to get into discussions with the international experts invited to the workshop. In particular, recent theoretical results concerning propagation delays, collective dynamics, and applications to neuroscience were discussed intensively.

APPLIED MATHEMATICS AND SIMULATION FOR SEMICONDUCTORS — AMASIS 2015 Berlin, March 11–13 Organized by: WIAS (RG 1 and RG 3), Università della Svizzera Italiana Lugano Supported by: DFG, WIAS

The workshop was devoted to modeling, mathematical analysis, and numerical schemata for the simulation of latest semiconductor device designs and materials as well as advances in the actual simulation of such devices. In particular, we were interested in the mathematics involved in novel applications like organic electronics and a new generation of strained germanium-based laser designs.



Fifty-nine scientists from Austria, France, Germany, Great Britain, the Netherlands, Switzerland, Taiwan, and the United States participated in the workshop. Sixteen invited lectures and thirteen contributed talks were presented.

INTERNATIONAL WORKSHOP "STRUCTURED NONPARAMETRIC MODELING"

Berlin, June 4–6

Organized by: WIAS (RG 6)

Supported by: Collaborative Research Center (SFB) 649 "Economic Risk", DFG Research Unit (FOR) 1735 "Structural Inference in Statistics: Adaptation and Efficiency", International Research Training Group (IRTG) 1792 "High Dimensional Non Stationary Time Series", WIAS

The aim of this meeting was bringing together leading scientists working in the areas of mathematical statistics and econometrics for discussing the challenging problems and major directions of modern statistical science. The workshop focused particularly on high-dimensional models under certain structural assumptions like sparsity or approximate sparsity. The program featured 24 invited lectures of high-calibre scientists from reputed universities.

The workshop was also open to young scientists working in different fields of statistics and econometrics all over the world and particularly to the students and young researchers working in Berlin in SFB 649, FOR 1735, and IRTG 1792. The young scientists were invited to offer a poster presentation. This meeting gave them an opportunity of discussion with leading specialists in the fields of statistics and econometrics.

The conference was attended by about 90 participants mainly from Germany and the United States as well as from Korea, France, Russia, UK, and the Netherlands.

MATERIALS WITH DISCONTINUITIES — SAMM 2015 Stuttgart, September 7–11 Organized by: WIAS (RG 1), Universität Stuttgart Supported by: Dr. Klaus Körper Stiftung, Universität Stuttgart, WIAS



The series of SAMM—Summer Schools in Applied Mathematics and Mechanics annually organized by GAMM (International Association of Applied Mathematics and Mechanics) Juniors—aims at fostering the exchange between young scientists in mechanical engineering and applied mathematics by providing insight into recent developments and novel methods in a current research topic of interdisciplinary interest.

SAMM 2015 was devoted to the modeling, analysis, and simulation of materials with discontinuities caused by dissipative processes such as phase transition or separation processes, plastification, damage, and fracture. In minicourses held by Helmut Abels (Regensburg), Sören Bartels (Freiburg), Dorothee Knees (Kassel), and Christian Miehe (Stuttgart), the school gave an overview on thermodynamical modeling, mathematical solution concepts, and numerical schemes for dissipative processes, minimization problems for functions of bounded variation, and phase field models. More than 30 junior scientists, mainly Ph.D. students, both from mathematics and engineering participated in the summer school.



RECENT DEVELOPMENTS IN INVERSE PROBLEMS Berlin, September 17–18 Organized by: WIAS (RG 4 and RG 6) Supported by: WIAS

The workshop brought together experts from the German and international inverse problems community and young scientists. This event was a part of the "Chemnitz Symposium on Inverse Problems", previously held in Chemnitz (2014), Shanghai (2013), and Canberra (2012).

The focus was on ill-posedness phenomena, regularization theory, and on the analytical, numerical, and stochastic treatment of applied inverse problems from natural sciences, engineering, and finance.

The two-day workshop attracted 60 participants from 12 countries. There were four plenary talks. Simon R. Arridge (University College London), Christian Clason (Universität Duisburg-Essen), Otmar Scherzer (University of Vienna), and Samuli Siltanen (University of Helsinki) presented important recent trends in the field. Contributed talks were presented in two parallel sessions, among them 12 by Ph.D. students, who talked about their work.

The workshop was jointly organized by the WIAS research groups *Stochastic Algorithms and Nonparametric Statistics* (Peter Mathé) and *Nonlinear Optimization and Inverse Problems* (Guanghui Hu).

WAVES, SOLITONS AND TURBULENCE IN OPTICAL SYSTEMS (WASTOS 2015) Berlin, October 12–14 Organized by: WIAS (RG 2) Supported by: Einstein Center for Mathematics Berlin, Research Center MATHEON, WIAS

Nonlinear optical systems display a great variety of complex dynamical behaviors in space and time. Along with the regular dynamical regimes associated with continuous waves, periodic and quasiperiodic patterns or solitons, high-dimensional irregular dynamics with a very large number of exited modes can be observed. The understanding of mechanisms underlying such kind of behavior, known as optical turbulence, is, perhaps, one of the most difficult and challenging problems in nonlinear optics. The three-day workshop was aimed at bringing applied mathematicians and theoretical and experimental physicists together to discuss recent advances concerning experimental findings and theoretical investigation of such dynamical phenomena, as optical wave turbulence, optical solitons and rogue waves, supercontinua generation, spatio-temporal dynamics in active and passive optical cavities, and effects related to the control of optical systems by delayed feedback. The program featured 31 invited and contributed talks presented by speakers from 11 countries and was attended by 39 registered participants.

FESTIVE EVENT ON THE OCCASION OF THE 200TH BIRTHDAY OF KARL WEIERSTRASS Berlin, October 31 Organized by: WIAS

Supported by: BBAW, HU Berlin, Deutsche Mathematiker-Vereinigung, Einstein Center for Mathematics Berlin, Berlin Mathematical School, Springer

The 200th birthday of the eminent Berlin mathematician Karl Weierstrass, whose name WIAS bears, was honored by a festive event in the worthy premises of the Berlin-Brandenburg Academy of Sciences (BBAW). A number of addresses were made by outstanding personalities, among them Germany's Minister of Education and Research, Prof. Johanna Wanka. The scientific part of the program consisted of nine talks on historical and mathematical aspects of Weierstrass, delivered by eminent international historians. These nine speakers delivered short versions of their contributions to a Festschrift that was published shortly before by Springer and was edited by the former director of WIAS, Jürgen Sprekels, jointly with the current Authorised Representative of the Director, Wolfgang König. About 600 personalities, mainly mathematicians and historians, from all over Northeast Germany had been invited to attend the event, and more than 120 of them came to enjoy it. DIRECT AND INVERSE PROBLEMS FOR PDES WITH RANDOM COEFFICIENTS Berlin, November 9–13 Organized by: WIAS (RG 3 and RG 4) Supported by: Research Center MATHEON, WIAS

Validated predictive computations in a wide range of scientific and engineering applications require some form of uncertainty quantification. The goal of this workshop was to bring together researchers from scientific computing with those working in optimal control and inverse problems to discuss different applications, the analysis and numerical treatment of PDEs with stochastic data. Sixty-eight participants from ten countries discussed various topics related to efficient numerical methods for the direct problem, control problems with uncertainties, sparse and low-rank tensor representations, and inverse problems with random data.

THEORY AND APPLICATIONS OF PARTIAL DIFFERENTIAL EQUATIONS — PDE 2015 Berlin, November 30 – December 4 Organized by: WIAS (RG 1, ERC 1, and ERC 2), Universität Kassel Supported by: DFG, WIAS



PDE 2015 - Theory and Applications of Partial Differential Equations

The workshop was organized by Hans-Christoph Kaiser, Alexander Mielke, Joachim Rehberg, Elisabetta Rocca, Marita Thomas, and Enrico Valdinoci from WIAS and Dorothee Knees from Universität Kassel.

Its aim was to bring together analysts furthering the theory of PDEs and scientists working on applications involving nonsmooth PDEs. Within PDE theory, the workshop focused on harmonic and geometric analysis and inequalities, (nonsmooth) evolution equations, and elliptic systems. Applications to problems with free and moving boundaries as well as dissipative solids were discussed.

The generous funding through the German Research Foundation (DFG) made it possible to invite 20 researchers from eight different countries. In total, 100 researchers from 16 countries participated in the workshop, contributing alltogether 48 talks and poster presentations.

4TH ANNUAL ERC BERLIN-OXFORD YOUNG RESEARCHERS MEETING ON APPLIED STOCHASTIC ANALYSIS Berlin, December 7–9 Organized by: WIAS (RG 6), TU Berlin, Oxford University Supported by: European Research Council, WIAS

After the third meeting in January 2015, and also after a significant presence of this community through invited and contributed talks in July at SPA 2015 in Oxford, this was the fourth Berlin-Oxford meeting on applied stochastic analysis. As in previous years, there was an emphasis on the powerful insights of pathwise analysis (Lyons' rough paths, Hairer's regularity structures, paracontrolled distributions à la Gubinelli–Imkeller– Perkowski), especially in the context of nonlinear (stochastic) partial differential equations. However, these ideas are applicable in many other areas of applied mathematics. As presented in talk by Terry Lyons (Oxford) himself, there have been striking applications in deep learning: The best presently available algorithm for handwritten Chinese character recognition is indeed a rough path inspired and based on iterated integrals.

The three-day workshop attracted around 56 participants and featured 27 invited speakers, mainly early career researchers from Berlin, Oxford, and additionally some people from Warwick, Imperial College London, Paris, and Rennes.



The workshop was jointly organized by the WIAS research group *Stochastic Algorithms and Nonparametric Statistics* (Peter Friz, ERC funded), Technische Universität (TU) Berlin (Martina Hofmanova), Humboldt-Universität zu Berlin (Nicolas Perkowski), and Oxford University (Terry Lyons, ERC funded; Ilya Chevyrev, Xi Geng).

STOCHASTIC LIMIT ANALYSIS FOR REACTING PARTICLE SYSTEMS Berlin, December 16–18 Organized by: WIAS (RG 5) Supported by: Einstein Center for Mathematics Berlin, Collaborative Research Center (SFB) 1114 "Scaling Cascades in Complex Systems"

This workshop was organized by the WIAS Research Group RG 5 *Interacting Random Systems* (Wolfgang König, Michiel Renger, Robert Patterson).It presented and facilitated discussion on approaches to systems of many particles, which at some level of modeling undergo spatial motion and stochastically interact when they collide or at least get very close. Classic applications of such systems include gas dynamics, particle coagulation, and chemical reactions, but zoological and other application areas were also considered. Hence, this workshop lay in the intersection of the interests of (at least) WIAS research groups RG 1 *Partial Differential Equations* and RG 5. The three mornings of the workshop were devoted to two minicourses delivered by the eminent international experts James Norris (Cambridge) and Vassili Kolokoltsov (Warwick); in the afternoons, several guests and WIAS members gave accounts on their research results. About 50 people from Berlin and from other cities attended the workshop.

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

JUNIOR FEMALE RESEARCHERS IN PROBABILITY

Berlin, October 22-23

Organized by: DFG Research Training Group 1845 "Stochastic Analysis with Applications in Biology, Finance and Physics"

Supported by: Technische Universität Berlin, Universität Potsdam, Berlin Mathematical School, WIAS

The goal of the workshop was to offer junior female researchers in stochastics a platform to talk about their own research work and to get acquainted with important research topics presented by well-established female researchers. To cover various topics in probability and its applications, several invited talks were given, as well as a number of contributed talks. The workshop was one of the activities of the DFG Graduate School in Stochastic Processes for the support of young females in this field. About 50 participants enjoyed the talks and the relaxed atmosphere provided by the WIAS premises and organization.

A.4.3 Oberwolfach Workshops co-organized by WIAS

WORKSHOP "INTERPLAY OF ANALYSIS AND PROBABILITY IN APPLIED MATHEMATICS" Mathematisches Forschungsinstitut Oberwolfach, July 26 – August 1 Organized by: Volker Betz (Darmstadt), Wolfgang König (RG 5), Florian Theil (Coventry), Johannes Zimmer (Bath)

This workshop brought together about 50 analysts and probabilists working on problems at some of the many interfaces of these two fields. Most of the problems discussed during the meeting have their origin in physics or chemistry. The workshop was grouped around the four themes (1) condensation in random structures, (2) disordered systems, (3) discrete-to-continuum transitions, and (4) atomistic and molecular systems. The organizers feel that the communication between the two communities has become a lot more intense and natural since the last of the three Oberwolfach workshops that had this purpose. Early-career researchers received broad space to present their results.

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

- 1. U. BANDELOW, member of the Program Committee, *CLEO*®/*Europe EQEC 2015*, Munich, June 21–25.
- <u>A. CAIAZZO</u>, organizer of the minisymposium "Boundary Challenges in Clinically Relevant Physiological Flow Simulations", 4th International Conference on Computational & Mathematical Biomedical Engineering, Ecole Normale Supérieure de Cachan, Cachan, France, June 29 – July 1.
- 3. <u>D. HÖMBERG</u>, organizer of the minisymposium "Recent Results on Analysis and Optimal Control of Phase Field Models", *27th IFIP TC7 Conference 2015 on System Modelling and Optimization*, Sophia Antipolis, France, June 29 July 3.
- 4. <u>V. JOHN</u>, organizer of the minisymposium "Finite Element Methods for Convection-dominated Problems", *European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2015)*, Ankara, Turkey, September 14–18.
- L. KAMENSKI, organizer of the minisymposium "Anisotropic Mesh Adaptation", International Conference on Scientific Computation and Differential Equations (SciCADE 2015), Universität Potsdam, Campus Griebnitzsee, September 14–18.
- 6. <u>O. KLEIN</u>, member of the Steering Committee, 10th International Symposium on Hysteresis Modeling and Micromagnetics (HMM), Iasi, Romania, May 18–20.
- 7. <u>W. KÖNIG</u>, co-organizer, *Workshop "Interplay of Analysis and Probability in Applied Mathematics"*, Mathematisches Forschungsinstitut Oberwolfach, July 26 August 1.
- 8. <u>M. LANDSTORFER</u>, organizer and chair of the minisymposium "Recent Developments on Electrochemical Interface Modeling", *8th International Congress on Industrial and Applied Mathematics (ICIAM 2015)*, International Council for Industrial and Applied Mathematics, Beijing, China, August 10–14.
- 9. <u>A. MIELKE</u>, member of the International Scientific Committee, *2nd International Conference on Continuous Media with Microstructure (CMwM2015)*, Łagów, Poland, March 2–5.
- <u>O. OMEL'CHENKO</u>, organizer of the minisymposium "Emergent Dynamics and Control", *The 8th International Conference on Chaotic Modeling, Simulation and Applications (CHAOS2015)*, Institut Henri Poincaré, Paris, France, May 26–29.
- 11. <u>R.I.A. PATTERSON</u>, co-organizer of the minisymposium "Real World Phenomena Explained by Microscopic Particle Models", *8th International Congress on Industrial and Applied Mathematics (ICIAM 2015)*, International Council for Industrial and Applied Mathematics, Beijing, China, August 10.
- <u>D. PESCHKA</u>, co-organizer of the minisymposium "Free Boundary Problems in Applications: Recent Advances in Modelling, Simulation and Optimization", 8th Vienna International Conference on Mathematical Modelling (MATHMOD 2015), Technische Universität Wien, Institut für Analysis und Scientific Computing, Vienna, Austria, February 17–20.
- 13. ——, co-organizer of the minisymposium "Recent Progress in Modeling and Simulation of Multiphase Thin-film Type Problems", 8th International Congress on Industrial and Applied Mathematics (ICIAM 2015), International Council for Industrial and Applied Mathematics, Beijing, China, August 10–14.
- 14. <u>D.R.M. RENGER</u>, co-organizer of the minisymposium "Real World Phenomena Explained by Microscopic Particle Models", *8th International Congress on Industrial and Applied Mathematics (ICIAM 2015)*, International Council for Industrial and Applied Mathematics, Beijing, China, August 10.
- 15. <u>E. ROCCA</u>, co-organizer of the special session "Applied Analysis", *86th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2015)*, Lecce, Italy, March 23–27.

- 16. ——, member of the Scientific and Organizing Committee, *INdAM Workshop "Special Materials in Complex Systems SMaCS 2015"*, Rome, Italy, May 18–22.
- 17. ——, course director, *Mathematical Thermodynamics of Complex Fluids*, Fondazione CIME "Roberto Conti" (International Mathematical Summer Center), Cetraro, Italy, June 29 July 3.
- N. ROTUNDO, co-organizer of the minisymposium "Numerical and Analytical Aspects in Semiconductor Theory", 8th International Congress on Industrial and Applied Mathematics (ICIAM 2015), International Council for Industrial and Applied Mathematics, Beijing, China, August 10–14.
- 19. <u>H. SI</u>, co-organizer, *24th International Meshing Roundtable*, University of Texas at Austin, AT&T Conference Center, Austin, USA, October 12–14.
- <u>V. SPOKOINY</u>, co-organizer, Frontiers of High Dimensional Statistics, Optimization, and Econometrics, Higher School of Economics, Laboratory of Stochastic Analysis and its Applications, Moscow, Russian Federation, February 25–27.
- 21. ——, organizer, *Spring School "Structural Inference in Statistics" 2015*, Humboldt-Universität zu Berlin, DFG Research Unit 1735, Sylt, March 16–20.
- 22. ——, head of the Organizing Committee, *Optimization and Applications in Control and Data Science*, Moscow Institute of Physics and Technology, PreMoLab, Russian Federation, May 13–15.
- 23. J. SPREKELS, member of the Scientific Committee, 2nd International Conference on Continuous Media with Microstructure (CMwM2015), Łagów, Poland, March 2–5.
- 24. <u>M. THOMAS</u>, co-organizer of the minisymposium "Analysis of Nonsmooth PDE Systems with Application to Material Failure", *8th International Congress on Industrial and Applied Mathematics (ICIAM 2015)*, International Council for Industrial and Applied Mathematics, Beijing, China, August 10–14.
- 25. <u>E. VALDINOCI</u>, co-organizer, 2° Corso Intensivo di Calcolo delle Variazioni, Dipartimento di Matematica e Informatica di Catania, Italy, June 15–20.
- 26. <u>A.G. VLADIMIROV</u>, member of the Program Committee, *CLEO*®/*Europe EQEC* 2015, Munich, June 21–25.
- 27. ——, member of the Program Committee, *International Workshop "Nonlinear Photonics: Theory, Materials, Applications"*, St. Petersburg State University, St. Petersburg, Russian Federation, June 29 July 2.
- _____, member of the Program Committee, International Symposium on Physics and Applications of Laser Dynamics, Laboratoire Matériaux Optiques, Photonique et Systèmes (LMOPS), Metz, France, November 4– 6.
- 29. <u>W. WAGNER</u>, member of the Program Committee, *10th IMACS Seminar on Monte Carlo Methods*, Johannes Kepler Universität Linz, Linz, Austria, July 6–10.
- 30. <u>M. WOLFRUM</u>, co-organizer of the minisymposium "Coupled Oscillator Systems and their Mean-field Dynamics", *EQUADIFF 2015*, Lyon, France, July 6–10.
- , co-organizer of the minisymposium "Delay-equations for Optoelectronic Systems", XXXV Dynamics Days Europe 2015, University of Exeter, Centre for Systems, Dynamics and Control, Exeter, UK, September 7–10.
- <u>S. YANCHUK</u>, co-organizer of the minisymposium "Delay-equations for Optoelectronic Systems", XXXV Dynamics Days Europe 2015, University of Exeter, Centre for Systems, Dynamics and Control, Exeter, UK, September 7–10.
- , co-organizer, Workshop on Control of Self-organizing Nonlinear Systems, SFB 910 "Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application", Lutherstadt Wittenberg, September 14–16.

A.6 Publications

A.6.1 Monographs

- A. MIELKE, T. ROUBÍČEK, Rate-independent Systems. Theory and Application, vol. 193 of Applied Mathematical Sciences, Springer International Publishing, New York, 2015, vii+660 pages.
- [2] V. SPOKOINY, <u>TH. DICKHAUS</u>, *Basics of Modern Mathematical Statistics*, vol. 18 of Springer Texts in Statistics, Springer, Berlin et al., 2015, 296 pages.

Monographs (to appear)

[1] <u>W. KÖNIG</u>, *The Parabolic Anderson Model: Random Walks in Random Potential*, Pathways in Mathematics, Springer.

A.6.2 Editorship of Proceedings and Collected Editions

- P. FRIZ, J. GATHERAL, A. GULISASHVILI, A. JAQUIER, J. TEICHMANN, eds., Large Deviations and Asymptotic Methods in Finance, vol. 110 of Springer Proceedings in Mathematics & Statistics, Springer, Berlin et al., 2015, ix+590 pages.
- [2] D. HÖMBERG, G. HU, eds., Issue on the workshop "Electromagnetics Modelling, Simulation, Control and Industrial Applications", vol. 8, no. 3 of Discrete Contin. Dyn. Syst. Ser. S, American Institute of Mathematical Sciences, Springfield, 2015, 259 pages.
- [3] P. COLLI, G. GILARDI, <u>D. HÖMBERG</u>, <u>E. ROCCA</u>, eds., Special Issue dedicated to Jürgen Sprekels on the Occasion of his 65th Birthday, vol. 35, no. 6 of Discrete Contin. Dyn. Syst. Ser. A, American Institute of Mathematical Sciences, Springfield, 2015, 472 pages.
- [4] P. EXNER, W. KÖNIG, H. NEIDHARDT, eds., Mathematical Results in Quantum Mechanics. Proceedings of the QMath12 Conference, World Scientific Publishing, Singapore, 2015, xii+383 pages.
- [5] B. FIEDLER, M. HARAGUS, <u>A. MIELKE</u>, G. RAUGEL, Y. YI, eds., Special Issue in Memoriam of Klaus Kirchgässner, vol. 27 of J. Dynam. Differential Equations, no. 3–4 (pp. 333–1006), Springer International Publishing, Cham et al., 2015, 674 pages.
- [6] ST. BOSIA, M. ELEUTERI, <u>E. ROCCA</u>, <u>E. VALDINOCI</u>, eds., *Preface: Special issue on rate-independent evolutions and hysteresis modelling*, vol. 8 of Discrete and Continuous Dynamical Systems Series S, no. 4, American Institute of Mathematical Sciences, Springfield, 2015, 167 pages.
- [7] E. VALDINOCI, ed., Contemporary PDEs between theory and applications, vol. 35 of Discrete and Continuous Dynamical Systems Series A, no. 12, American Institute of Mathematical Sciences, Springfield, 2015, 625 pages.

Proceedings and Collected Editions (to appear)

[1] M. DIMIAN, P. GUREVICH, <u>O. KLEIN</u>, D. KNEES, D. RACHINSKII, S. TIKHOMIROV, eds., Proceedings of MURPHYS-HSFS-2014 (the 7th Multi-Rate Processes and Hysteresis (MURPHYS) workshop, in conjunction with the second International Workshop on Hysteresis and Slow-Fast Systems (HSFS)), Special Edition of Journal of Physics: Conference Series, IOP Publishing. 171

[2] <u>W. KÖNIG</u>, J. SPREKELS, eds., Karl Weierstraβ (1815–1897): Aspekte seines Lebens und Werkes—Aspects of his Life and Work, Mathematik – Analysis, Springer Spektrum, Wiesbaden.

A.6.3 Outstanding Contributions to Monographs

- S. AMIRANASHVILI, Chapter 3: Hamiltonian Framework For Short Optical Pulses, in: New Approaches to Nonlinear Waves, E. Tobisch, ed., vol. 908 of Lecture Notes in Physics, Springer International Publishing, Cham, 2015, pp. 153–196.
- B. HILLER, CH. HAYN, <u>H. HEITSCH</u>, <u>R. HENRION</u>, H. LEÖVEY, A. MÖLLER, W. RÖMISCH, *Chapter 14: Methods for Verifying Booked Capacities*, *in: Evaluating Gas Network Capacities*, Th. Koch, B. Hiller, M.E. Pfetsch, L. Schewe, eds., MOS-SIAM Series on Optimization, SIAM, Philadelphia, 2015, pp. 291–315.
- [3] <u>H. HEITSCH, R. HENRION</u>, H. LEÖVEY, R. MIRKOV, A. MÖLLER, W. RÖMISCH, I. WEGNER-SPECHT, *Chapter 13: Empirical Observations and Statistical Analysis of Gas Demand Data, in: Evaluating Gas Network Capacities*, Th. Koch, B. Hiller, M.E. Pfetsch, L. Schewe, eds., MOS-SIAM Series on Optimization, SIAM, Philadelphia, 2015, pp. 273–290.
- [4] <u>A. MIELKE</u>, Chapter 5: Variational Approaches and Methods for Dissipative Material Models with Multiple Scales, in: Analysis and Computation of Microstructure in Finite Plasticity, S. Conti, K. Hackl, eds., vol. 78 of Lecture Notes in Applied and Computational Mechanics, Springer International Publishing, Heidelberg et al., 2015, pp. 125–155.
- [5] H.-J. MUCHA, H.-G. BARTEL, J. DOLATA, C. MORALES-MERINO, An Introduction to Clustering with Applications to Archaeometry, in: Mathematics and Archaeology, J.A. Barcelo, I. Bogdanovic, eds., CRC Press, Boca Raton, FL, 2015, pp. 190–213.

Contributions to Monographs (to appear)

 <u>A. MIELKE</u>, On Evolutionary Γ - Convergence for Gradient Systems, A. Muntean, J.D. Rademacher, A. Zagaris, eds., Lecture Notes in Applied Mathematics and Mechanics, Springer International Publishing, Heidelberg et al.

A.6.4 Articles in Refereed Journals²

- [1] P. COLLI, G. GILARDI, J. SPREKELS, A boundary control problem for the pure Cahn–Hilliard equation with dynamic boundary conditions, Adv. Nonlinear Anal., 4 (2015), pp. 311–325.
- J. ELSCHNER, G. HU, Corners and edges always scatter, Inverse Problems, 31 (2015), pp. 015003/1– 015003/17.
- [3] ——, Elastic scattering by unbounded rough surfaces: Solvability in weighted Sobolev spaces, Appl. Anal., 94 (2015), pp. 251–278.
- [4] J. ELSCHNER, G. HU, M. YAMAMOTO, Uniqueness in inverse elastic scattering from unbounded rigid surfaces of rectangular type, Inverse Probl. Imaging, 9 (2015), pp. 127–141.
- [5] G. Hu, J. Li, H. Liu, Uniqueness in determining refractive indices by formally determined far-field data, Appl. Anal., 94 (2015), pp. 1259–1269.
- [6] G. HU, X. LIU, F. QU, B. ZHANG, Variational approach to rough surface scattering problems with Neumann and generalized impedance boundary conditions, Comm. Math. Sci., 13 (2015), pp. 511–537.



²Articles that have been written by long-term guests and scholarship holders during their stay at WIAS have been listed in front of those written by the WIAS staff members.

- S. SIMONELLA, M. PULVIRENTI, On the evolution of the empirical measure for hard-sphere dynamics, Bull. Inst. Math. Acad. Sin., 10 (2015), pp. 171–204.
- [8] S. SIMONELLA, H. SPOHN, From Newton to Boltzmann: Hard spheres and short-range potentials, Bull. Amer. Math. Soc. (N.S.), 52 (2015), pp. 533–538.
- [9] N. AHMED, G. MATTHIES, Higher order continuous Galerkin–Petrov time stepping schemes for transient convection-diffusion-reaction equations, ESAIM Math. Model. Numer. Anal., 49 (2015), pp. 1429–1450.
- [10] N. AHMED, V. JOHN, Adaptive time step control for higher order variational time discretizations applied to convection-diffusion equations, Comput. Methods Appl. Mech. Engrg., 285 (2015), pp. 83–101.
- [11] <u>S. AMIRANASHVILI</u>, R. ČIEGIS, <u>M. RADZIUNAS</u>, Numerical methods for generalized nonlinear Schrödinger equations, Kinet. Relat. Models, 8 (2015), pp. 215–234.
- [12] F. ANKER, S. GANESAN, V. JOHN, E. SCHMEYER, A comparative study of a direct discretization and an operator-splitting solver for population balance systems, Comput. Chem. Engng., 75 (2015), pp. 95– 104.
- [13] <u>CH. BAYER</u>, H.A. HOEL, A. KADIR, P. PLECHAC, M. SANDBERG, A. SZEPESSY, Computational error estimates for Born–Oppenheimer molecular dynamics with nearly crossing potential surfaces, Appl. Math. Res. Express, 2015 (2015), pp. 329–417.
- [14] S. BIRKHOLZ, <u>C. BRÉE</u>, A. DEMIRCAN, G. STEINMEYER, *Predictability of rogue events*, Phys. Rev. Lett., 114 (2015), pp. 213901/1–213901/5.
- [15] C. BRÉE, M. KRETSCHMAR, T. NAGY, H.G. KURZ, U. MORGNER, M. KOVAČEV, Impact of spatial inhomogeneities on on-axis pulse reconstruction in femtosecond filaments, J. Phys. B, 48 (2015), pp. 094002/1– 094002/6.
- [16] I. BREMER, R. HENRION, A. MÖLLER, Probabilistic constraints via SQP solver: Application to a renewable energy management problem, Comput. Manag. Sci., 12 (2015), pp. 435–459.
- [17] <u>A. CAIAZZO</u>, R. GUIBERT, Y. BOUDJEMLINE, I.E. VIGNON-CLEMENTEL, Efficient blood flow simulations for the design of stented valve reducer in enlarged ventricular outflow tracts, Cardiovasc. Eng. Technol., 6 (2015), pp. 485–500.
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- [19] <u>A. CAIAZZO</u>, I. RAMIS-CONDE, Multiscale modeling of palisade formation in glioblastoma multiforme, J. Theor. Biol., 383 (2015), pp. 145–156.
- [20] <u>K. DISSER</u>, Well-posedness for coupled bulk-interface diffusion with mixed boundary conditions, Analysis (Berlin), 35 (2015), pp. 309–317.
- [21] <u>K. DISSER</u>, <u>H.-CHR. KAISER</u>, J. <u>REHBERG</u>, Optimal Sobolev regularity for linear second-order divergence elliptic operators occurring in real-world problems, SIAM J. Math. Anal., 47 (2015), pp. 1719–1746.
- [22] <u>K. DISSER</u>, <u>M. LIERO</u>, On gradient structures for Markov chains and the passage to Wasserstein gradient flows, Netw. Heterog. Media, 10 (2015), pp. 233–253.
- [23] K. DISSER, M. MEYRIES, J. REHBERG, A unified framework for parabolic equations with mixed boundary conditions and diffusion on interfaces, J. Math. Anal. Appl., 430 (2015), pp. 1102–1123.
- [24] D. BOTHE, <u>W. DREYER</u>, Continuum thermodynamics of chemically reacting fluid mixtures, Acta Mech., 226 (2015), pp. 1757–1805.
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- [137] M. SÁEZ, <u>E. VALDINOCI</u>, On the evolution by fractional mean curvature, Preprint no. 2183, WIAS, Berlin, 2015.
- [138] T. AHNERT, A. MÜNCH, B. NIETHAMMER, <u>B. WAGNER</u>, Stability of concentrated suspensions under Couette and Poiseuille flow, Preprint no. 2159, WIAS, Berlin, 2015.
- [139] W. WAGNER, A random cloud model for the Wigner equation, Preprint no. 2083, WIAS, Berlin, 2015.
- [140] ——, A random walk model for the Schrödinger equation, Preprint no. 2109, WIAS, Berlin, 2015.
- [141] M. WOLFRUM, O. OMEL'CHENKO, J. SIEBER, Regular and irregular patterns of self-localized excitation in arrays of coupled phase oscillators, Preprint no. 2069, WIAS, Berlin, 2015.
- [142] <u>M. WOLFRUM</u>, S. GUREVICH, <u>O. OMEL'CHENKO</u>, *Turbulence in the Ott–Antonsen equation for arrays of coupled phase oscillators*, Preprint no. 2135, WIAS, Berlin, 2015.
- [143] S. YANCHUK, G. GIACOMELLI, Dynamical systems with multiple, long delayed feedbacks: Multiscale analysis and spatio-temporal equivalence, Preprint no. 2125, WIAS, Berlin, 2015.
- [144] S. YANCHUK, P. PERLIKOWSKI, M. WOLFRUM, A. STEFAŃSKI, T. KAPITANIAK, Amplitude equations for collective spatio-temporal dynamics in arrays of coupled systems, Preprint no. 2070, WIAS, Berlin, 2015.

A.7.2 Preprints/Reports in other Institutions

 R. ALLEZ, J. BUN, J.-P. BOUCHAUD, The eigenvectors of Gaussian matrices with an external source, arXiv:1412.7108, Cornell University Library, arXiv.org, Ithaca, USA, 2015.

- [2] J. BUN, <u>R. ALLEZ</u>, J.-P. BOUCHAUD, M. POTTERS, *Rotational invariant estimator for general noisy matrices*, arXiv:1502.06736, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [3] <u>P. FRIZ</u>, A. SHEKHAR, On the existence of SLE trace: Finite energy drivers and non-constant SkS, arXiv:1212.5888, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [4] <u>R. HILDEBRAND</u>, L. LOKUTSIEVSKIY, M. ZELIKIN, *Typicalness of chaotic fractal behaviour of integral vortexes in Hamiltonian systems with discontinuous right hand side*, arXiv:1506.02320, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [5] <u>G. HU</u>, M. SALO, E.V. VESALAINEN, Shape identification in inverse medium scattering problems with a single far-field pattern, arXiv:1507.07846, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [6] <u>A. MIELKE</u>, M.A. PELETIER, <u>D.R.M. RENGER</u>, *A generalization of Onsager's reciprocity relations to gradient flows with nonlinear mobility*, arXiv:1510.06219, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [7] D. BELOMESTNY, ST. HAEFNER, <u>T. NAGAPETYAN</u>, M. URUSOV, *Higher order variance reduction for discretised diffusions via regression*, arXiv:1510.03141, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [8] J. BEHRNDT, M.M. MALAMUD, <u>H. NEIDHARDT</u>, Scattering matrices and Dirichlet-to-Neumann maps, arXiv:1510.06219, Cornell University Library, arXiv.org, Ithaca, USA, 2015.
- [9] E.K. YAPP, <u>R.I.A. PATTERSON</u>, J. AKROYD, S. MOSBACH, E.M. ADKINS, J.H. MILLER, M. KRAFT, Numerical simulation and parametric sensitivity study of optical band gap in a laminar co-flow ethylene diffusion flame, Technical report no. 159, University of Cambridge, c4e-Preprint Series, Cambridge, UK, 2015.
- [10] K.F. LEE, <u>R.I.A. PATTERSON</u>, <u>W. WAGNER</u>, M. KRAFT, Stochastic weighted particle methods for population balance equations with coagulation, fragmentation and spatial inhomogeneity, Technical report no. 154, University of Cambridge, c4e-Preprint Series, Cambridge, UK, 2015.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Main and Plenary Talks

- D. HÖMBERG, Modelling, analysis and simulation of multifrequency induction hardening, XXIV Congress on Differential Equations and Applications (CEDYA)/XIV Congress on Applied Mathematics (CMA), June 8–12, Universidad de Cádiz, Spain, June 11.
- 2. <u>H. NEIDHARDT</u>, *Trace formulas for non-additive perturbations*, Conference "Spectral Theory and Applications", May 25–29, AGH University of Science and Technology, Krakow, Poland, May 28.
- M. RADZIUNAS, Computation and analysis of longitudinal optical modes in multisection ring and edgeemitting semiconductor lasers, 20th International Conference on Mathematical Modeling and Analysis (MMA 2015), May 25–29, Sigulda, Latvia, May 27.
- 4. <u>V. SPOKOINY</u>, *Feature selection by "simplest accepted" rule*, Information Technologies and Systems 2015, September 6–11, Russian Academy of Sciences, Institute for Information Transmission Problems, Sochi, Russian Federation, September 7.

A.8.2 Scientific Talks (Invited)

- 1. G. Hu, Shape identification in inverse medium scattering with a single far-field pattern, Workshop "Inverse Problems for PDEs", June 2–3, Université de Reims Champagne-Ardenne, France, June 2.
- 2. ——, Shape identification in inverse medium scattering with a single far-field pattern, Tsing Hua University, Yau Mathematical Sciences Center, Beijing, China, June 9.
- 3. ——, Direct and inverse acoustic, elastic and electromagnetic scattering problems, Beijing Computational Science Research Center, China, June 11.
- 4. _____, Direct and inverse acoustic scattering by a collection of extended and point-like scatterers, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, June 13.
- J. SPREKELS, Optimal boundary control problems for Cahn-Hilliard systems with dynamic boundary conditions, INdAM Workshop "Special Materials in Complex Systems – SMaCS 2015", May 18–22, Rome, Italy, May 21.
- 6. <u>R. ALLEZ</u>, *A continuous approach to random matrix theory*, Stochastic Analysis Seminar, Imperial College London, Department of Mathematics, UK, February 10.
- 7. <u>U. BANDELOW</u>, Applied mathematical research in photonics at WIAS Berlin, Innovation Days 2015, December 8–9, Leibniz-Gemeinschaft, Berlin, December 9.
- 8. <u>CH. BAYER</u>, *The forward-reverse method for conditional diffusion processes*, Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2015), January 6–9, King Abdullah University of Science and Technology (KAUST), Jeddah, Saudi Arabia, January 6.
- 9. ——, The forward-reverse method for conditional diffusion processes, Oberseminar Finanz- und Versicherungsmathematik, Technische Universität München, Fakultät für Mathematik, January 19.
- Asymptotics beats Monte Carlo: The case of correlated local vol baskets, Groupe de Travail: Finance Mathématique, Probabilités Numériques et Statistique des Processus, Université Paris Diderot, Laboratoire de Probabilités et Modèles Aléatoires, France, February 19.
- 11. ——, *Pricing under rough volatility*, Berlin-Princeton-Singapore Workshop on Quantitative Finance, June 29 July 1, National University of Singapore, Centre for Quantitative Finance, Singapore, June 29.

- , The forward-reverse method for conditional Markov processes, MInisymposium "Multilevel Monte Carlo Methods and Applications" of the 8th International Congress on Industrial and Applied Mathematics (ICIAM2015), August 10–14, International Council for Industrial and Applied Mathematics, Beijing, China, August 10.
- The forward-reverse method for conditional Markov processes, International Conference on Scientific Computation and Differential Equations, Universität Potsdam, Institut für Mathematik, September 16.
- 14. ——, *Pricing under rough volatility*, Imperial College London, Department of Mathematics, UK, November 3.
- 15. _____, SDE based regression for random PDEs, Direct and Inverse Problems for PDEs with Random Coefficients, WIAS Berlin, November 13.
- 16. ——, *Rough paths and rough partial differential equations*, 2 talks, University of Oslo, Department of Mathematics, Norway, November 16–18.
- 17. ——, *Pricing under rough volatility*, Finanzmathematik, University of Vienna, Faculty of Mathematics, Austria, November 26.
- L. BLANK, CGS Taking advantage of the irregular convergence behavior, Università della Svizzera Italiana, Institute of Computational Science, Lugano, Switzerland, December 16.
- <u>C. BréE</u>, Impact of resonance-enhanced ionization on femtosecond filamentation, International Workshop "Nonlinear Photonics: Theory, Materials, Applications", Session: Extreme and Relativistic Nonlinear Optics, June 28 – July 4, St. Petersburg State University, St. Petersburg, Russian Federation, July 2.
- A model of intense laser-matter interaction based on complex-rotated Floquet resonances, 24th Annual International Laser Physics Workshop (LPHYS'15), Seminar 5: Nonlinear Optics & Spectroscopy, August 21–25, Shanghai, China, August 23.
- 21. ——, Numerical modelling of femtosecond filamentation, Leibniz-Universität Hannover, Institut für Quantenoptik, Hannover, September 7.
- 22. <u>A. CAIAZZO</u>, *Multiscale modeling of weakly compressible elastic materials in harmonic regime*, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Numerische Simulation, Bonn, May 21.
- 23. , A Stokes-residual based backflow stabilization for incompressible flows, XXIV Congreso de Ecuaciones Diferenciales y Aplicaciones, June 8–12, Universidad de Cádiz, Cádiz, Spain, June 10.
- Modeling and simulation of fluid flows through a porous interface, Besançon Week on Numerical Analysis: XFEM, Nitsche FEM, Adaptive FEM, Artificial Boundary Conditions, June 15–21, Université de Franche Comté, Besançon, France, June 19.
- Assessment of Kalman filtering for parameter identification in one-dimensional blood flow model, 4th International Conference on Computational & Mathematical Biomedical Engineering, June 29 – July 1, Ecole Normale Supérieure de Cachan, Cachan, France, June 29.
- Multiscale modeling of weakly compressible elastic materials, Workshop on Aktive Drag Reduction, November 9–10, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, Aachen, November 10.
- 27. <u>E. CINTI</u>, A quantitative weighted isoperimetric inequality via the ABP method, Oberseminar Analysis, Universität Bonn, Institut für Angewandte Mathematik, February 5.
- Quantitative isoperimetric inequality via the ABP method, Università di Bologna, Dipartimento di Matematica, Bologna, Italy, July 17.
- <u>A. CIPRIANI</u>, Rates of convergence for extremes of geometric random variables and marked point processes, Università degli Studi di Milano-Bicocca, Dipartimento di Matematica Applicazioni, Milano, Italy, March 30.



- 30. ——, Thick points for generalized Gaussian fields with different cut-offs, Indian Statistical Institute, Theoretical Statistics and Mathematics Unit, Kolkata, India, April 8.
- 31. ——, *Extremes of the supercritical Gaussian free field*, Seminar Series in Probability and Statistics, Technical University of Delft, Applied Mathematics, Netherlands, June 11.
- 32. ——, *Extremes of the supercritical Gaussian free field*, Probability Seminar, Leiden University, Netherlands, June 18.
- *Extremes of the super critical Gaussian free field*, Workshop "Women in Probability 2015", July 3–4, Technische Universität München, July 3.
- , Rates of convergence for extremes of geometric random variables and marked point processes, Workshop "Interplay of Analysis and Probability in Applied Mathematics", July 26 – August 1, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, July 28.
- 35. <u>F. DASSI</u>, Achievements and challenges in anisotropic mesh generation, Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milano, Italy, November 17.
- <u>TH. DICKHAUS</u>, Simultaneous test procedures in high dimensions: The extreme value approach, 4th Annual International Conference on CMCGS 2015, January 26–27, Global Science and Technology Forum (GSTF), Singapore, January 26.
- , Self-concordant profile empirical likelihood ratio tests for the population correlation coefficient: A simulation study, 12th Workshop on Stochastic Models, Statistics and Their Applications, February 16– 20, Wrocław University of Technology, Poland, February 17.
- 38. <u>K. DISSER</u>, *Asymptotic behavior of a rigid body with a cavity filled by a viscous liquid*, Oberseminar "Analysis", Universität Kassel, Institut für Mathematik, Kassel, January 12.
- Asymptotic behavior of a rigid body with a cavity filled by a viscous liquid, Seminar "Dynamische Systeme", Technische Universität München, Zentrum Mathematik, München, February 2.
- 40. ——, Asymptotic behavior of a rigid body with a cavity filled by a viscous liquid, Workshop "Young Researchers in Fluid Dynamics", June 18–19, Technische Universität Darmstadt, Fachbereich Mathematik, Darmstadt, June 18.
- Asymptotic behavior of a rigid body with a cavity filled by a viscous liquid, Mathematical Thermodynamics of Complex Fluids, June 29 – July 3, Centro Internazionale Matematico Estivo (CIME), Cetraro, Italy, June 30.
- 42. <u>W. DREYER</u>, *Stochastic modelling of many-particle electrodes*, Solid State Electrochemistry Workshop 2015, September 6–9, Kloster Roggenburg, September 7.
- 43. ——, *Stochastic theory of many-particle systems*, 12th Hirschegg Workshop on Conservation Laws, September 13–19, Hirschegg, Kleinwalsertal, Austria, September 15.
- 44. <u>P. DVURECHENSKY</u>, Semi-supervised pagerank model learning with gradient-free optimization methods, Traditional Youth School "Control, Information and Optimization", June 14–20, Moscow, Russian Federation, June 17.
- 45. ——, Stochastic intermediate gradient method: Convex and strongly convex cases, Information Technologies and Systems 2015, September 6–11, Russian Academy of Sciences, Institute for Information Transmission Problems, Sochi, Russian Federation, September 9.
- 46. <u>M. EIGEL</u>, *Stochastic adaptive FEM*, Forschungsseminar Numerische Mathematik, Humboldt-Universität zu Berlin, Institut für Mathematik, January 28.
- 47. ——, *Guaranteed error bounds for adaptive stochastic Galerkin FEM*, Technische Universität Braunschweig, Institut für Wissenschaftliches Rechnen, April 1.

- 48. ——, Adaptive stochastic Galerkin FEM with hierarchical tensor representations, 2nd GAMM AGUQ Workshop on Uncertainty Quantification, September 10–11, Chemnitz, September 10.
- 49. <u>M.H. FARSHBAF SHAKER</u>, Relating phase field and sharp interface approaches to structural topology optimization, National Institute for Mathematical Sciences, Division of Computational Mathematics, Daejeon, Korea (Republic of), May 13.
- _____, Introduction into optimal control of partial differential equations, 2 talks, National Institute for Mathematical Sciences, Division of Computational Mathematics, Daejeon, Korea (Republic of), May 14– 18.
- , A deep quench approach to the optimal control of an Allen–Cahn equation with dynamic boundary conditions, National Institute for Mathematical Sciences, Division of Computational Mathematics, Daejeon, Korea (Republic of), May 20.
- A relaxation approach to vector-valued Allen–Cahn MPEC problems, 27th IFIP TC7 Conference 2015 on System Modelling and Optimization, Minisymposium 20: Recent Results on Analysis and Optimal Control of Phase Field Models, June 29 July 3, Sophia Antipolis, France, July 2.
- 53. ——, Multi-material phase field approach to structural topology optimization and its relation to sharp interface approach, University of Tokyo, Graduate School of Mathematical Sciences, Japan, October 6.
- 54. ——, Multi-material phase field approach to structural topology optimization and its relation to sharp interface approach, Ehime University, Department of Mathematics, Matsuyama, Japan, October 16.
- 55. ——, Optimal boundary control of a viscous Cahn–Hilliard system with dynamic boundary condition and double obstacle potentials, Conference "Developments of the Theory of Evolution Equations as Applications of the Analysis for Nonlinear Phenomena", October 21–23, Kyoto University, Japan, October 22.
- 56. <u>F. FLEGEL</u>, Localization of the first Dirichlet-eigenvector in the heavy-tailed random conductance model, Workshop "Interplay of Analysis and Probability in Applied Mathematics", July 26 – August 1, Mathematisches Forschungsinstitut Oberwolfach, July 30.
- 57. ——, Localization of the first Dirichlet-eigenvector in the heavy-tailed random conductance model, Summer School 2015 of the RTG 1845 Berlin-Potsdam "Stochastic Analysis with Applications in Biology, Finance and Physics", September 28 October 3, Levico Terme, Italy, October 1.
- <u>S.P. FRIGERI</u>, Recent results on optimal control for Cahn-Hilliard/Navier-Stokes systems with nonlocal interactions, Control Theory and Related Topics, April 13–14, Politecnico di Milano, Italy, April 13.
- 59. ——, On a diffuse interface model of tumor growth, INdAM Workshop "Special Materials in Complex Systems SMaCS 2015", May 18–22, Rome, Italy, May 22.
- On a nonlocal diffuse interface model for binary incompressible fluids with different densities, Mathematical Thermodynamics of Complex Fluids, June 28 – July 3, Fondazione CIME "Roberto Conti" (International Mathematical Summer Center), Cetraro, Italy, July 2.
- 61. <u>P. FRIZ</u>, *Rough paths*, Kolloquium, Westfählische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, January 15.
- 62. ——, *Lecture Series on Rough Path*, 4 talks, Junior Hausdorff Trimester Program "Optimal Transportation", January 5 – April 24, Hausdorff Research Institute for Mathematics, Bonn, March 23–25.
- 63. ——, *Rough Paths and Regularity Structures*, 4 talks, Courses for Graduates, April 21–23, Cambridge University, Faculty of Mathematics, April 21–23.
- 64. ——, *Rough Paths and Regularity Structures*, 4 talks, Courses for Graduates, April 28–30, Cambridge University, Faculty of Mathematics, April 28–30.
- 65. ——, *Rough Paths and Regularity Structures*, 4 talks, Courses for Graduates, May 4–7, Cambridge University, Faculty of Mathematics, May 4–7.



- *Eikonal equations and fully non-linear SPDEs*, 38th Conference on Stochastic Processes and their Applications, July 13–17, University of Oxford, Oxford-Man Institute of Quantitative Finance, UK, July 15.
- 67. ——, *Rough paths and regularity structures*, 38th Conference on Stochastic Processes and their Applications, July 13–17, University of Oxford, Oxford-Man Institute, UK, July 16.
- 68. J. FUHRMANN, Boundary heat and mass transfer: Analytical and numerical approaches, Summer School of the International Max Planck Research School in Process and Systems Engineering, August 31 – September 2, Magdeburg, September 1.
- <u>A. GLITZKY</u>, Finite volume discretized reaction-diffusion systems in heterostructures, Conference on Partial Differential Equations, March 25–29, Technische Universität München, Zentrum Mathematik, München, March 28.
- <u>A. GONZÁLEZ CASANOVA SOBERÓN</u>, Modeling the Lenski experiment, Genealogies in Evolution: Looking Backward and Forward, Workshop of the Priority Program (SPP) 1590 "Probabilistic Structures in Evolution", October 5–6, Goethe-Universität Frankfurt, October 6.
- 71. ——, An individual-based model for the Lenski experiment, and the deceleration of the relative fitness, Workshop on Probabilistic Models in Biology, October 24–30, Playa del Carmen, Mexico, October 28.
- <u>C. GUHLKE</u>, Revision of the Poisson-Nernst-Planck equations in the context of thermodynamic consistency, 7th International Workshop and Summer School on Nonequilibrium Thermodynamics (IWNET 2015), July 5–10, Hilvarenbeek, Netherlands, July 10.
- 73. ——, *Stochastic modeling of many-particle electrodes*, Group Seminar Multiphysikalische Modellierung, Helmholtz-Institut Ulm für elektrochemische Energiespeicherung, November 18.
- 74. <u>O. GUN</u>, *Branching random walks in random environments on hypercubes*, Workshop on Random Walk in Random Environment, March 22–27, European Institute for Statistics, Probability, Stochastic Operations Research and their Applications (EURANDOM), Eindhoven, Netherlands, March 27.
- Fluid and diffusion limits for the Poisson encounter-mating model, Mini-Workshop on Population Dynamics, April 6–17, Bögaziçi University Istanbul, Department of Mathematics, Istanbul, Turkey, April 6.
- *Stochastic encounter-mating model*, Mathematical Model in Ecology and Evolution (MMEE 2015), July 7–13, Collège de France, Paris, France, July 8.
- M. HEIDA, Modeling of fluid interfaces, Jahrestagung der Deutschen Mathematiker-Vereinigung, Minisymposium "Mathematics of Fluid Interfaces", September 21–25, Universität Hamburg, Fakultät für Mathematik, Informatik und Naturwissenschaften, Hamburg, September 23.
- <u>CH. HEINEMANN</u>, Well-posedness of strong solutions for a damage model in 2D, Universitá di Brescia, Department DICATAM – Section of Mathematics, Italy, March 13.
- <u>CH. HEINEMANN</u>, On elastic Cahn–Hilliard systems coupled with evolution inclusions for damage processes, 86th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2015), Young Researchers' Minisymposium 2, March 23–27, Lecce, Italy, March 23.
- 80. ——, Solvability of differential inclusions describing damage processes and applications to optimal control problems, Universität Essen-Duisburg, Fakultät für Mathematik, Essen, December 3.
- <u>H. HEITSCH</u>, Optimization of booked capacity in gas transport networks using nonlinear probabilistic constraints, 2nd International Symposium on Mathematical Programming (ISMP 2015), Cluster "Optimization in Energy Systems", July 13–17, Pittsburgh, USA, July 17.
- 82. <u>R. HENRION</u>, *Conditioning of linear-quadratic two-stage stochastic optimization problems*, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, March 26.
- 83. ——, *Calmness as a constraint qualification for MPECs*, International Conference on Variational Analysis, Optimization and Quantitative Finance in Honor of Terry Rockafellar's 80th Birthday, May 18–22, Université de Limoges, France, May 21.

- 84. ——, On some relations between probability functions and variational analysis, International Workshop "Variational Analysis and Applications", August 28 – September 5, Erice, Italy, August 31.
- (Sub-) Gradient formulae for probability functions with Gaussian distribution, PGMO Days 2015

 Gaspard Monge Program for Optimization and Operations Research, October 27–28, ENSTA ParisTech, Palaiseau, France, October 28.
- 86. ——, (Sub-)Gradient formulae for probability functions with applications to power management, Universidad de Chile, Centro de Modelamiento Matemático, Santiago de Chile, Chile, November 25.
- <u>R. HILDEBRAND</u>, Geometry of barriers for 3-dimensional cones, Optimization and Applications in Control and Data Science, May 13–15, Moscow Institute of Physics and Technology, PreMoLab, Moscow, Russian Federation, May 15.
- <u>CH. HIRSCH</u>, Asymptotic properties of collective-rearrangement algorithms, International Conference on Geometry and Physics of Spatial Random Systems, September 6–11, Karlsruher Institut für Technology (KIT), Bad Herrenalb, September 7.
- 89. <u>M. HOFMANN</u>, *Numerical solution of the time dependent Schrödinger equation*, Seminar Week, Leibniz-Universität Hannover, Institut für Quantenoptik, Ultrafast Laser Laboratory, Dahnsdorf, October 7.
- 90. <u>D. Hömberg</u>, Optimal coefficient control for semilinear parabolic equations, Fudan University, School of Mathematical Sciences, Shanghai, China, March 10.
- 91. ——, *A crash course on optimal control*, Fudan University, School of Mathematical Sciences, Shanghai, China, March 18.
- 92. ——, Nucleation, growth, and grain size evolution in multiphase materials, INdAM Workshop "Special Materials in Complex Systems SMaCS 2015", May 18–22, Rome, Italy, May 21.
- 93. ——, The digital factory A perspective for a closer cooperation between math and industry, Workshop "Mathematics and Computer Science in Practice: Potential and Reality", December 9–11, Prague, Czech Republic, December 9.
- 94. <u>B. JAHNEL</u>, Classes of non-ergodic interacting particle systems with unique invariant measure, Kac-Seminar, April 30 – May 3, Utrecht University, Department of Mathematics, Netherlands, May 1.
- Classes of nonergodic interacting particle systems with unique invariant measure, Workshop "Recent Trends in Stochastic Analysis and Related Topics", September 20–21, Universität Hamburg, September 21.
- 96. ——, Classes of nonergodic interacting particle systems with unique invariant measure, Kyoto University, Research Institute for Mathematical Sciences, Kyoto, Japan, November 16.
- 97. V. JOHN, A survey on the analysis and numerical analysis of some turbulence models, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, München, June 23.
- <u>L. KAMENSKI</u>, A simple implementation for variational mesh generation by means of a geometric discretization, International Workshop on Moving Mesh and High Order Numerical Methods, August 5–8, Xiamen University, Fujian, China, August 7.
- On the conditioning of the linear finite element equations with arbitrary anisotropic grids, International Conference on Scientific Computation and Differential Equations (SciCADE 2015), September 14–18, Universität Potsdam, Campus Griebnitzsee, September 15.
- P. KEELER, When do wireless network signals appear Poisson?, 18th Workshop on Stochastic Geometry, Stereology and Image Analysis, March 22–27, Universität Osnabrück, Lingen, March 24.
- 101. ——, When do wireless network signals appear Poisson?, Simons Conference on Networks and Stochastic Geometry, May 18–21, University of Texas, Austin, USA, May 20.

- 102. ——, *The Poisson–Dirichlet process and coverage in mobile phone networks*, Stochastic Processes and Special Functions Workshop, August 13–14, The University of Melbourne, Melbourne, Australia, August 14.
- 103. _____, Large-deviation theory and coverage in mobile phone networks, Seminar "Applied Probability", The University of Melbourne, Department of Mathematics and Statistics, Australia, August 17.
- 104. <u>O. KLEIN</u>, *A representation result for rate-independent systems*, 10th International Symposium on Hysteresis Modeling and Micromagnetics (HMM), May 18–20, Iasi, Romania, May 19.
- 105. <u>W. KÖNIG, Cluster size distribution in classical many-body systems with Lennard–Jones-type potential,</u> Basque Center for Applied Mathematics, Bilbao, Spain, January 20.
- 106. ——, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Heriot-Watt University, Department of Mathematics, Analysis Seminar, Edinburgh, UK, January 23.
- 107. ——, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, University of Warwick, Mathematics Institute, Coventry, UK, February 11.
- 108. ——, *Cluster size distribution in classical many-body systems with Lennard–Jones potential*, 18th Workshop on Stochastic Geometry, Stereology and Image Analysis, March 22–26, Universität Osnabrück, Lingen, March 24.
- 109. ——, *Moment asymptotics for a branching random walk in random environment*, Applied Mathematics Seminars, University of Warwick, Mathematics Institute, Coventry, UK, November 6.
- 110. <u>M. LANDSTORFER</u>, *Theory, structure and experimental justification of the metal/electrolyte interface*, Workshop on Mathematical Modelling of Synthetic Nanopores, March 4–5, Technische Universität Darmstadt, March 5.
- 111. ——, Theory, structure and experimental justification of the metal/electrolyte interface, Minisymposium "Recent Developments on Electrochemical Interface Modeling" of the 8th International Congress on Industrial and Applied Mathematics (ICIAM 2015), August 10–14, International Council for Industrial and Applied Mathematics, Beijing, China, August 11.
- 112. ——, *Thermodynamics of the metal/electrolyte interface*, Solid State Electrochemistry Workshop 2015, September 6–9, Kloster Roggenburg, September 7.
- 113. <u>M. LIERO</u>, OLEDS eine heiβe Sache?, Organische Leuchtdioden, Workshop im Handlungsfeld Lichttechnik, OpTec Berlin Brandenburg e.V., Berlin, May 18.
- 114. ——, On dissipation distances for reaction-diffusion equations The Hellinger–Kantorovich distance, Workshop "Collective Dynamics in Gradient Flows and Entropy Driven Structures", June 1–5, Gran Sasso Science Institute, L'Aquila, Italy, June 3.
- 115. ——, On p(x)-Laplace thermistor models describing electrothermal feedback in organic semiconductor devices, Università di Pavia, Dipartimento di Matematica, Pavia, Italy, November 17.
- 116. <u>A. LINKE</u>, *Robust discretization of the Coriolis force in Navier–Stokes flows on unstructured grids*, Workshop "Galerkin Methods with Applications in Weather and Climate Forecasting", March 23–27, International Centre for Mathematical Sciences, Edinburgh, UK, March 24.
- 117. ——, Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations, Technische Universität Wien, Analysis und Scientific Computing, Wien, August 26.
- 118. ——, *Toward pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Université de Montpellier, Institut Montpelliérain Alexander Grothendieck, Montpellier, France, November 24.
- 119. ——, Über neue Entwicklungen bei der Diskretisierung der inkompressiblen Navier-Stokes-Gleichungen: Druckrobustheit und Konstruktion von Benchmarks, Universität Paderborn, Theoretische Physik, Paderborn, December 2.

- 120. <u>P. MATHÉ</u>, *IBC for unbounded operators*, Workshop on Information-Based Complexity and Model Selection, April 9–10, Université Pierre et Marie Curie, Institut Henri Poincaré, Paris, France, April 9.
- 121. ——, *IBC for Bayesian approximation*, Information-Based Complexity, April 27 May 2, Polish Academy of Sciences, Banach Center, Bedlewo, Poland, April 29.
- 122. ——, *Minicourse on Computational Statistics*, 5 talks, Fudan University, The School of Mathematical Sciences, Shanghai, China, May 12–22.
- 123. ——, *Some IBC for ill-posed equations*, Regularization Theory of Unstructured Data, May 15–16, Fudan University, Shanghai, China, May 16.
- 124. ——, *Minimax signal detection in statistical inverse problems*, Algorithms and Complexity for Continuous Problems, September 21–25, Schloss Dagstuhl, September 25.
- 125. <u>M. MAURELLI</u>, Stochastic 2D Euler equations: A poorly correlated multiplicative noise regularizes the twopoint motion, Universität Augsburg, Institut für Mathematik, March 24.
- 126. ——, Enhanced Sanov theorem for Brownian rough paths and an application to interacting particles, Seminar Stochastic Analysis, Imperial College London, UK, October 20.
- 127. <u>A. MIELKE</u>, The Chemical Master Equation as a discretization of the Fokker–Planck and Liouville equation for chemical reactions, Colloquium of Collaborative Research Center/Transregio "Discretization in Geometry and Dynamics", Technische Universität Berlin, Institut für Mathematik, Berlin, February 10.
- 128. ——, *The Chemical Master Equation as entropic gradient flow*, Conference "New Trends in Optimal Transport", March 2–6, Universität Bonn, Institut für Angewandte Mathematik, March 2.
- 129. ——, *Mathematical modeling for finite-strain elastoplasticity*, Intensive Period on Variational Methods for Plasticity and Dislocations, March 16–20, International School of Advanced Studies (SISSA), Trieste, Italy, March 16.
- 130. ——, *The multiplicative strain decomposition in finite-strain elastoplasticity*, Intensive Period on Variational Methods for Plasticity and Dislocations, March 16–20, International School of Advanced Studies (SISSA), Trieste, Italy, March 17.
- 131. ——, Abstract approach to energetic solutions for rate-independent solutions, Intensive Period on Variational Methods for Plasticity and Dislocations, March 16–20, International School of Advanced Studies (SISSA), Trieste, Italy, March 18.
- 132. ——, *Existence results in finite-strain elastoplasticity*, Intensive Period on Variational Methods for Plasticity and Dislocations, March 16–20, International School of Advanced Studies (SISSA), Trieste, Italy, March 19.
- 133. ——, *A mathematical approach to finite-strain viscoplasticity*, Intensive Period on Variational Methods for Plasticity and Dislocations, March 16–20, International School of Advanced Studies (SISSA), Trieste, Italy, March 20.
- 134. ——, *Evolutionary* Γ -convergence for gradient systems explained via applications, Symposium "Variational Methods for Stationary and Evolutionary Problems", University of Warwick, Mathematics Institute, Warwick, UK, May 12.
- Homogenizing the Penrose–Fife system via evolutionary Γ -convergence, INdAM Workshop "Special Materials in Complex Systems SMaCS 2015", May 18–20, Rome, Italy, May 19.
- Evolutionary Γ-convergence for generalized gradient systems, Workshop "Gradient Flows", June 22–23, Université Pierre et Marie Curie, Laboratoire Jacques-Louis Lions, Paris, France, June 22.
- 137. ——, Geometric approaches at and for theoretical and applied mechanics, Phil Holmes Retirement Celebration, October 8–9, Princeton University, Mechanical and Aerospace Engineering, New York, USA, October 8.

- 138. ——, *Evolutionary relaxation of a two-phase model*, Mini-Workshop "Scales in Plasticity", November 8– 14, Mathematisches Forschungsinstitut Oberwolfach, November 11.
- 139. <u>H.-J. MUCHA</u>, *Inequality measures and clustering*, International Workshop on Partial Orders in Applied Sciences, April 9–10, Università degli Studi di Firenze, Centro Studi Cisl, Italy, April 9.
- 140. ——, Validation of K-means clustering: Why is bootstrapping better than subsampling?, European Conference on Data Analysis 2015, September 2–4, University of Essex, Department of Mathematical Sciences, Colchester, UK, September 2.
- 141. , *A fast pre-clustering method by iterative binary binning*, Herbsttagung der AG Datenanalyse und numerische Klassifikation, November 20–21, Karlsruher Institut für Technologie, November 21.
- 142. <u>CH. MUKHERJEE</u>, *Compactness, large deviations and the mean-field polaron problem*, Workshop "Interplay of Analysis and Probability in Applied Mathematics", July 27–31, Mathematisches Forschungsinstitut Oberwolfach, July 28.
- 143. <u>R. MÜLLER</u>, *Modeling of ion transport in nanopores*, Workshop "Multiscale Transport of Particles", September 14–16, Wolfgang Pauli Institute, Vienna, Austria, September 15.
- 144. <u>H. NEIDHARDT</u>, *Boundary triplets and trace formulas*, Workshop "Spectral Theory and Weyl Function", January 5–9, Mathematisches Forschungsinstitut Oberwolfach, January 5.
- 145. ——, Boundary triplet approach and tensor products, Seminar "Angewandte Analysis und Numerische Mathematik", Technische Universität Graz, Institut für Numerische Mathematik, Graz, Austria, January 29.
- 146. <u>O. OMEL'CHENKO</u>, *Controlling unstable chaos in systems of coupled oscillators*, The 8th International Conference on Chaotic Modeling, Simulation and Applications (CHAOS2015), Minisymposium "Emergent Dynamics and Control", May 25–30, Institut Henri Poincaré, Paris, France, May 28.
- 147. ——, *Chimera states in systems with control*, EQUADIFF 2015, Minisymposium 3 "Coupled Oscillator Systems and their Mean-Field Dynamics", July 6–10, Lyon, France, July 9.
- 148. ——, *Chimera states for any taste*, Dynamics of Coupled Oscillators: 40 Years of the Kuramoto Mode, July 27–31, Max Planck Institute for the Physics of Complex Systems, Dresden, July 27.
- 149. ——, *Creative control of chimera states*, XXXV Dynamics Days Europe 2015, Minisymposium "Controlling Complex Networks: Interplay of Structure, Noise, and Delay", September 6–11, University of Exeter, Centre for Systems, Dynamics and Control, UK, September 9.
- 150. ——, *Paradoxes of the Kuramoto model*, Seminar of the Department of Mathematics, Lomonosov Moscow State University, Russian Federation, November 25.
- 151. <u>ST. PATRIZI</u>, Dislocations dynamics: From microscopic models to macroscopic crystal plasticity, Analysis Seminar, The University of Texas at Austin, Department of Mathematics, USA, January 21.
- 152. ——, Dislocations dynamics: From microscopic models to macroscopic crystal plasticity, Seminar, King Abdullah University of Science and Technologie, SRI – Center for Uncertainty Quantification in Computational Science & Engineering, Jeddah, Saudi Arabia, March 25.
- 153. ——, On a long range segregation model, Seminario di Analisi Matematica, Sapienza Università di Roma, Dipartimento di Matematica "Guido Castelnuovo", Italy, April 20.
- 154. ——, On a long range segregation model, Seminar, Università degli Studi di Salerno, Dipartimento di Matematica, Italy, May 19.
- 155. <u>R.I.A. PATTERSON</u>, *Uniqueness and regularity for coagulation-advection problems*, Workshop on Theory and Numerics of Kinetic Equations, June 1–4, Universität Saarbrücken, June 2.
- 156. J. PELLERIN, Tackling the geometrical complexity of structural models in mesh generation, Meshing Workshop, March 19–20, Technische Universität Bergakademie Freiberg, Institut für Geophysik & Geoinformatik, Freiberg, March 20.

- 157. ———, Voronoi-based remeshing of surface structural models: Latest advancements, Société TOTAL E&P RECHERCHE DEVELOPPEMENT SAS, Pau, France, June 25.
- 158. D. PESCHKA, Modeling and applications of bilayer flows, Seminar of the Research Training Group GRK 1276 "Structure Formation and Transport in Complex Systems", Universität des Saarlandes, Institut für Theoretische Physik, Saarbrücken, January 27.
- 159. ——, *Thin-film equations with free boundaries*, Jahrestagung der Deutschen Mathematiker-Vereinigung, Minisymposium "Mathematics of Fluid Interfaces", September 21–25, Universität Hamburg, Fakultät für Mathematik, Informatik und Naturwissenschaften, Hamburg, September 23.
- <u>A. PIMENOV</u>, Theoretical analysis of pulse timing jitter in mode-locked semiconductor lasers, International Symposium "Semiconductor Nanophotonics", November 2–3, Technische Universität Berlin, November 2.
- 161. J. POLZEHL, Statistical problems in diffusion weighted MR, University of Minnesota, Biostatistics-Statistics Working Group in Imaging, Minneapolis, USA, January 30.
- 162. ——, *Noise quantification in MR experiments*, Joint Statistical Meetings 2015, August 10–13, Seattle, USA, August 12.
- —, Analysing dMRI data: Consequences of low SNR, SAMSI Working group "Structural Connectivity", Statistical and Applied Mathematical Sciences Institute (SAMSI), Research Triangle Park, USA, December 8.
- 164. <u>M. RADSZUWEIT</u>, A non-isothermal phase-field model for damage in biphasic brittle materials, 13th US National Congress on Computational Mechanics, July 26–30, San Diego, California, USA, July 27.
- 165. <u>M. RADZIUNAS</u>, *Modeling, simulation and analysis of nonlinear dynamics in multisection semiconductor lasers*, Research Seminar, Gediminas Technical University, Department of Mathematical Modelling, Vilnius, Lithuania, April 16.
- 166. ——, Nonlinear dynamics in mode locked lasers: Modeling, simulations and analysis, 5th International Conference "Telecommunications, Electronics and Informatics" (ICTEI 2015), May 20–24, Chisinau, Moldova, May 21.
- 167. J. REHBERG, On maximal parabolic regularity and its applications, Oberseminar "Mathematische Optimierung", Technische Universität München, Lehrstuhl für Optimalsteuerung, München, May 6.
- 168. ——, On maximal parabolic regularity, The Fourth Najman Conference on Spectral Problems for Operators and Matrices, September 20–25, University of Zagreb, Department of Mathematics, Opatija, Croatia, September 23.
- 169. <u>S. REICHELT</u>, *Two-scale homogenization of reaction-diffusion systems involving different diffusion length scales*, CASA Colloquium, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), Eindhoven, Netherlands, March 11.
- 170. <u>D.R.M. RENGER</u>, *The inverse problem: From gradient flows to large deviations*, Workshop "Analytic Approaches to Scaling Limits for Random System", January 26–30, Universität Bonn, Hausdorff Research Institute for Mathematics, January 26.
- 171. ——, Large deviations for reacting particle systems: The empirical and ensemble processes, Workshop "Interplay of Analysis and Probability in Applied Mathematics", July 26 August 1, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, July 30.
- 172. ——, The empirical process of reacting particles: Large deviations and thermodynamic principles, Minisymposium "Real World Phenomena Explained by Microscopic Particle Models" of the 8th International Congress on Industrial and Applied Mathematics (ICIAM 2015), August 8–22, International Council for Industrial and Applied Mathematics, Beijing, China, August 10.

- 173. ——, From large deviations to Wasserstein gradient flows in multiple dimensions, Workshop on Gradient Flows, Large Deviations and Applications, November 22–29, EURANDOM, Mathematics and Computer Science Department, Eindhoven, Netherlands, November 23.
- 174. <u>E. ROCCA</u>, Optimal control of a nonlocal convective Cahn–Hilliard equation by the velocity, Numerical Analysis Seminars, Durham University, UK, March 13.
- 175. J.G.M. SCHOENMAKERS, Uniform approximation of the CIR process via exact simulation at random times, Berlin-Princeton-Singapore Workshop on Quantitative Finance, June 29 – July 1, National University of Singapore, Centre for Quantitative Finance, Singapore, July 1.
- 176. <u>H. Sı</u>, *TetGen, a Delaunay-based tetrahedral mesh generator*, Commissariat à l'Énergie Atomique et aux Énergies Alternatives, Bruyères-le-Châtel, France, July 10.
- 177. <u>R. SOARES DOS SANTOS</u>, *Random walk on a dynamic random environment consisting of a system of independent simple symmetric random walks*, Oberseminar Stochastik, Technische Universität Darmstadt, Fachbereich Mathematik, Darmstadt, January 22.
- 178. ——, *Random walk on random walks*, YEP XII: Workshop on Random Walk in Random Environment, March 23–27, Technical University of Eindhoven, EURANDOM, Netherlands, March 24.
- 179. ———, *Random walk on random walks*, Mathematical Physics Seminar, Université de Genève, Section de Mathématiques, Genève, Switzerland, April 27.
- 180. ——, *Mass concentration in the parabolic Anderson model*, Oberseminar Stochastik, Johannes-Gutenberg-Universität, Institut für Mathematik, Mainz, November 17.
- 181. <u>V. SPOKOINY</u>, Bootstrap confidence sets under model misspecification, Optimization and Statistical Learning, January 11–16, Institut National de Recherche en Informatique et en Automatique (INRIA), Les Houches, France, January 15.
- 182. ——, Mini Course "Methods of Model Selection", 6 talks, Methods of Model Selection, February 16 March 3, Independent University of Moscow, Moscow Center for Continuous Mathematical Education, Russian Federation, February 16 – March 3.
- 183. ——, Bootstrap based methods in model selection, WISE-CASE Workshop on Econometrics and Statistics, July 4–5, Xiamen University, China, July 4.
- 184. ——, Bootstrap calibrated model selection, CRC 649 "Economic Risk" Conference in Motzen, July 16– 18, Humboldt-Universität zu Berlin, Motzen, July 17.
- 185. ——, *Predictive modeling: Methods and applications*, Skolkov Institute of Science and Technology, Moscow, Russian Federation, August 27.
- 186. ——, Bootstrap tuning in model selection, Lomonosov State University, Faculty of Computer Sciences, Moscow, Russian Federation, September 18.
- 187. ——, Nonparametric regression estimation in error-in-variable models, Inverse Problems in Econometrics, October 2–3, Northwestern University, Evanston, USA, October 2.
- 188. ——, *Bootstrap confidence sets*, Welcome Workshop 2015 of the International Research Training Group "High Dimensional Non Stationary Time Series", October 5, Grünheide, October 5.
- 189. ——, Bootstrap-based methods for model, Meeting in Mathematical Statistics 2015 (MMS 2015), December 14–18, Fréjus, France, December 17.
- 190. J. SPREKELS, Optimal boundary control problems for Cahn–Hilliard systems with singular potentials and dynamic boundary conditions, Romanian Academy, Simeon Stoilow Institute of Mathematics, Bucharest, March 18.

- 191. <u>K. TABELOW</u>, *msPOAS An adaptive denoising procedure for dMRI data*, Riemannian Geometry in Shape Analysis and Computational Anatomy, February 23–27, Universität Wien, Erwin Schrödinger International Institute for Mathematical Physics, Austria, February 25.
- 192. , *To smooth or not to smooth in fMRI*, Seminar "Bildgebende Verfahren in den Neurowissenschaften: Grundlagen und aktuelle Ergebnisse", Universitätsklinikum Jena, IDIR, Medical Physics Group, April 17.
- 193. <u>M. THOMAS</u>, Rate-independent damage models with spatial BV-regularization Existence & fine properties of solutions, Oberseminar "Angewandte Analysis", Universität Freiburg, Abteilung für Angewandte Mathematik, Freiburg, February 10.
- 194. ——, *Coupling rate-independent and rate-dependent processes: Existence results*, Applied Mathematics Seminar, Università di Pavia, Dipartimento di Matematica, Pavia, Italy, March 5.
- 195. ——, Coupling rate-independent and rate-dependent processes: Existence and evolutionary Gamma convergence, INdAM Workshop "Special Materials in Complex Systems SMaCS 2015", May 18–22, Rome, Italy, May 19.
- 196. ——, Evolutionary Gamma convergence with application to damage and delamination, Seminar DI-CATAM, Università di Brescia, Dipartimento di Matematica, Brescia, Italy, June 3.
- 197. ——, Analysis of nonsmooth PDE systems with application to material failure—towards dynamic fracture, Minisymposium "Analysis of Nonsmooth PDE Systems with Application to Material Failure" of the 8th International Congress on Industrial and Applied Mathematics (ICIAM 2015), August 10–14, International Council for Industrial and Applied Mathematics, Beijing, China, August 12.
- 198. <u>E. VALDINOCI</u>, *Nonlocal problems Theory and applications*, 5 talks, School/Workshop "Phase Transition Problems and Nonlinear PDEs", March 9–11, Università di Bologna, Dipartimento di Matematica, March 9–11.
- 199. ——, Nonlocal minimal surfaces, Seminario di Calcolo delle Variazioni & Equazioni alle Derivate Parziali, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Italy, March 13.
- 200. ——, Minimal surfaces and phase transitions with nonlocal interactions, Analysis Seminar, University of Edinburgh, School of Mathematics, UK, March 23.
- 201. ——, What is the (fractional) Laplacian?, Perlen-Kolloquium, Universität Basel, Fachbereich Mathematik, Switzerland, May 22.
- 202. ——, Nonlocal problems and applications, 3 talks, Summer School on "Geometric Methods for PDEs and Dynamical Systems", June 8–11, École Normale Supérieure de Lyon, Unité de Mathématiques Pures et Appliquées and Institut de Mathématiques, Equipe d'Analyse, Université Bordeaux 1, Porquerolles, France, June 9–10.
- 203. ——, Nonlocal Problems in Analysis and Geometry, 5 talks, 2° Corso Intensivo di Calcolo delle Variazioni, June 15–20, Dipartimento di Matematica e Informatica di Catania, Italy, June 15–19.
- 204. ——, Some models arising in crystal dislocations, Global Dynamics in Hamiltonian Systems, June 28 July 4, Universitat Politècnica de Catalunya (BarcelonaTech), Girona, Spain, June 29.
- 205. ——, Dislocation dynamics in crystals: Nonlocal effects, collisions and relaxation, Mostly Maximum Principle, September 16–18, Castello Aragonese, Agropoli, Italy, September 16.
- 206. _____, Dislocation dynamics in crystals: Nonlocal effects, collisions and relaxation, Second Workshop on Trends in Nonlinear Analysis, September 24–26, GNAMPA, Universitá degli Studi die Cagliari, Dipartimento di Matematica e Informatica, Cagliari, Italy, September 26.
- 207. <u>A.G. VLADIMIROV</u>, *Modelling of mode-locked semiconductor lasers*, 24th International SAOT Workshop on Design, Modelling and Simulation of Lasers, June 17–20, Erlangen, June 19.

- 208. ——, *Control of cavity solitons by time-delayed optical feedback*, International Conference "Dynamics, Bifurcations and Strange Attractors", July 20–24, Nizhny Novgorod, Russian Federation, July 22.
- 209. <u>W. WAGNER</u>, *Probabilistic models for the Schrödinger equation*, 6th Workshop "Theory and Numerics of Kinetic Equations", June 1–4, Universität Saarbrücken, June 2.
- 210. ——, Stochastic weighted algorithms for population balance equations with multi-dimensional type space, 10th IMACS Seminar on Monte Carlo Methods, July 6–10, Johannes Kepler Universität Linz, Linz, Austria, July 6.
- 211. <u>U. WILBRANDT</u>, *Classical iterative subdomain methods for the Stokes–Darcy problem*, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, Aachen, June 11.
- 212. <u>S. YANCHUK</u>, *Multiscale jittering in oscillators with pulsatile delayed feedback*, Short Thematic Program on Delay Differential Equations, May 11–15, The Fields Institute for Research in Mathematical Sciences, Toronto, Canada, May 14.
- 213. ——, Pattern formation in systems with multiple delayed feedbacks, Minisymposium "Time-delayed Feedback" of the SIAM Conference on Applications of Dynamical Systems, May 17–21, Society for Industrial and Applied Mathematics, Snowbird/Utah, USA, May 20.
- 214. ——, Delay-induced patterns in a two-dimensional lattice of coupled oscillators, 10th Colloquium on the Qualitative Theory of Differential Equations, July 1–4, University of Szeged, Bolyai Institute, Szeged, Hungary, July 4.
- 215. ——, How time delays influence dynamics, School of the International Research Training Group 1740
 "Dynamical Phenomena in Complex Networks", July 20–21, Humboldt-Universität zu Berlin, Institut für Physik, Berlin, July 20.
- 216. ——, Dynamic jittering and exponentially large number of periodic spiking solutions in oscillators with pulsatile delayed feedback, XXXV Dynamics Days Europe 2015, Minisymposium "Delay-equations for Optoelectronic Systems", September 7–10, University of Exeter, Centre for Systems, Dynamics and Control, Exeter, UK, September 7.
- 217. ——, Stability of plane wave solutions in complex Ginzburg–Landau equation with delayed feedback, Jahrestagung der Deutschen Mathematiker-Vereinigung, Minisymposium "Topics in Delay Differential Equations", September 21–25, Universität Hamburg, Fakultät für Mathematik, Informatik und Naturwissenschaften, Hamburg, September 22.
- 218. ——, *Time delays and plasticity in neuronal networks*, Seminar "Self-assembly and Self-organization in Computer Science and Biology", September 27 October 2, Leibniz-Zentrum für Informatik, Schloss Dagstuhl, September 28.

A.8.3 Talks for a More General Public

- 1. <u>A. CIPRIANI</u>, *Perkolation, ein Spiel von zufälligen Pflasterungen*, 20. Berliner Tag der Mathematik (20th Berlin Day of Mathematics), Beuth Hochschule für Technik Berlin, May 9.
- 2. <u>CH. D'ALONZO</u>, *Mit Mathematik das Rechnen vereinfachen (vermeiden?)*, 20. Berliner Tag der Mathematik (20th Berlin Day of Mathematics), Beuth Hochschule für Technik Berlin, May 9.
- 3. <u>F. FLEGEL</u>, Kuriositäten aus der Wahrscheinlichkeitsrechnung, Girls' Day, WIAS Berlin, April 23.
- 4. <u>C. GUHLKE</u>, *Modellierung von Lithium-Ionen-Batterien: Warum wir von Luftballons viel lernen können!*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2015, WIAS at Leibniz Association Headquarters, Berlin, June 13.

- 5. <u>B. JAHNEL</u>, *Die Poesie der Logik*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2015, WIAS at Leibniz Association Headquarters, Berlin, June 13.
- 6. W. KÖNIG, Was ist Zufall und wie kam er in die Mathematik?, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2015, WIAS at Leibniz Association Headquarters, Berlin, June 13.
- 7. ——, Unendlichkeit in der Wahrscheinlichkeitsrechnung, MathInside Mathematik ist überall, Urania, Berlin, November 10.
- Unendlichkeit in der Wahrscheinlichkeitsrechnung, 2 talks, Tag der Wissenschaften 2015, Weinberg-Gymnasium Kleinmachnow, Kleinmachnow, December 8.
- 9. <u>S. REICHELT</u>, Achilles und die Schildkröte, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2015, WIAS at Leibniz Association Headquarters, Berlin, June 13.
- 10. <u>D.R.M. RENGER</u>, *Minimierung in unendlich vielen Dimensionen*, 20. Berliner Tag der Mathematik (20th Berlin Day of Mathematics), Beuth Hochschule für Technik Berlin, May 9.
- 11. <u>H. STEPHAN</u>, *Primzahlen und Pseudoprimzahlen*, 20. Berliner Tag der Mathematik (20th Berlin Day of Mathematics), Beuth Hochschule für Technik Berlin, May 9.
- 12. <u>M. WOLFRUM</u>, Nichtlineare Dynamik: Ordnung und Chaos in optoelektronischen Bauelementen, MathInside – Mathematik ist überall, Urania, Berlin, November 10.

A.8.4 Posters

- A. KOZIUK, Bootstrap log-likelihood ratio test for linear hypothesis in problem with instrumental variables under both strong and weak identification, WIAS Workshop "Structured Nonparametric Modeling", Berlin, June 4–6.
- 2. V. WIEDMEYER, <u>F. ANKER</u>, A. VOIGT, <u>V. JOHN</u>, K. SUNDMACHER, *Crystal shape evolution in a continuous helically coiled flow tube crystallizer (HCFT)*, 10th European Congress of Chemical Engineering (ECCE10), Nice, France, September 28–29.
- P. FARRELL, Simulating semiconductor devices: Generalisations of the Scharfetter–Gummel scheme to non-Boltzmann statistics, 36. Norddeutsches Kolloquium über Angewandte Analysis und Numerische Mathematik (NoKo 2015), Jacobs University Bremen, April 24–25.
- 4. <u>C. GUHLKE</u>, Modeling of electron transfer reactions in the context of non-equilibrium thermodynamics, 13th International Fischer Symposium (IFS), Lübeck, June 7–11.
- 5. <u>M. HOFMANN</u>, *Ab-initio description of optical nonlinearities in femtosecond filaments*, International Workshop "Waves, Solitons and Turbulence in Optical Systems" (WASTOS15), Berlin, October 12–14.
- 6. <u>M. HOFMANN</u>, <u>C. BRÉE</u>, On the role of Freeman resonances in pump-probe measurements of the nonlinear refractive index, CLEO/Europe-EQEC 2015 Conference, München, June 19–25.
- B. JAHNEL, Classes of non-ergodic interacting particle systems with unique invariant measure, Workshop "Interacting Particles Systems and Non-Equilibrium Dynamics", Institut Henri Poincaré, Paris, France, March 9–13.
- 8. <u>V. JOHN</u>, S. LE BORNE, K. SUNDMACHER, *Numerische Lösungsverfahren für gekoppelte Populationsbilanzsysteme zur dynamischen Simulation multivariater Feststoffprozesse am Beispiel der formselektiven Kristallisation*, Evaluation Colloquium of the Priority Program (SPP) 1679 "Dyn-Sim-FP – Dynamische Simulation vernetzter Feststoffprozesse", Frankfurt/Main, January 13.
- 9. <u>V. JOHN</u>, S. ROCKEL, ST. SOBOLEV, *Viscoelastic mantle flow Numerical modeling of geological phenomena*, 4th Annual GEOSIM Workshop, Potsdam, November 17–18.



- 10. <u>M. KANTNER</u>, *Multi-scale modeling and simulation of electrically pumped single-photon sources*, International Nano-Optoelectronics Workshop (iNOW 2015), Tokio, Japan, August 3–7.
- 11. H.-J. MUCHA, Vergleich römischer und neuzeitlicher Ziegel aus Mainz mittels Clusteranalyse mit Variablenselektion, Tagung "Archäometrie und Denkmalpflege 2015", Mainz, March 27.
- 12. J. POLZEHL, K. TABELOW, Bias in low SNR diffusion MRI experiments: Problems and solution, 21th Annual Meeting of the Organization for Human Brain Mapping, Honolulu, USA, June 14–18.
- 13. J. POLZEHL, <u>K. TABELOW</u>, H.U. VOSS, *Towards higher spatial resolution in DTI using smoothing*, 21th Annual Meeting of the Organization for Human Brain Mapping, Honolulu, USA, June 14–18.
- 14. <u>D. PUZYREV</u>, Instabilities of laser cavity solitons induced by delayed feedback, CLEO/Europe-EQEC 2015 Conference, München, June 21–25.
- 15. ——, Delay induced multistability and wiggling movement of laser cavity solitons, International Workshop "Waves, Solitons and Turbulence in Optical Systems" (WASTOS15), Berlin, October 12–14.
- 16. <u>M. RADZIUNAS</u>, R. HERRERO, M. BOTEY, K. STALIUNAS, *Beam shaping in spatially modulated broad area edge-emitting semiconductor lasers*, CLEO/Europe-EQEC 2015 Conference, München, June 21–25.
- 17. <u>M. RADZIUNAS</u>, V. TRONCIU, E. LUVSANDAMDIN, CH. KÜRBIS, A. WICHT, H. WENZEL, *Coexistence of multiple stable continuous-wave states in micro-integrated external-cavity diode lasers*, CLEO/Europe-EQEC 2015 Conference, München, June 21–25.
- <u>K. SCHILDKNECHT</u>, A multivariate multiple permutation test for epigenetic data, IXth International Conference for Multiple Comparison Procedures, Hyderabad, India, September 2–5.
- 19. J. KRÄMER, M. DEPPE, K. GÖBEL, <u>K. TABELOW</u>, H. WIENDL, S. MEUTH, *Recovery of thalamic microstructural damage after Shiga toxin 2-associated hemolytic-uremic syndrome*, 21th Annual Meeting of the Organization for Human Brain Mapping, Honolulu, USA, June 14–18.
- <u>K. TABELOW</u>, M. DELIANO, M. JÖRN, R. KÖNIG, A. BRECHMANN, J. POLZEHL, Towards a population analysis of behavioral and neural state transitions during associative learning, 21th Annual Meeting of the Organization for Human Brain Mapping, Honolulu, USA, June 14–18.
- H.U. VOSS, J. DYKE, D. BALLON, N. SCHIFF, <u>K. TABELOW</u>, Magnetic resonance advection imaging (MRAI) depicts vascular anatomy, 21th Annual Meeting of the Organization for Human Brain Mapping, Honolulu, USA, June 14–18.
- <u>M. THOMAS</u>, Coupling rate-independent and rate-dependent processes: Existence results, 86th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2015), GAMM Juniors Poster Session, Lecce, Italy, March 23–27.
- 23. <u>M. WOLFRUM</u>, *Chimera states with global feedback*, Workshop on Control of Self-Organizing Nonlinear Systems, Wittenberg, September 14–16.

A.8.5 Contributions to Exhibitions

- 1. J. FUHRMANN, H. SI, Tetrahedralizations and finite volume models in numerical modeling, Hannover Messe 2015, April 16.
- N. ROTUNDO, L. HELTAI, Analysis, convergence and experiments on the distributional immersed interface method, The 13th European Finite Element Fair at Charles University of Prague, Faculty of Mathematics and Physics, June 5–7, Prague, Czech Republic, June 6.

A.9 Visits to other Institutions⁴

- 1. G. Hu, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, June 8–14.
- 2. N. AHMED, Technische Universität Dresden, Institut für Numerische Mathematik, March 3–6.
- 3. <u>R. ALLEZ</u>, University of Cambridge, Statistical Laboratory, UK, January 9–16.
- 4. _____, University of Cambridge, Statistical Laboratory, UK, January 22–26.
- 5. , University of Cambridge, Statistical Laboratory, UK, January 29 February 16.
- 6. , University of Cambridge, Statistical Laboratory, UK, February 26 March 2.
- 7. ——, University of Cambridge, Statistical Laboratory, UK, March 18–30.
- 8. ——, University of Cambridge, Statistical Laboratory, UK, July 1–13.
- 9. <u>CH. BAYER</u>, King Abdullah University of Science and Technology (KAUST), Division Computer, Electrical and Mathematical Science and Engineering, Jeddah, Saudi Arabia, January 6–15.
- 10. ——, University of Oslo, Department of Mathematics, Norway, November 16–20.
- 11. , University of Vienna, Faculty of Mathematics, Austria, November 23–27.
- 12. L. BLANK, Università della Svizzera Italiana, Institute of Computational Science, Lugano, Switzerland, December 14–18.
- 13. <u>A. CAIAZZO</u>, National Laboratory for Scientific Computing, Hemodynamics Modeling Laboratory, Quitandinha-Petrópolis, Brazil, November 30 – December 11.
- 14. ——, Universidad de Chile, Center for Mathematical Modeling, Santiago de Chile, Chile, December 14– 18.
- 15. E. CINTI, Universität Bonn, Institut für Angewandte Mathematik, February 3–6.
- 16. _____, Università di Bologna, Dipartimento di Matematica, Italy, March 7 April 8.
- 17. ——, Universitat Politecnica de Catalunya, Departament de Matematica Aplicada I, Barcelona, Spain, April 8 – May 15.
- 18. ——, Università di Bologna, Dipartimento di Matematica, Italy, May 15–24.
- _____, Università di Bologna, Dipartimento di Scienze per la Qualità della Vita, Bologna, Italy, July 10– 20.
- <u>A. CIPRIANI</u>, Indian Statistical Institute, Theoretical Statistics and Mathematics Unit, Kolkata, India, April 4–14.
- 21. _____, Universität Zürich, Institut für Mathematik, Zürich, Switzerland, September 4–9.
- , University of Technology, Faculty of Electrical Engineering, Mathematics and Computer Science, Delft, Netherlands, November 22–28.
- 23. F. DASSI, Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milano, Italy, November 14-18.
- 24. K. DISSER, Technische Universität München, Zentrum Mathematik, München, February 1–6.
- 25. ——, Heinrich-Heine Universität Düsseldorf, Lehrstuhl für Partielle Differentialgleichungen, Düsseldorf, April 1 September 30.
- M.H. FARSHBAF SHAKER, National Institute for Mathematical Sciences, Division of Computational Mathematics, Daejeon, Korea (Republic of), May 12–21.



⁴Only stays of more than three days are listed.

- , University of Tokyo, Graduate School of Mathematical Sciences, and Ehime University, Department of Mathematics, Matsuyama, Japan, October 5–20.
- 28. S.P. FRIGERI, Politecnico di Milano, Dipartimento di Matematica, Milan, Italy, November 9–13.
- 29. , Università di Pavia, Dipartimento di Matematica, Pavia, Italy, December 14–18.
- 30. J. FUHRMANN, Norwegian University of Science and Technology, Department of Physics, Trondheim, June 4–7.
- <u>A. GONZÁLEZ CASANOVA SOBERÓN</u>, Centro de Investigación en Matemáticas, Department of Probability and Statistics, Guanajuato, Mexico, October 31 – November 13.
- , Universidad Nacional Autónoma de México, Institute of Mathematics, Mexico City, Mexico, November 14-24.
- 33. CH. HEINEMANN, Università di Pavia, Dipartimento di Matematica, Italy, March 9–13.
- 34. _____, Universität Essen-Duisburg, Fakultät für Mathematik, Essen, November 30 December 4.
- 35. <u>R. HENRION</u>, Universidad de Chile, Centro de Modelamiento Matemático, Santiago de Chile, Chile, November 18–27.
- 36. <u>D. HÖMBERG</u>, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, February 1–5.
- 37. , Fudan University, School of Mathematical Sciences, Shanghai, China, March 10–20.
- 38. ——, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, August 21 – September 10.
- Morwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, November 23 December 3.
- <u>G. Hu</u>, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, November 19 December 1.
- 41. V. JOHN, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, March 8–13.
- 42. ——, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, December 14– 18.
- 43. L. KAMENSKI, Xiamen University, School of Mathematical Sciences, China, July 28 August 4.
- 44. , Xiamen University, School of Mathematical Sciences, China, August 10–21.
- 45. <u>P. KEELER</u>, Institut National de Recherche en Informatique et en Automatique (INRIA), Research Group DYOGENE, Paris, France, March 9–17.
- 46. ——, The University of Melbourne, Department of Mathematics and Statistics, Melbourne, Australia, July 31 – September 6.
- 47. W. KÖNIG, Heriot-Watt-University, Department of Mathematics, Edinburgh, UK, January 21–24.
- 48. _____, University of Warwick, Mathematics Institute, Coventry, UK, February 9–14.
- 49. ——, University of Warwick, Mathematics Institute, Coventry, UK, April 27 May 1.
- 50. , University of Warwick, Mathematics Institute, Coventry, UK, November 2–8.
- 51. ——, Courant Institute, Department of Mathematics, New York, USA, November 24 December 3.
- 52. M. LIERO, Technische Universität München, Zentrum Mathematik, München, February 1–6.
- 53. , Università di Pavia, Dipartimento di Matematica, Pavia, Italy, November 15–21.
- 54. P. MATHÉ, Fudan University, The School of Mathematical Sciences, Shanghai, China, May 6–30.

- 55. _____, Technische Universität Chemnitz, Fachbereich Mathematik, November 30 December 4.
- 56. <u>M. MAURELLI</u>, Universität Augsburg, Institut für Mathematik, March 23–27.
- 57. , Università di Pisa, Dipartimento di Matematica, Italy, June 3–13.
- <u>H. NEIDHARDT</u>, Technische Universität Graz, Institut f
 ür Numerische Mathematik, Graz, Austria, January 26–31.
- 59. ——, Kyoto University, Research Institute for Mathematical Sciences (RIMS), Kyoto, Japan, September 5–20.
- 60. Hiroshima University, Institute of Engineering, Hiroshima, Japan, September 20–27.
- ——, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, Marseille, France, November 30 – December 10.
- <u>O. OMEL'CHENKO</u>, Lomonosov Moscow State University, Faculty of Physics, Department of Mathematics, Moscow, Russian Federation, November 20–26.
- 63. ST. PATRIZI, The University of Texas at Austin, Department of Mathematics, USA, January 19 February 5.
- 64. , King Abdullah University of Science and Technologie, SRI Center for Uncertainty Quantification in Computational Science & Engineering, Jeddah, Saudi Arabia, March 15–25.
- , Università degli Studi di Roma "La Sapienza", Dipartimento di Matematica "Guido Castelnuovo", Italy, March 27 – May 22.
- 66. J. PELLERIN, TOTAL E&P RECHERCHE DEVELOPPEMENT SAS, Pau, France, June 22 July 10.
- 67. J. POLZEHL, University of Minnesota, School of Statistics, USA, January 22 February 19.
- 68. <u>M. RADZIUNAS</u>, Gediminas Technical University, Department of Mathematical Modeling and Analysis, Vilnius, Lithuania, April 15–19.
- 69. J. REHBERG, Technische Universität München, Lehrstuhl für Optimalsteuerung, München, May 5–8.
- N. ROTUNDO, International School of Advanced Studies (SISSA), Mathematics, Trieste, Italy, January 19– 23.
- 71. _____, International School of Advanced Studies (SISSA), Mathematics, Trieste, Italy, February 16–20.
- 72. _____, International School of Advanced Studies (SISSA), Mathematics, Trieste, Italy, November 12–24.
- <u>R. SCALA</u>, Universidade Nova de Lisboa, Faculdade de Ciencias e Tecnologia, Caparica, Portugal, December 16–20.
- <u>G. SCHMIDT</u>, Università degli Studi di Roma "La Sapienza", Dipartimento di Matematica, Italy, September 16–30.
- 75. R. SOARES DOS SANTOS, Université Claude Bernard, Institut Camille Jordan, Lyon, France, April 6–13.
- 76. ——, Université de Genève, Section de Mathématiques, Genève, Switzerland, April 26–29.
- 77. _____, Johannes-Gutenberg-Universität, Institut für Mathematik, Mainz, November 16–20.
- 78. ——, Université Claude Bernard, Institut Camille Jordan, Lyon, France, November 22–29.
- <u>V. SPOKOINY</u>, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, Russian Federation, February 28 – March 6.
- Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, Pre-MoLab, Moscow, Russian Federation, June 27–30.
- Skolkov Institute of Science and Technology, Moscow, Russian Federation, August 26 September 6.

- 82. , Moscow Institute of Physics and Technology, PreMoLab, Russian Federation, November 23–28.
- 83. J. SPREKELS, Romanian Academy, Simeon Stoilow Institute of Mathematics, Bucharest, March 16–20.
- 84. M. THOMAS, Universität Freiburg, Abteilung für Angewandte Mathematik, Freiburg, February 5–11.
- 85. ——, Polytechnic University of Turin, Department of Mathematics, Turin, Italy, February 26 March 1.
- 86. ——, University of Pavia, Department of Mathematics, Pavia, Italy, March 2–6.
- 87. , University of Brescia, Department of Mathematics, Brescia, Italy, June 1–5.
- 88. _____, Universität Wien, Fakultät für Mathematik, Wien, Austria, June 22–26.
- 89. <u>E. VALDINOCI</u>, University of Edinburgh, School of Mathematics, UK, January 27 February 2.
- 90. , Université de Picardie Jules Verne, Faculté des Sciences, Amiens, France, February 2–8.
- 91. , Università di Bologna, Dipartimento di Matematica, Italy, March 9–13.
- 92. , University of Edinburgh, School of Mathematics, UK, March 16–29.
- 93. _____, Columbia University, Department of Mathematics, New York, USA, March 29 May 16.
- 94. _____, University of Edinburgh, School of Mathematics, UK, May 16–21.
- 95. , Universität Basel, Departement Mathematik und Informatik, Switzerland, May 21–24.
- 96. , University of Edinburgh, School of Mathematics, UK, June 2–8.
- 97. , Universidad Autónoma de Madrid, Department of Mathematics, Spain, June 22–28.
- 98. ——, Université de Picardie Jules Verne, Faculté de Mathématiques et d'Informatique, Amiens, France, September 24 – October 2.
- 99. <u>B. WAGNER</u>, University of Oxford, Mathematical Institute, UK, March 16–20.
- 100. ——, University of Oxford, Mathematical Institute, UK, November 4–18.
- 101. <u>U. WILBRANDT</u>, Indian Institute of Science, Supercomputer Education & Research Centre, Bangalore, March 3-15.
- 102. <u>M. ZHILOVA</u>, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, Russian Federation, February 23 – March 6.

A.10 Academic Teaching⁵

Winter Semester 2014/2015

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

⁵SWS = semester periods per week

26. S. YANCHUK, Angewandte Analysis (research seminar), Humboldt-Universität zu Berlin, 2 SWS.

Summer Semester 2015

- 1. <u>S. AMIRANASHVILI</u>, *Theorie nichtlinearer Phänomene in der Photonik* (lecture), Humboldt-Universität zu Berlin, 3 SWS.
- 2. L. RECKE, <u>U. BANDELOW</u>, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
- 3. CH. BAYER, Stochastik I (lecture), Humboldt-Universität zu Berlin, 4 SWS.
- 4. _____, Berufsbezogenes Fachseminar Stochastik (seminar), Humboldt-Universität zu Berlin, 2 SWS.
- 5. , Stochastik I (practice), Humboldt-Universität zu Berlin, 2 SWS.
- 6. <u>K. DISSER</u>, *Lineare Algebra I* (lecture), Heinrich-Heine-Universität Düsseldorf, 4 SWS.
- 7. _____, Analysis: Navier-Stokes-Gleichungen (seminar), Heinrich-Heine-Universität Düsseldorf, 2 SWS.
- 8. _____, Lineare Algebra I (practice), Heinrich-Heine-Universität Düsseldorf, 4 SWS.
- 9. <u>W. DREYER</u>, *Grundlagen der Kontinuumstheorie II: Kontinuumsphysik* (lecture), Technische Universität Berlin, 4 SWS.
- 10. M.H. FARSHBAF SHAKER, Lineare Algebra für Ingenieure (lecture), Technische Universität Berlin, 2 SWS.
- 11. P. FRIZ, Rough Paths and Regularity Structures (lecture), Technische Universität Berlin, 2 SWS.
- 12. ——, Rough Paths and Related Topics (senior seminar), Technische Universität Berlin, 2 SWS.
- 13. D. BECHERER, J. BLATH, <u>P. FRIZ</u>, <u>W. KÖNIG</u>, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS.
- 14. <u>A. GLITZKY</u>, <u>A. MIELKE</u>, J. SPREKELS, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
- <u>D. HÖMBERG</u>, Variational Calculus and Optimal Control of Ordinary Differential Equations (13 two-hour lectures from Aug. 21 to Sept. 10, 2015) (lecture), Norwegian University of Science and Technology, Trondheim, – SWS.
- 16. ——, Variationsrechnung und optimale Steuerung partieller Differentialgleichungen (lecture), Technische Universität Berlin, 4 SWS.
- 17. <u>V. JOHN</u>, *Numerical Methods for Convection-Dominated and Turbulent Flow Problems* (lecture), Freie Universität Berlin, 2 SWS.
- 18. ——, Numerical Methods for Convection-Dominated and Turbulent Flow Problems (practice), Freie Universität Berlin, 2 SWS.
- 19. L. KAMENSKI, Analysis I (lecture), Freie Universität Berlin, 4 SWS.
- 20. , Analysis I (practice), Freie Universität Berlin, 2 SWS.
- 21. W. KÖNIG, Zufällige Netzwerke für Kommunikation (seminar), Technische Universität Berlin, 2 SWS.
- 22. A. LINKE, Numerik mit partiellen Differentialgleichungen (lecture), Technische Universität Dresden, 3 SWS.
- 23. _____, Optimierung und Numerik (lecture), Technische Universität Dresden, 3 SWS.
- 24. _____, Numerik mit partiellen Differentialgleichungen (practice), Technische Universität Dresden, 1 SWS.
- 25. _____, Optimierung und Numerik (practice), Technische Universität Dresden, 1 SWS.

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- 26. <u>R. MÜLLER</u>, *Iterative Verfahren für lineare Gleichungssysteme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
- 27. <u>V. SPOKOINY</u>, W. HÄRDLE, M. REISS, G. BLANCHARD, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
- 28. <u>H. STEPHAN</u>, *Funktionalanalytische Methoden in der klassischen Physik II* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
- 29. K. TABELOW, Mathematik (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
- 30. B. WAGNER, Asymptotische Analysis II (lecture), Technische Universität Berlin, 2 SWS.
- 31. _____, Mathematische Modellierung (lecture), Technische Universität Berlin, 4 SWS.
- 32. _____, Dünne Schichten Freie Randwertprobleme (seminar), Technische Universität Berlin, 2 SWS.
- 33. <u>M. WOLFRUM</u>, B. FIEDLER, ST. LIEBSCHER, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.
- 34. S. YANCHUK, Angewandte Analysis (research seminar), Humboldt-Universität zu Berlin, 2 SWS.

Winter Semester 2015/2016

- 1. <u>S. AMIRANASHVILI</u>, <u>U. BANDELOW</u>, *Nichtlineare Dynamik in der Photonik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
- 2. L. RECKE, <u>U. BANDELOW</u>, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
- 3. <u>M. EIGEL</u>, *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, <u>P. FRIZ</u>, <u>W. KÖNIG</u>, ET AL., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
- 7. <u>A. GLITZKY</u>, <u>A. MIELKE</u>, 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. <u>A. MIELKE</u>, <u>K. DISSER</u>, Mehrdimensionale Variationsrechnung/BMS Advanced Course on Multidimensional Calculus of Variations (lecture), Humboldt-Universität zu Berlin, 4 SWS.
- 10. ——, Mehrdimensionale Variationsrechnung/BMS Advanced Course on Multidimensional Calculus of Variations (practice), Humboldt-Universität zu Berlin, 2 SWS.
- 11. R.I.A. PATTERSON, Stochastic Process Convergence (lecture), Technische Universität Berlin, 2 SWS.
- 12. J.G.M. SCHOENMAKERS, Berechnungs- und Simulationsmethoden in der Finanzmathematik (lecture), Humboldt-Universität zu Berlin, 3 SWS.
- 13. <u>V. SPOKOINY</u>, W. HÄRDLE, M. REISS, G. BLANCHARD, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
- 14. K. TABELOW, Mathematik (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
- 15. <u>M. WOLFRUM</u>, 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 http: //www.wias-berlin.de/jobs/fellowship.jsp?lang=1). The institute offers postgraduate fellowships with a duration of six to twelve months. These fellowships are designed to enable highly-qualified young scientists to participate in the research into the mathematical problems in the institute's main application areas and thus to further their education and training.

The fellowships can be started anytime in the year. The application deadlines are February 28 and August 31 of each year.

In 2015, Dr. Sergio Simonella (Technische Universität München) and Dr. Tigran Nagapetyan (Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern) worked as fellowship holders at WIAS.

A.12 Visiting Scientists⁶

A.12.1 Guests

- 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.
- 2. N. AKHMEDIEV, Australian National University, Institute of Advanced Studies, Optical Science Group, Canberra, October 4–16.
- 3. R. ARKHIPOV, Berlin, January 15-31.
- 4. L. AVENA, University of Leiden, Mathematical Institute, Leiden, Netherlands, November 2-6.
- 5. G.R. BARRENECHEA, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, August 30 September 7.
- J. BEHRNDT, Technische Universität Graz, Institut f
 ür Numerische Mathematik, Graz, Austria, August 24 September 6.
- 7. T. BENACCHIO, Met Office, Dynamics Research, Exeter, UK, September 10–21.
- 8. C. BERTOGLIO, Universidad de Chile, Center for Mathematical Modeling, Santiago, March 2–6.
- 9. O. BLONDEL, Université Claude Bernard Lyon 1, Institut Camille Jordan, Villeurbanne, France, May 21–28.
- 10. N. BOCHKINA, University of Edinburgh, The School of Mathematics, UK, April 12–17.
- 11. A. BOITSEV, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, St. Petersburg, Russian Federation, November 9–14.
- J. BRASSEUR, Université de Lyon, Ecole Normale Supérieure de Lyon, Département de Mathématiques, Lyon, France, May 25 – August 21.
- 13. V.M. BUCHSTABER, Steklov Mathematical Institute, Department of Geometry and Topology, Moscow, Russian Federation, January 7–10.
- C. BUCUR, Università degli Studi di Milano, Dipartimento di Matematica, Milano, Italy, February 23 March 8.
- 15. ST. BÜRGER, Technische Universität Chemnitz, Fakultät für Mathematik, March 16–20.
- 16. O. BURYLKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, Ukraine, November 24 December 23.
- 17. X. CABRÉ, Universitat Politècnica de Catalunya, Institució Catalana de Recerca i Estudis Avancats, Departament de Matemàtica Aplicada I, Barcelona, Spain, November 23–29.
- Z. CAO, Beihang University, School of Instrument Science and Opto-Electronic Engineering, Beijing, China, August 13–16.
- 19. A. CARPENTIER, Universität Potsdam, Institut für Mathematik, Potsdam, October 1 December 31.
- 20. C. CAVATERRA, Università degli Studi di Milano, Dipartimento di Matematica, Italy, April 19-29.
- 21. ____, June 14–20.
- 22. ____, September 21-24.
- 23. X. CHEN, Yale University, Department of Economics, New Haven, USA, October 20–25.

⁶Only stays of more than three days are listed.

- 24. A. CHIARINI, Université d'Aix-Marseille, Centre de Mathématiques et d'Informatique, Marseille, France, October 23–28.
- 25. H. CHIBA, Kyushu University, Institute of Mathematics for Industry, Fukuoka, Japan, July 12–26.
- 26. R. ČIEGIS, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, January 12–24.
- 27. ____, September 20–25.
- 28. P. COLLI, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, June 7–12.
- M. Cozzi, Università degli Studi di Milano, Dipartimento di Matematica "Federigo Enriques", Milano, Italy, February 23 – March 6.
- 30. M. DAI, University of Illinois at Chicago, Department of Mathematics, Statistics and Computer Science, Chicago, USA, March 29 April 7.
- 31. S. DAMES, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, Center for Applied Statistics and Economics, May 8, 2014 January 31, 2015.
- 32. M. DEL PINO, Universidad de Chile, Departamento de Ingeniería Matemática y Centro de Modelamiento Matemático, Santiago, Chile, January 27 February 2.
- 33. A. DIEB, Ibn Khaldoun University, Department of Mathematics, Tiaret, Algeria, November 22, 2015 January 31, 2016.
- 34. A.L. DINIZ, CEPEL Brazilian Electric Energy Research Center, Rio de Janeiro, Brazil, September 13–16.
- 35. S. DIPIERRO, University of Edinburgh, School of Mathematics, Edinburgh, UK, February 12–20.
- P. DVURECHENSKII, Moscow Institute of Physics and Technology, PreMoLab, Russian Federation, April 27– 30.
- 37. M. EGERT, Technische Universität Darmstadt, Fachbereich Mathematik, Darmstadt, February 9–13.
- 38. M. FATHI, University of California, Department of Mathematics, Berkeley, USA, November 1–4.
- E. FEIREISL, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, Czech Republic, March 30 – April 3.
- M. FRÉMOND, Università degli Studi di Roma "Tor Vergata", Dipartimento di Ingegneria Civile e Ingegneria Informatica, Italy, June 1–5.
- 41. S.K. GANESAN, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, June 15–18.
- 42. Y. GAO, Université Paris-Sud, Laboratoire d'Analyse Numérique, Orsay, France, September 21 October 2.
- 43. A. GASNIKOV, Moscow Institute of Physics and Technology, PreMoLab, Russian Federation, June 6–11.
- 44. G. GIACOMELLI, Institute of Complex Systems, Florence, Italy, July 22 September 9.
- 45. G. GILARDI, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, June 7–12.
- 46. N. GOERIGK, Elektronische Fahrwerksysteme GmbH, Gaimersheim, October 11–16.
- 47. A. GOLDENSCHLUGER, University of Haifa, Department of Statistics, Israel, August 13 September 13.
- M. GROZA, Université de Nice Sophia Antipolis, Laboratoire de Mathématiques "J.A. Dieudonné", Nice, France, February 8–14.
- 49. S. GUREVICH, Wilhelms-Universität Münster, Institut für Theoretische Physik, March 9–14.
- F. HAMEL, Université d'Aix-Marseille, Institut de Mathématiques de Marseille, Marseille, France, May 24– 29.

- R. HAZRA, Indian Statistical Institute, Department Theoretical Statistics and Mathematics, Kolkata, India, September 10–18.
- 52. M. HEIDA, Technische Universität Dortmund, Fakultät für Mathematik, Dortmund, March 23–27.
- L. HELTAI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, April 13–24.
- 54. ____, September 24 October 9.
- 55. —, December 7–15.
- 56. M. HERRMANN, Westfälische Wilhelms-Universität Münster, Angewandte Mathematik, Münster, November 16–19.
- 57. B. HOFMANN, Technische Universität Chemnitz, Fakultät für Mathematik, September 14–18.
- 58. J. HOROWITZ, Northwestern University, Department of Economics, Evanston, Illinois, USA, May 31 June 7.
- V. KLINSHOV, Russian Academy of Sciences, Institute of Applied Physics, Nizhny Novgorod, Russian Federation, February 9 – March 31.
- Y. KLOCHKOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 "High Dimensional Non Stationary Time Series", October 1 – December 31.
- 61. D. KNEES, Universität Kassel, Institut für Mathematik, Kassel, August 1–7.
- 62. ____, November 27 December 4.
- P. KNOBLOCH, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, August 31 September 4.
- A. KOZIUK, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russian Federation, June 3–8.
- M. KRAFT, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, July 20 August 21.
- 66. C. KREISBECK, Universität Regensburg, Institut für Mathematik, Regensburg, September 20-30.
- P. KREJČÍ, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, Czech Republic, May 23–29.
- 68. K.F. LAM, Universität Regensburg, Fakultät für Mathematik, Regensburg, December 13–18.
- 69. G. Li, University of Cambridge, Faculty of Mathematics, UK, June 9–19.
- 70. X. LIU, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, China, April 13–19.
- H. MAI, ENSAE ParisTech, Centre de Recherche en Economie et Statistique, Laboratoire de Statistique, Malakoff, France, October 6–11.
- 72. D. MAIA, National Institute for Space Research, Laboratório Associado de Computação e Matemática Aplicada, São José dos Campos, Brazil, October 8 – December 31.
- 73. M.M. MALAMUD, Institute of Applied Mathematics and Mechanics, Partial Differential Equations, Slavyansk, Ukraine, April 1–30.
- 74. M. MALIOUTOV, Northeastern University, Department of Mathematics, Boston, USA, January 7–11.
- 75. ____, June 15–24.
- 76. E. MAMMEN, Universität Mannheim, Institut für Informatik und Wirtschaftsinformatik, May 29 June 2.

- 77. M. MILIČEVIĆ, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, Freiburg, December 6–11.
- CH. MUKHERJEE, Technische Universität München, Lehrstuhl für Wahrscheinlichkeitstheorie, March 23– 31.
- 79. O. MUSCATO, Università degli Studi di Catania, Dipartimento di Matematica e Informatica (DMI), Italy, March 9–13.
- 80. ____, July 26 August 7.
- 81. M. Musso, Universidad de Chile, Departamento de Ingeniería Matemática y Centro de Modelamiento Matemático, Santiago, Chile, January 27 – February 2.
- TH.N. NGUYEN, Université Paris-Sud, Département de Mathématiques de la Faculté des Sciences d'Orsay, Paris, France, July 13–16.
- 83. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Madrid, Spain, June 8–12.
- 84. T. ORENSHTEIN, Université Claude Bernard Lyon 1, Institut Camille Jordan, France, June 29 July 3.
- 85. Ł. PŁOCINICZAK, Wrocław University of Technology, Institute of Mathematics and Computer Science, Poland, April 20 May 9.
- 86. R. RICHTER, Max-Planck-Institut Halbleiterlabor, München, August 28 September 1.
- 87. ____, October 8–12.
- 88. CH. RITTER, Université Catholique de Louvain, Louvain School of Statistics, Biostatistics and Actuarial Sciences, Louvain-la-Neuve, France, December 14–17.
- 89. T. ROUBÍČEK, Charles University, Mathematical Institute, Prague, Czech Republic, April 7 May 7.
- 90. T. ROUBIČEK, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, November 4 December 4.
- 91. S. RUBINO, Universidad de Sevilla, Facultad de Matemáticas, Sevilla, Spain, January 17–29.
- 92. M. SAEZ, Pontificia Universidad Católica de Chile, Facultad de Matemáticas, Santiago de Chile, September 7–13.
- 93. G. SAVARÉ, Università di Pavia, Dipartimento di Matematica, Pavia, Italy, June 17-21.
- 94. K. SCHADE, Technische Universität Darmstadt, Fachbereich Mathematik, Darmstadt, February 9–13.
- 95. M. SCHONBEK, University of California, Department of Mathematics, Santa Cruz, USA, March 16–20.
- 96. , March 30 April 4.
- 97. B. SEGUIN, University of Dundee, Department of Mathematics, Dundee, UK, June 7–11.
- 98. U. SHARMA, Eindhoven University of Technology, Department of Mathematics and Computer Science, Eindhoven, Netherlands, November 17–20.
- 99. N. SOAVE, Justus-Liebig-Universität Gießen, Mathematisches Institut, Gießen, July 19 August 1.
- 100. K. STURM, Universität Duisburg-Essen, Fakultät für Mathematik, January 5–16.
- 101. ____, July 20-24.
- 102. ____, September 12–18.
- 103. A. SUVORIKOVA, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 "High Dimensional Non Stationary Time Series", October 1, 2014 – March 31, 2016.

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- 104. A.F.M. TER ELST, The University of Auckland, Department of Mathematics, Auckland, New Zealand, December 5–19.
- 105. E. TOBISCH, Johannes Kepler Universität, Institut für Analysis, Linz, Austria, October 11–17.
- 106. M. TRETYAKOV, University of Nottingham, School of Mathematical Sciences, UK, April 13–24.
- 107. D. TURAEV, Imperial College London, Department of Mathematics, UK, May 21-30.
- 108. V. ULYANOV, Lomonosov Moscow State University, Department of Mathematical Statistics, Probability Theory, Statistics, Russian Federation, July 20 – August 3.
- 109. A. WAHAB, COMSATS Institute of Information Technology, Mathematics Department, Wah Cantt, Pakistan, August 7–14.
- 110. H. WEN, University of Oxford, Department of Physics, Oxford, UK, October 11–16.
- 111. H. Wu, Fudan University, School of Mathematical Sciences, Shanghai, China, May 12–16.
- 112. _____, September 30 October 14.
- 113. T. YIN, Chongqing University, College of Mathematics and Statistics, China, July 11 August 10.
- 114. S. YOSHIKAWA, Ehime University, Department of Engineering for Production and Environment, Matsuyama, Japan, January 19–23.
- 115. V. ZAGREBNOV, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, Marseille, France, June 10–24.
- 116. CH. ZANINI, Politecnico di Torino, Dipartimento di Matematica, Turin, Italy, July 29 August 4.
- 117. A.D. ZARNESCU, University of Sussex, School of Mathematical and Physical Sciences, Brighton, UK, March 16-21.
- 118. P.A. ZEGELING, Utrecht University, Mathematical Institute, Utrecht, Netherlands, May 24–29.

A.12.2 Scholarship Holders

- 1. F. CAFORIO, Università degli Studi di Trento, Italy, Erasmus+ Traineeship, February 16 May 15.
- 2. F. CAFORIO, Università degli Studi di Trento, Italy, Erasmus+ Traineeship, September 1 October 31.
- F. DASSI, Politecnico di Milano, Italy, Leibniz-DAAD Research Fellowship, October 1, 2014 September 30, 2015.
- T. NAGAPETYAN, Fraunhofer-Institut f
 ür Techno- und Wirtschaftsmathematik, Kaiserslautern, Weierstrass Postdoctoral Fellowship Program, June 1, 2014 – May 31, 2015.
- S. SIMONELLA, Technische Universität München, Zentrum Mathematik, Weierstrass Postdoctoral Fellowship Program, December 1, 2014 – May 31, 2015.

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

- N. ABATANGELO, Università di Milano, Dipartimento di Matematica, doctoral candidate, January 1 December 1.
- L. ADAMYAN, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 "High Dimensional Non Stationary Time Series", doctoral candidate, December 1–31.

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- T. AHNERT, Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, doctoral candidate, January 1 – November 30.
- 4. S. BERGMANN, Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, doctoral candidate, January 1 December 31.
- 5. C. BUCUR, Università di Milano, Dipartimento di Matematica, doctoral candidate, January 1 June 30.
- 6. M. Cozzı, Università di Milano, Dipartimento di Matematica, doctoral candidate, January 1 December 31.
- 7. M. DZIWNIK, Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, doctoral candidate, January 1 October 31.
- K. EFIMOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group 1792 "High Dimensional Non Stationary Time Series Analysis", doctoral candidate, January 1 – December 31.
- 9. T. GONZÁLEZ GRANDÓN, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, doctoral candidate, October 1 December 31.
- Y. KLOCHKOV, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 "High Dimensional Non Stationary Time Series", doctoral candidate, October 1 – December 31.
- J.P. PADE, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, International Research Training Group 1740 "Dynamical Phenomena in Complex Networks: Fundamentals and Applications", doctoral candidate, January 1 – July 22.
- 12. M. PANOV, Russian Academy of Science, Institute for Information Transmission Problems, doctoral candidate, January 1 – December 31.
- S. ROCKEL, Freie Universität Berlin, Institut für Mathematik, Helmholtz-Kolleg GEOSIM, doctoral candidate, January 1 – December 31.
- 14. ST. RUSCHEL, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, International Research Training Group 1740 "Dynamical Phenomena in Complex Networks: Fundamentals and Applications", doctoral candidate, January 1 – December 31.
- A. SUVORIKOVA, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group 1792 "High Dimensional Non Stationary Time Series Analysis", doctoral candidate, January 1 – December 31.

A.13 Guest Talks

- 1. T.B. ARMSTRONG, Yale University, Department of Economics, New Haven, USA, Adaptive testing on a regression function at a point, May 27.
- 2. A. ARNOLD, Technische Universität Wien, Institut für Analysis und Scientific Computing, Wien, Austria, *Entropy method for hypocoercive & non-symmetric Fokker–Planck equations with linear drift*, November 6.
- 3. A. AZOUANI, Mohamed Premier University, National School of Applied Sciences, Al Hoceima, Morocco, Feedback control of nonlinear dissipative dynamical systems using general interpolant observables and continuous data assimilation, January 27.
- 4. N. BALDIN, Humboldt-Universität zu Berlin, Institut für Mathematik, *A new estimator for the volume of a convex set*, February 10.
- 5. V. BALLY, Université de Marne-la-Vallée, Laboratoire d'Analyse et de Mathématiques, Marne-la-Vallée, France, *Convergence and regularity of probability laws by using an interpolation method*, November 25.
- 6. G.R. BARRENECHEA, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Stabilising some inf-sup stable pairs on anisotropic quadrilateral meshes*, September 3.
- 7. J. BEHRNDT, Technische Universität Graz, Institut für Numerische Mathematik, Graz, Austria, *Selfadjoint realizations of the Laplacian on bounded Lipschitz domains*, September 2.
- 8. T. BENACCHIO, Met Office, Dynamics Research, Exeter, UK, *Towards scalable numerical weather and cli*mate prediction with mixed finite element discretizations, September 11.
- 9. M. BIBINGER, Humboldt-Universität zu Berlin, Institut für Mathematik, *Statistics of discretely observed semi-martingales under noise*, January 14.
- 10. N. BOCHKINA, University of Edinburgh, The School of Mathematics, UK, *Statistical inference in possibly misspecified nonregular models*, April 15.
- 11. A. BOITSEV, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, St. Petersburg, Russian Federation, *Boundary triplets for sum of tensor products of operators*, November 11.
- 12. C. BONADONNA, Université de Genève, Section des Sciences de la Terre et de l'Environnement, Genève, Switzerland, *Volcanic plumes and particle sedimentation*, November 26.
- 13. CH. BREUNIG, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *Testing the specification in random coefficient models*, July 8.
- 14. O. BURYLKO, National Academy of Sciences, Institute of Mathematics, Kiev, Ukraine, *Weak chimeras in minimal networks of coupled phase oscillators*, January 13.
- 15. A. CARPENTIER, University of Cambridge, Statistical Laboratory, Cambridge, UK, *Inference problems in high dimensional linear models*, June 17.
- 16. S.-K. CHAO, Humboldt-Universität zu Berlin, School of Business and Economics, *FASTEC: Factorisable sparse tail event curves*, May 13.
- 17. X. CHEN, Yale University, Department of Economics, New Haven, USA, *Optimal sup-norm rates, adaptivity* and inference in nonparametric instrumental variables regression, October 21.
- 18. Y. CHEN, National University of Singapore, Department of Statistics & Applied Probability, Singapore, *An adaptive functional autoregressive forecasting model to predict electricity price curves*, June 24.
- 19. H. CHIBA, Kyushu University, Institute of Mathematics for Industry, Fukuoka, Japan, *Renormalization group methods for ODEs/PDEs*, July 23.



- 20. R. ČIEGIS, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, On efficient numerical methods for unidirectional models of nonlinear optics, September 24.
- 21. H. DIETERT, University of Cambridge, Faculty of Mathematics, Cambridge, UK, *Stability and bifurcation for the Kuramoto model*, December 1.
- 22. A.L. DINIZ, CEPEL Brazilian Electric Energy Research Center, Rio de Janeiro, Brazil, *Dynamic piecewise linear models for nonlinear optimization with application to power generation problems*, September 15.
- 23. A.L. DONTCHEV, University of Michigan, Mathematics Department, Ann Arbor, USA, *Newton methods for* variational inequalities, October 22.
- 24. M. EGERT, Technische Universität Darmstadt, Fachbereich Mathematik, Darmstadt, On Kato's square root problem, February 11.
- 25. M. ELLER, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, *Unique continuation and Carle*man estimates for linear PDE, October 14.
- 26. M. FATHI, University of California, Department of Mathematics, Berkeley, USA, *A gradient flow approach to large deviations for diffusion processes*, November 2.
- 27. S.K. GANESAN, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, *Finite element algorithms for massively parallel architectures*, June 16.
- 28. Y. GAO, Université Paris-Sud, Laboratoire d'Analyse Numérique, Orsay, France, Finite volume methods for first order stochastic conservation laws, September 24.
- 29. A. GASNIKOV, Moscow Institute of Physics and Technology (MIPT), PreMoLab, Russian Federation, *On optimization aspects of finding Wasserstain(–Kantorovich) barycenter*, June 10.
- 30. N. GOERIGK, Elektronische Fahrwerksysteme GmbH, Gaimersheim, *On indecomposable polyhedra and the number of Steiner points*, October 14.
- 31. H. GOTTSCHALK, Bergische Universität Wuppertal, Fachgruppe Mathematik und Informatik, *Probabilistic failure mechanisms in fatigue life and optimal reliability via shape control*, June 23.
- 32. J.A. GRIEPENTROG, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, On the positivity and the long-time behavior of solutions to discrete-time evolution systems of nonlocally interacting particles, January 21.
- 33. S. GUREVICH, Wilhelms-Universität Münster, Institut für Theoretische Physik, *Control and selection of spatio-temporal patterns in dynamic self-assembly systems*, March 10.
- 34. F. HAMEL, Université d'Aix-Marseille, Institut de Mathématiques de Marseille, France, *Transition fronts for monostable reaction-diffusion equations*, May 27.
- 35. R. HAZRA, Indian Statistical Institute, Department Theoretical Statistics and Mathematics, Kolkata, India, *Stability of point process, regular variation and branching random walk*, September 16.
- 36. L. HELTAI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modelling, and Applications, Trieste, Italy, *Coupling isogeometric analysis and reduced basis methods for complex geometrical parametrizations*, April 16.
- 37. B. HILDER, Universität Stuttgart, Fachbereich Mathematik, Stuttgart, *Analysis der Embedded Cell Methode in 2D*, November 18.
- 38. S. HIRSCH, Charité Universitätsmedizin Berlin, Institut für Radiologie, Berlin, *Compression-sensitive* Magnetic Resonance Elastography and poroelasticity, June 25.
- 39. M. HOFMANOVÁ, Technische Universität Berlin, Institut für Mathematik, *Stochastic mean curvature flow*, October 14.

- 40. TH. HOHAGE, Universität Göttingen, Institut für Numerische und Angewandte Mathematik, Variational regularization of statistical inverse problems, April 22.
- 41. H. HORNG-SHING LU, National Chiao Tung University, Institute of Statistics, China, *Network analysis of big data*, May 20.
- 42. M. JIRAK, Humboldt-Universität zu Berlin, Institut für Mathematik, *Rate of convergence in the (weighted) CLT under weak dependence*, January 20.
- 43. E. KLANN, Technische Universität Berlin, Institut für Mathematik, *Geometric inverse problems with applications in tomography*, June 16.
- 44. M. KLOFT, Humboldt-Universität zu Berlin, Institut für Informatik, On the statistical properties of ℓ_p -norm multiple kernel learning, May 6.
- 45. D. KNEES, Universität Kassel, Institut für Mathematik, Kassel, Global spatial regularity for elasticity models with nonsmooth constraints, August 4.
- 46. K. KNIGHT, University of Toronto, Department of Statistics, Canada, 1 ∞ estimation in regression, April 29.
- 47. P. KNOBLOCH, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, *On linearity* preservation and discrete maximum principle for algebraic flux correction schemes, September 1.
- 48. M. KRAFT, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, *Industry* 4.0, the internet of things and the J-Park simulator, August 5.
- 49. C. KREISBECK, Universität Regensburg, Institut für Mathematik, Regensburg, *Homogenization of layered materials with rigid components in single-slip finite plasticity*, September 23.
- 50. J. LADENBAUER, Technische Universität Berlin, Institut für Softwaretechnik und Theoretische Informatik, Low-dimensional spike rate dynamics of coupled adaptive model neurons, May 12.
- 51. M. LADKAU, Humboldt-Universität zu Berlin, Institut für Mathematik, *Stochastic volatility Libor modeling and efficient algorithms for optimal stopping problems*, July 14.
- 52. S. LANGE, Heinrich-Hertz-Institut Berlin, Abteilung Photonische Komponenten, Optical feedback effects in monolithically integrated laser Mach–Zehnder modulator transmitter PICs, February 12.
- 53. G. LI, University of Cambridge, Faculty of Mathematics, UK, *Microscopic effects on Brownian coagulation*, June 18.
- 54. X. LI, Eidgenössische Technische Hochschule Zürich, D-MATH, Zürich, Switzerland, A lower bound for disconnection by simple random walk, November 16.
- 55. X. LIU, Chinese Academy of Sciences, Academy of Mathematics and Systems Science, Institute of Applied Mathematics, Beijing, China, *Locating buried objects in a two-layered medium*, April 14.
- 56. M.M. MALAMUD, Institute of Applied Mathematics and Mechanics, Institute of Applied Mathematics and Mechanics, Slavyansk, Ukraine, *Spectral shift functions for pairs of non-selfadjointness operators*, April 22.
- 57. M. MALIOUTOV, Northeastern University, Department of Mathematics, Boston, USA, SCOT modeling, training and homogeneity testing, June 16.
- 58. M. MARSCHALL, Technische Universität Berlin, Institut für Mathematik, *Sparse-grid Bayesian inversion*, June 30.
- 59. R. MASSON, Université de Nice Sophia Antipolis, Laboratoire de Mathématiques J.A. Dieudonné, Nice, France, *Gradient scheme discretizations of two phase porous media flows in fractured porous media*, February 10.

A.13 Guest Talks

- 60. D. MAZZOLENI, Università degli Studi di Torino, Dipartimento di Matematica "G. Peano", Italy, *Existence, regularity and surgery results for solutions of spectral problems*, March 6.
- 61. H. MEINLSCHMIDT, Technische Universität Darmstadt, Fachbereich Mathematik, *Optimalsteuerung des 3D Thermistor-Problems*, January 27.
- 62. A. MIJATOVIĆ, Imperial College London, Imperial Probability Centre, London, UK, *On the Poisson equation* for the Metropolis–Hastings chains: Variance reduction for ergodic average, July 22.
- 63. M. MILIČEVIĆ, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, Freiburg, *Iterative methods for TV regularization and application to a damage model*, December 9.
- 64. P. MÖRTERS, University of Bath, Department of Mathematical Sciences, Bath, UK, *Robustness of spatial preferential attachment networks*, November 18.
- 65. O. MUSCATO, Università degli Studi di Catania, Dipartimento di Matematica e Informatica (DMI), Italy, Electro-thermal transport in silicon carbide semiconductors via hydrodynamic models, August 5.
- 66. A. NAUMOV, LOMONOSOV MOSCOW State University, Faculty of Computational Mathematics and Cybernetics, Moscow, Russian Federation, *Limit theorems for random matrices and their applications*, August 25.
- 67. TH.N. NGUYEN, Université Paris-Sud, Département de Mathématiques de la Faculté des Sciences d'Orsay, Paris, France, Large time behavior for a nonlocal ordinary differential equation — Generation of interface for the mass conserved Allen–Cahn equation, July 15.
- 68. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Madrid, Spain, *Local error* estimates for the SUPG method applied to evolutionary convection-reaction-diffusion equations, June 11.
- 69. T. ORENSHTEIN, Université Claude Bernard Lyon 1, Institut Camille Jordan, France, *Excited mob*, July 1.
- 70. N. PERKOWSKI, Humboldt-Universität zu Berlin, Institut für Mathematik, *Paracontrolled KPZ equation*, October 14.
- 71. S. PEROTTO, Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milano, Italy, Adaptive Hierarchical Model (HiMod) reduction for initial boundary value problems, March 3.
- 72. J. PETERS, Eidgenössische Technische Hochschule Zürich, Seminar for Statistics, Switzerland, *Invariant* prediction and causal inference, January 21.
- 73. CH. PFLAUM, Friedrich-Alexander-Universität Erlangen-Nürnberg, Technische Fakultät, Erlangen, Discretization of elliptic differential equations with variable coefficients on sparse grids, November 19.
- 74. Ł. PŁOCINICZAK, Wrocław University of Technology, Institute of Mathematics and Computer Science, Poland, Anomalous nonlinear diffusion in porous media: Analytical approximations, April 28.
- 75. C. RAUTENBERG, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, Analysis and approximation of evolutionary quasi-variational inequalities, June 24.
- 76. T. ROUBIČEK, Charles University, Mathematical Institute, Prague, Czech Republic, Damage with plasticity at small strains — An overview of various models, April 29.
- 77. T. ROUBIČEK, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, *Modeling of lithospheric faults Demands, options, concepts*, November 12.
- 78. S. RUBINO, Universidad de Sevilla, Facultad de Matemáticas, Sevilla, Spain, *Finite element approximation of an unsteady projection-based VMS turbulence model with wall laws*, January 22.
- 79. L. RUTHOTTO, Emory University, Department of Mathematics and Computer Science, Atlanta, USA, *Numerical methods for hyperelastic image registration*, May 19.
- 80. G. SAVARÉ, Università di Pavia, Dipartimento di Matematica, Pavia, Italy, *Visco-energetic solutions to rateindependent problems*, June 19.

- 81. K. SCHADE, Technische Universität Darmstadt, Fachbereich Mathematik, *Dynamics of nematic liquid crystal flows: The quasilinear approach*, February 11.
- 82. K. SCHMIDT, Technische Universität Berlin, Institut für Mathematik, Berlin, On optimal basis functions for thin conducting sheets in electromagnetics and on efficient calculation of the photonic crystal bandstructure, June 4.
- 83. S. SCHMITZ, Siemens AG, Large Gas Turbines, PG GT LGT EN MT 3 2, Berlin, *Probabilistic design in gas turbine engineering*, October 19.
- 84. B. SEGUIN, University of Dundee, Department of Mathematics, Dundee, UK, *Plant cell wall biomechanics: Model and multiscale analysis*, June 10.
- 85. S. SERFATY, Université Pierre et Marie Curie Paris 6 (UPMC), Laboratoire Jacques-Louis Lions (LJLL), Paris, France, *Crystallization questions for large systems with Coulomb and Riesz interactions*, January 8.
- 86. U. SHARMA, Eindhoven University of Technology, Department of Mathematics and Computer Science, Eindhoven, Netherlands, *Quantification of coarse-graining error in overdamped/non-overdamped Langevin dynamics*, November 18.
- 87. E. SPADARO, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, Lower semicontinuous functionals defined on spaces of multiple-valued maps, September 16.
- M. SPECOVIUS-NEUGEBAUER, Universität Kassel, Institut für Mathematik, Kassel, How do cracks propagate? Some ideas related to the energy criterion, March 4.
- 89. E. SPOHR, Universität Duisburg-Essen, Fakultät für Chemie, Essen, *MD Simulations of structure and reac*tion dynamics at the liquid/solid electrode interface, February 10.
- 90. A. STIVALA, The University of Melbourne, Melbourne School of Psychological Sciences, Social Networks Laboratory (MELNET), Australia, *Modeling large social networks via snowball samples*, June 12.
- 91. A.F.M. TER ELST, The University of Auckland, Department of Mathematics, Auckland, New Zealand, *The Dirichlet-to-Neumann operator on rough domains*, December 9.
- 92. S. TIKHOMIROV, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Shadowing and random walks*, January 20.
- M. TRABS, Université Paris-Dauphine, Centre de Recherche en Mathématique de la Decision (CEREMADE), Low-rank volatility estimation for high-dimensional Lévy processes and low frequency observations, July 1.
- 94. M. TRETYAKOV, University of Nottingham, School of Mathematical Sciences, UK, *Long-time numerical inte*gration of stochastic gradient systems, April 21.
- 95. D. TURAEV, Imperial College London, Department of Mathematics, UK, *Chaotic dynamics in nonholonomic systems*, May 28.
- 96. ——, On a periodically perturbed Lorenz attractor, August 11.
- 97. W. VAN ACKOOIJ, Electricité de France R&D, Clamart, France, *Probabilistic optimization via approximate p* -efficient points and bundle methods, April 16.
- 98. A. WAHAB, COMSATS Institute of Information Technology, Mathematics Department, Wah Cantt, Pakistan, *Time reversal algorithms for inverse source problems*, August 11.
- 99. M. WAHL, Universität Mannheim, Lehrstuhl für Statistik, Nonparametric estimation in the presence of complex nuisance components, February 4.
- 100. M. YAMAMOTO, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Inverse problems* for integro-hyperbolic equations: Kelvin–Voigt model and viscoelasticity, March 17.


A.13 Guest Talks

- 101. T. YIN, Chongqing University, College of Mathematics and Statistics, China, *Numerical methods for time*dependent scattering problems, July 21.
- 102. S. YOSHIKAWA, Ehime University, Department of Engineering for Production and Environment, Matsuyama, Japan, *Refined proofs of existence and error estimate for the structure-preserving finite difference scheme for the Cahn–Hilliard equation*, January 20.
- 103. V. ZAGREBNOV, Université d'Aix-Marseille, Centre de Mathématiques et Informatique, Marseille, France, Dynamical semigroups for unbounded repeated harmonic perturbation, June 17.
- 104. CH. ZANINI, Politecnico di Torino, Dipartimento di Matematica, Turin, Italy, *Viscous and rate-independent damage models in non-smooth domains*, August 4.
- 105. P.A. ZEGELING, Utrecht University, Mathematical Institute, Utrecht, Netherlands, Adaptive grids for detecting non-monotone waves and instabilities in a non-equilibrium PDE model from porous media, May 28.

A Facts and Figures

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 **B**road-**A**rea 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: http://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 **B**lock **O**riented **P**rocess 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: http://www.wias-berlin.de/software/BOP

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

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

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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.

 $\texttt{ClusCorr98}^{\textcircled{0}}$ runs in the host application Excel 2013.

Further information: http://www.wias-berlin.de/software/ClusCorr98

DiPoG (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@wias-berlin.de)

The program package DiPoG (Direct and inverse Problems for optical Gratings) provides simulation and optimization tools for periodic diffractive structures with multilayer stacks.

The direct solver computes the field distributions and efficiencies of given gratings for TE and TM polarization as well as, under conical mounting, for arbitrary polygonal surface profiles. The inverse solver deals with the optimal design of gratings, realizing given optical functions, for example, far-field patterns, efficiency, or phase profiles. The algorithms are based on coupled generalized finite/boundary elements and gradient-type optimization methods.

For detailed information please see http://www.wias-berlin.de/software/DIPOG.

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.radziunas@wias-berlin.de)

LDSL-tool (Longitudinal Dynamics in Semiconductor Lasers) is a tool for the simulation and analysis of the nonlinear longitudinal dynamics in multisection semiconductor lasers and different coupled laser devices. This software is used to investigate and design laser devices that exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, mutual synchronization, and frequency entrainment by an external modulated optical or electrical signal.

LDSL-tool combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.

Detailed information: http://www.wias-berlin.de/software/ldsl

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

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 solidsolid 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 timeand 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.

Fore more information see http://www.wias-berlin.de/software/mefresim.

Par Moon (contact: U. Wilbrandt, phone: +49 30/20372-571, e-mail: ulrich.wilbrandt@wias-berlin.de)

Par MooN is a flexible finite element package for the solution of steady-state and time-dependent convectiondiffusion-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 Par MooN 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 (θ -schemes, DIRK schemes, Rosenbrock–Wanner schemes)
- the application of a multiple-discretization multi-level (MDML) preconditioner in Krylov subspace methods
- tools for using reduced-order models based on proper orthogonal decomposition (POD) are available
- hybrid parallelization with MPI and OpenMP

Par MooN is a joint development with the group of Prof. S. Ganesan (IISc Bangalore) and the group of Prof. Matthies (TU Dresden).

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de)

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

- iterative solvers for linear and nonlinear systems of equations
- sparse matrix structures with preconditioners and direct solver interfaces
- dimension-independent simplex grid handling in one, two, and three space dimensions
 - finite volume-based solution of coupled parabolic reaction-diffusion-convection systems 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 language Lua
- graphical user interface based on the FLTK toolkit
- modular build system and package manager for the installation of third-party software used in the code

Please see also http://www.wias-berlin.de/software/pdelib.



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)

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)

WIAS-TeSCA is a **T**wo- and thre**e**-dimensional **S**emi-**C**onductor **A**nalysis package. It serves to simulate numerically the charge carrier transport in semiconductor devices based upon the drift-diffusion model. This van Roosbroeck system is augmented by a vast variety of additional physical phenomena playing a role in the operation of specialized semiconductor devices as, e.g., the influence of magnetic fields, optical radiation, temperature, or the kinetics of deep (trapped) impurities.

The strategy of WIAS-TeSCA for solving the resulting highly nonlinear system of partial differential equations is oriented towards the Lyapunov structure of the system describing the currents of electrons and holes within the device. Thus, efficient numerical procedures for both the stationary and the transient simulation have been



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



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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 $\tt WIAS-TeSCA$ 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 http://www.wias-berlin.de/software/tesca.

WIAS-QW (contact: Th. Koprucki, phone: +49 30/20372-508, e-mail: thomas.koprucki@wias-berlin.de)

WIAS-QW is a numerical code for the simulation of strained multi-quantum-well structures. Based upon multiband kp models it allows to treat band mixing effects, confinement effects, crystal symmetry, and the influence of mechanical strain.

In particular, WIAS-QW calculates the

- subband dispersion
- eigenfunctions
- transition matrix elements
- miniband effects in multi-quantum-well structures

In dependence on the sheet carrier densities and the temperature, $\mathtt{WIAS-QW}$ calculates the

- optical response function
- gain spectrum
- radiative recombination rate
- carrier density distributions

Furthermore, the calculations can be performed self-consistently, comprising pure kp calculations, but also calculations that include the Hartree–Coulomb potential, obtained from Poisson's equation, as well as density-dependent exchange-correlation potentials accounting for the bandgap shift, which is one of the most prominent many-particle effects.

Please find further information under http://www.wias-berlin.de/software/qw.

WIAS Software Collection for Imaging (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

adimpro is a contributed package within the R-Project for Statistical Computing that contains tools for image processing, including structural adaptive smoothing of digital color images. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

The AWS for AMIRA (TM) plugin implements a structural adaptive smoothing procedure for two- and threedimensional images in the visualization software AMIRA (TM). It is available in the Zuse Institute Berlin's version of the software for research purposes (http://amira.zib.de/).

WIAS Software Collection for Neuroscience (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

dti is a contributed package within the R-Project for Statistical Computing. The package contains tools for the analysis of diffusion-weighted magnetic resonance imaging data (dMRI). It can be used to read dMRI data,

to estimate the diffusion tensor, for the adaptive smoothing of dMRI data, the estimation of the orientation density function or its square root, the estimation of tensor mixture models, the estimation of the diffusion kurtosis model, fiber tracking, and for the two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org). The multi-shell position-orientation adaptive smoothing (msPOAS) method for dMRI data is additionally available within the ACID toolbox for SPM (http://www.diffusiontools.com).

fmri is a contributed package within the R-Project for Statistical Computing that contains tools to analyze fMRI data with structure adaptive smoothing procedures. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).