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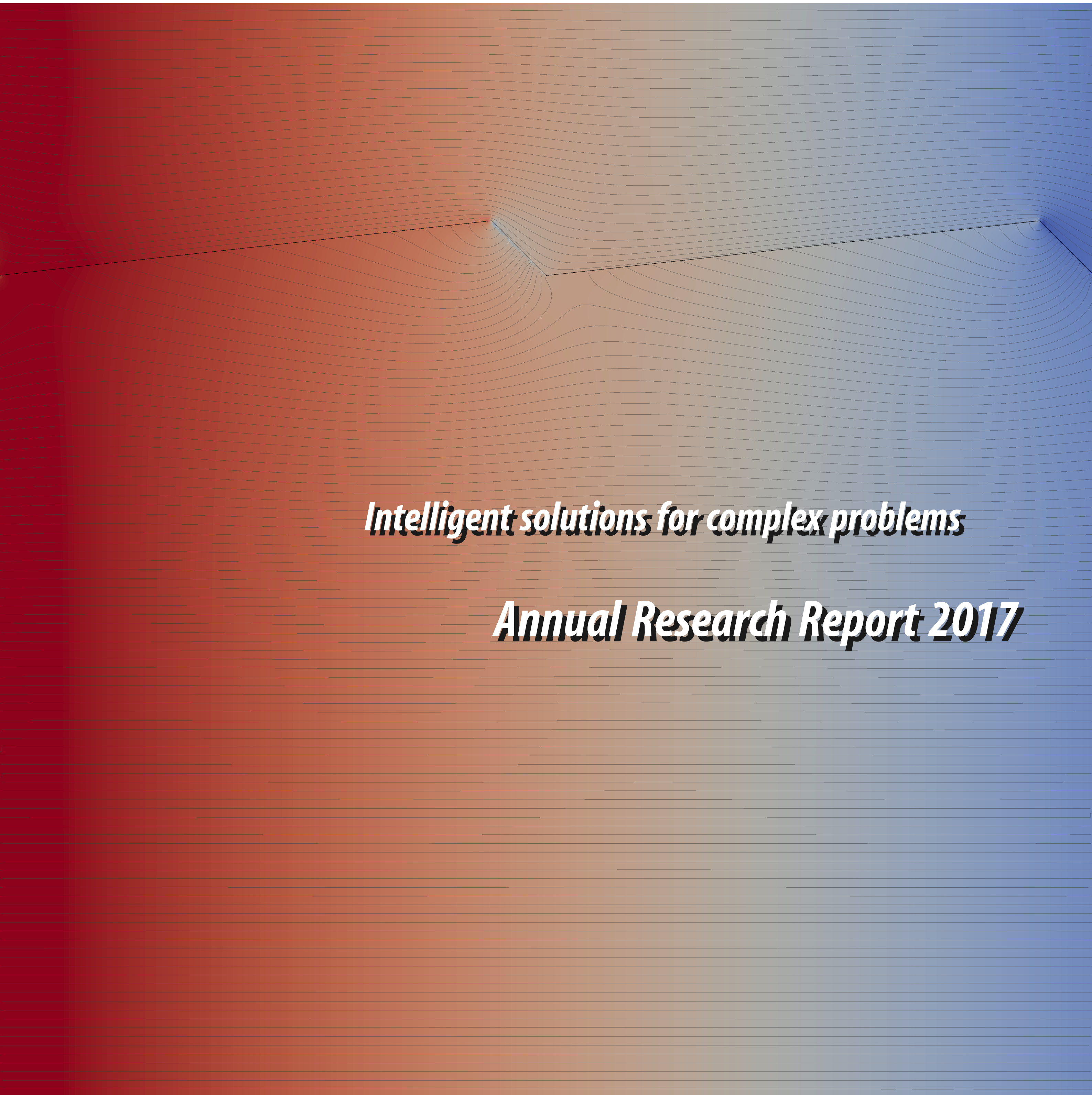

Intelligent solutions for complex problems

Annual Research Report 2017

Cover figure: Solution to the Stokes–Darcy coupled problem for a “river bed”; above black line: surface water (free flow), below: groundwater flow; computed by the finite element software package ParMooN.

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Prof. Dr. Michael Hintermüller, Director

The Weierstrass Institute for Applied Analysis and Stochastics, Leibniz Institute in Forschungsverbund Berlin e.V. (WIAS, member of the Leibniz Association), presents its Annual Report 2017. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2017. Following six selected scientific contributions that highlight some results presented in December in Lisbon during the joint workshop of WIAS with the Portuguese Centro Internacional de Matemática (CIM), see page 121, in the second part, a general introduction is given, followed by the report of the IMU Secretariat, the essential results of the research groups, and statistical data.

The most important event in 2017 was—after months of careful preparation—the evaluation of the Weierstrass Institute by the Senate of the Leibniz Association on July 6 and 7. In its statement of March 20, 2018, the Senate recommends the Federal Government and the Federal States of Germany the continued funding of WIAS and its next evaluation regularly in seven years time. It acknowledges WIAS as an internationally outstanding institution and states that its holistic approach to the solution of highly relevant mathematical problems represents an important unique feature. Moreover, WIAS maintains a cutting-edge position in the interlinking of different mathematical approaches and develops novel practice-oriented methods. The Senate underlines the outstanding research and publication output of the institute and praises the intense knowledge and technology transfer of WIAS via its cooperations with industry.

The high, world-wide appreciation of WIAS is documented especially by the fact that the institute has been the headquarters of the Secretariat of the International Mathematical Union (IMU) since 2011. Its staff, headed by the WIAS Authorized Representative and IMU Treasurer Prof. Alexander Mielke, has served mathematics and mathematicians all over the world ever since. In its evaluation statement, the Senate emphasizes its support for the current preparations of the institute to continue hosting the permanent headquarters of the IMU Secretariat. This decision at the upcoming General Assembly of the IMU in Sao Paulo in 2018 is important not only for mathematics and the Federal State of Berlin, but also for Germany's role within the global scientific community.

The evaluation report also very positively highlights the newly implemented *Flexible Research Platform*, which allows WIAS to flexibly bring in and pursue new research ideas, to support young scientists to become leaders in their fields, and to improve the gender balance in science. With the support of the WIAS Scientific Advisory Board, the institute implemented the new independent Weierstrass Group WG 1 *Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes*, headed by Dr. Marita Thomas, and the Focus Platform *Quantitative Analysis of Stochastic and Rough Systems*, headed by Dr. Christian Bayer and Prof. Peter Friz in RG 6 *Stochastic Algorithms and Nonparametric Statistics*. It is planned to further expand this platform in 2018, e.g., by implementing a new W2-S Professorship (limited to five years) with one of WIAS's Berlin partner universities.

Like the previous years, 2017 has proven to be a busy and fruitful year for the institute with 104 WIAS Preprints, 149 articles in refereed journals, four collected editions, and three million euros provided by grants. More details on this and further information can be found in the facts-and-figures part of this report. All important indicators of scientific productivity and quality again remained on an excellent level, continuing WIAS's successful track record.

In preparation for a spin-off, three former staff members of WIAS, Dr. Lennard Kamenski, Dr. Klaus Gärtner, and Dr. André Fiebach, received an EXIST Business Start-up Grant by the Federal Ministry for Economic Affairs and Energy of Germany for their project "MSim – Microelectronic Simulations". Dr. Pierre-Étienne Druet and Dr. Shalva Amiranashvili got Temporary Positions for Principal Investigators by the German Research Foundation DFG. The proposal of Dr. Manuel Landstorfer et al. for a cooperative project in der BMBF Call *Mathematics for Innovations as a Contribution to the German Energiewende* on the topic "Model-based assessment of the life span of aged Li batteries for second-life use for stationary energy storage" was approved as well, another step to advance the already very successful research in the field of lithium ion batteries at WIAS; see pages 108ff.

In the framework of the WIAS-coordinated Leibniz Network "Mathematical Modeling and Simulation" (MMS), twenty-eight institutes from all sections of the Leibniz Association work together. In February 2017, the 2nd Leibniz MMS Days took place at the Technische Informationsbibliothek in Hanover. The network applied successfully for financial support from the Leibniz Strategic Fund.

The Weierstrass Institute is committed to the implementation of the legally binding German policies and standards to achieve the goal of gender equality. In 2017, WIAS received the "audit berufundfamilie" (audit job and family) quality seal, which it got in December 2013 for the first time, for another three-years' term. New goals in this area were defined to maintain the high standards of WIAS as an employer who is paying particular attention to respecting a well-balanced work/life relation.

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

WIAS also expanded its scope into new applied problems from medicine, economy, science, and engineering. Besides the international workshops organized by the institute, the large number of invited lectures held by WIAS members at international meetings and research institutions, and the many renowned foreign visitors hosted by the institute, last year's positive development is best reflected by the acquisition of grants: altogether, 48 additional co-workers (+ 7 outside WIAS; Dec. 31, 2017) could be financed from third-party funds.

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

In addition to these "global" activities, on the "local" scale WIAS intensified its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. The highlight in this respect was also in 2017 the joint operation of the Research Center MATHEON "Mathematics for key technologies" located at the Technische Universität Berlin and currently funded by the "Einstein Foundation Berlin" in the framework of the "Einstein Center for Mathematics" (ECMath). WIAS is committed to the success of the center by providing considerable financial and personal resources; several members of WIAS play key roles in the scientific administration of the MATHEON.

In 2017, also the 25th anniversary of the foundation of the Forschungsverbund Berlin was celebrated, and MATHEON, the Berlin-based flagship research center, became 15, which was celebrated by an impressive event at Urania. The DFG representative indeed highlighted MATHEON as a "blueprint" for research centers of excellence, a very encouraging statement motivating the Berlin mathematicians in their application for the next-generation excellence cluster MATH+ in the currently running competition within the Excellence Strategy of the Federal Government and the Federal States of Germany administered by the German Research Foundation DFG. The corresponding proposal was successfully evaluated in September 2017. Currently, WIAS, together with its cooperation partners in Berlin, prepares the submission of the full proposal.

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.

Finally, let me emphasize that WIAS's primary aim remains unchanged: to combine fundamental research with application-oriented research, and to contribute to the advancement of innovative technologies through new scientific insights. The recent achievements give evidence that this concept, in combination with hard, continuing work on scientific details, eventually leads to success.

We hope that funding agencies, colleagues, and partners from industry, economy, and sciences will find this report informative and will be encouraged to cooperate with us. Enjoy reading...

Berlin, in March 2018

M. Hintermüller

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1 Scientific Highlights

- Hybrid Quantum-classical Modeling of Electrically Driven Quantum Light Sources
- Models and Numerical Methods for Electroosmotic Flows
- Mathematical Modeling, Simulation, and Optimization using the Example of Gas Networks
- Probabilistic Methods for Mobile Ad-hoc Networks
- Statistical Inference for Barycenters
- Gradient Structure for Flows of Concentrated Suspensions

1.1 Hybrid Quantum-classical Modeling of Electrically Driven Quantum Light Sources

Markus Kantner and Markus Mittnenzweig

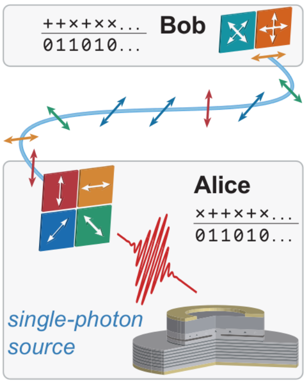

Fig. 1: *Quantum key distribution with single photons: A secret message is transferred from Alice to Bob using the BB84 protocol*

The quantum theory of light started more than a century ago when Max Planck calculated the black body radiation spectrum by assuming that light is emitted in discrete, fundamental units of energy that we denote today as *photons*. Based on the same hypothesis, which involves a particle-like conception of the electromagnetic field that was formerly understood as an entirely wave-like phenomenon, Albert Einstein gave an explanation of the photoelectric effect for which he was awarded with the Nobel prize in 1921. Subsequently, also wave-like properties of electrons in the form of matter waves were discovered, which finally lead to the advent of quantum mechanics – a scientific revolution continuing until the present day. The classical theory of electromagnetism was superseded in the following by quantum electrodynamics by the mid of the 20th century, which forms the basis of our modern understanding of light, matter, and their interaction on a fundamental level. Soon it was discovered that light can exist in different states, e.g., coherent states (lasers), thermal states (blackbody radiation) and more exotic states such as squeezed states. However, it was not until 1977 when H.J. Kimble et al. first demonstrated the emission of a single photon from a single atom at one time, which gave further evidence that light consists of photons. Such a single-photon state of the electromagnetic field is a truly non-classical state of light. The radiation generated by a single emitter shows phenomena like *photon anti-bunching* [1] (i.e., the photons emitted by the source tend to keep a distance due to non-classical intensity fluctuations) that can only be understood in terms of a quantized electromagnetic field theory.

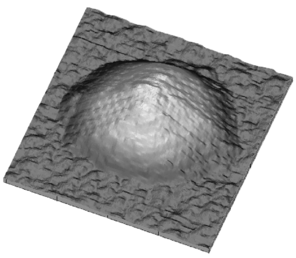

Fig. 2: *STM-image of an InAs semiconductor QD. Picture taken from Márquez et al., Appl. Phys. Lett.,* ***78*** *(2001), 2309.*

The insights obtained in quantum optics with single photons and entangled photon pairs stimulated progress in quantum information theory, which aims at, e.g., using single photons as *qubits* – units of quantum information – for optical quantum computing and information processing tasks. Some of the most promising applications in that field are the various cryptographic methods for secure data transmission based on *quantum key distribution* (e.g., BB84 protocol, E91 protocol); see Figure 1. The security of quantum key distribution relies on well-approved quantum mechanical effects (no-cloning theorem, collapse of the wave function etc.) rather than on assumptions on the available computational power or the efficiency of algorithms as in classical encryption methods.

The experimental preparation of single-photon states using single atoms requires a huge technical effort making the technology extremely expensive and inappropriate for real-world applications. However, with the advent of semiconductor quantum dots (QDs), which are nano-crystalline structures (see Figure 2) that provide an atom-like three-dimensional confinement of electrons within solid-state structures, the fundamental research in quantum optics merged with the well-developed semiconductor technology. Semiconductor QDs are frequently denoted as *artificial atoms* as they represent a solid-state analogue of a single atom with tailorable electro-optical properties. Moreover, QDs can be directly integrated into semiconductor devices and micro-resonators by standard manufacturing techniques, which has lead to many novel concepts for opto-electronic and photonic devices including single-photon sources and ultimately downsized QD nanolasers.

Today, semiconductor quantum optics is on the leap from the lab to commercial applications [1]. To support the development of novel devices, efficient mathematical models and simulation tools are needed to optimize particular device concepts, provide insights into internal physics, and reduce the development costs. In particular, for electrically driven devices, which are desirable for practical applications, the understanding of the current flow is an essential basis for the improvement of certain device designs. For example, Figure 3 shows a single-photon-emitting diode featuring an oxide-confined aperture that is intended to efficiently funnel the current (red lines) into the central QD above the aperture. The experimentally recorded electroluminescence map, however, revealed optical activity of parasitic QDs far away from the aperture. This counterintuitive phenomenon was eventually understood on the basis of carrier transport simulations using the van Roosbroeck system, which showed a rapid lateral current spreading right above the oxide explaining the observations [2]. On the other hand, the van Roosbroeck system makes no predictions on the quantum optical properties of the radiation emitted by the device. Hence, many important figures of merit, like, e.g., the second-order intensity correlation function related to the above-mentioned photon anti-bunching effect, are not accessible by the semi-classical transport model. In order to enable a quantum optical analysis of the device and to simulate electrically driven quantum light sources on a comprehensive level, one has to combine classical device physics with cavity quantum electrodynamics. In particular, it is required to connect semi-classical semiconductor transport theory (e.g., using the van Roosbroeck system) with quantum optical models from the theory of open quantum systems, as illustrated in Figure 4. This was recently achieved in [3] by coupling the van Roosbroeck system to a quantum master equation in Lindblad form.

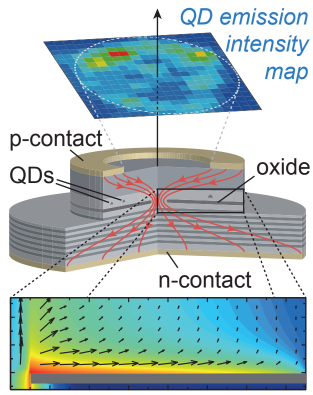

Fig. 3: *Lateral current spreading in an oxide-confined single-photon source leading to unwanted optical activity of parasitic QDs [2]*

The research on quantum-classical hybrid models at WIAS is embedded in the long-term collaborations with experimental groups on single-photon sources (Technische Universität Berlin, funded by DFG CRC 787 *Semiconductor Nanophotonics*). It was stimulated by the ERC-Advanced Grant *AnaMultiScale* on the analysis of multiscale systems driven by functionals that had a focus on the derivation of consistent multi-physics models obeying the fundamental laws of non-equilibrium thermodynamics.

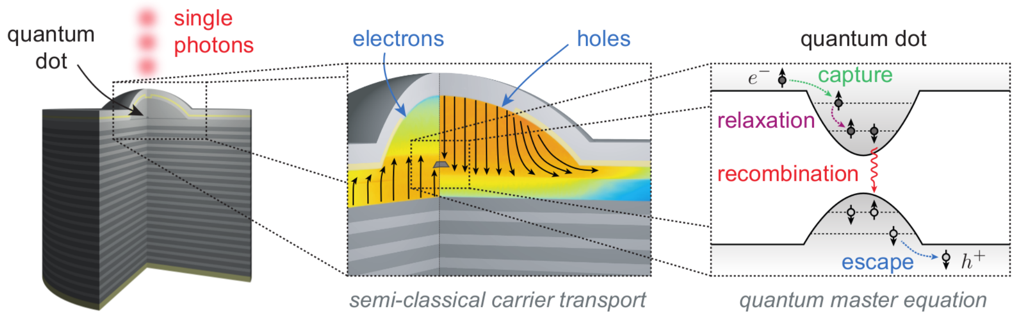

Fig. 4: *The hybrid quantum-classical modeling approach for quantum light sources combines semi-classical carrier transport theory with microscopic models for the QD-photon system*

Combining classical device physics with quantum mechanics

The van Roosbroeck system describes the transport of electrons and holes in macroscopic semiconductor structures in a semi-classical approximation. The charge transport is modeled by a system of reaction-drift-diffusion equations for the electron and hole densities n and p that are coupled to Poisson's equation describing their self-consistently generated electrostatic potential ϕ.

The gradient of the electrostatic potential in turn generates the drift part of the currents. Moreover, electron-hole pairs can be generated or recombine in the semiconductor material modeled by the net-recombination rate R. In [3], we introduced a hybrid quantum-classical model that self-consistently couples the van Roosbroeck system with a quantum master equation in Lindblad form, which is an operator equation describing the evolution of the quantum mechanical density matrix ρ:

$$-\nabla \cdot \varepsilon \nabla \phi = q\left(p - n + C + Q(\rho)\right), \tag{1}$$

$$\partial_t n - \frac{1}{q}\nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \phi), \tag{2}$$

$$\partial_t p + \frac{1}{q}\nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \phi), \tag{3}$$

$$\partial_t \rho = -\frac{i}{\hbar}[H, \rho] + \mathcal{D}(\rho; n, p, \phi). \tag{4}$$

The model system (1)–(4) is based on a Born approximation separating continuum and confined carriers where the transport of the freely roaming continuum carriers by drift and diffusion is described by the van Roosbroeck system (1)–(3), whereas the bound QD carriers evolve according to the Lindblad master equation (4). The coupling structure is illustrated in Figure 5. The Lindblad master equation models the evolution of an open quantum many-body system, where the internal Hamiltonian dynamics of the quantum system is described by the commutator term $\sim i[H, \rho]$ and the dissipative interaction with the macroscopic environment is mediated by the dissipation superoperator $\mathcal{D}(\rho; n, p, \phi)$. The latter includes, e.g., capture and escape of carriers from the continuum states to the confined QD states, spontaneous decay of bound excitons, and the emission of cavity photons from the system. The dissipative interactions can change the charge of the quantum system, while the Hamiltonian evolution leaves it invariant. The backaction of the quantum system on its macroscopic environment is reflected by novel coupling terms in the van Roosbroeck system, which are the scattering rates S_n, S_p describing the loss of continuum carriers in the continuity equations (2)–(3) for electrons and holes and the (net-)charge density $Q(\rho)$ of the QD contributing to the right-hand side of Poisson's equation (1). These macroscopic coupling terms can be expressed as expectation values of certain Hermitian operators, which depend on the state of the quantum mechanical density matrix ρ [3].

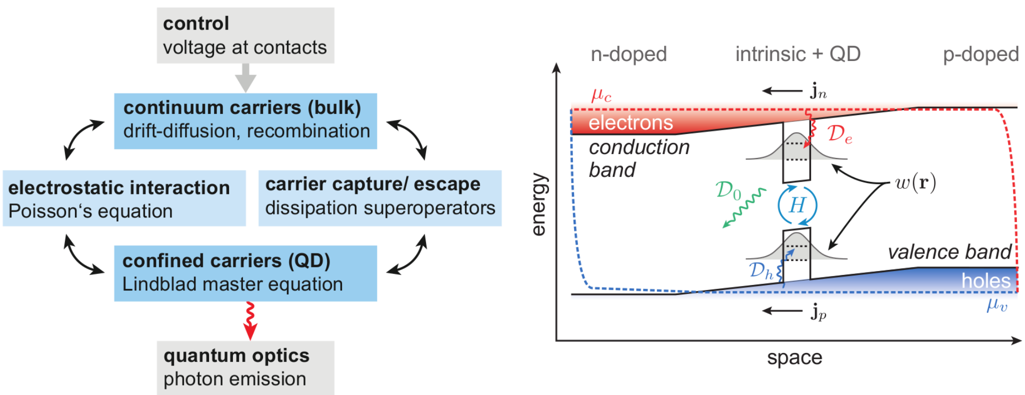

__Fig. 5:__ Illustration of the hybrid modeling approach and the structure of the couplings between the classical and the quantum mechanical subsystem

Consistency with thermodynamics and GENERIC structure

The consistency with fundamental laws of non-equilibrium thermodynamics is crucial in semiconductor device modeling, in particular, when it comes to multi-physics applications where mathematical models from different fields need to be coupled in a reasonable way. In [3], we showed that the hybrid model (1)–(4) meets this requirement. The central quantity in the analysis of the system's thermodynamic properties is the free energy functional

$$\mathcal{F}(n, p, \rho) = \mathcal{F}_{\text{classical}}(n, p) + \mathcal{F}_{\text{quantum}}(\rho) + U_{\phi}(p - n + Q(\rho)), \tag{5}$$

which comprises the free energy contributions of the quasi-free electrons and holes that are subject to the van Roosbroeck model, the free energy of the quantum system, and the electrostatic interaction energy U_{ϕ} generated by the Coulomb interaction of the charges in the system. Based on (5), it can be shown that the system guarantees a non-negative entropy production rate under direct-current bias conditions, which implies consistency with the second law of thermodynamics.

From a mathematical point of view the thermodynamic consistency of the hybrid system (1)–(4) is reflected by the fact that our model falls into the class of damped Hamiltonian systems within the GENERIC framework. GENERIC is an acronym for *General Equations for Non-Equilibrium Reversible Irreversible Coupling* and provides a thermodynamically consistent way of coupling reversible Hamiltonian dynamics with irreversible dissipative dynamics. In our case, a damped Hamiltonian GENERIC system is defined by a quadruple $(\mathbf{Z}, \mathcal{F}, \mathbb{K}, \mathbb{J})$, where $\mathbf{Z}$ is the state space, and $\mathcal{F}(z)$ is the free-energy functional on it. The state variable of the system is given by $z = (n, p, \rho)$. Moreover, the state space carries two geometric structures, namely the Poisson structure $\mathbb{J}$ that generates the Hamiltonian evolution and the Onsager operator $\mathbb{K}$ driving the dissipative dynamics. Together, the time evolution of the system is given by

$$\partial_t z = \mathbb{J}(z)\, D\mathcal{F}(z) - \mathbb{K}(z)\, D\mathcal{F}(z).$$

The Onsager operator $\mathbb{K}(z)$ is positive and symmetric, whereas $\mathbb{J}(z)$ is antisymmetric and satisfies the Jacobi identity. The second law of thermodynamics is encoded in the positivity and symmetry of $\mathbb{K}$ that follows from microscopic reversibility of the underlying microscopic dynamics. In our hybrid model, the evolution of the semi-classical part is purely dissipative such that the Poisson structure only acts on the quantum mechanical part via

$$\mathbb{J}(\rho)A = \frac{i}{\hbar}[\rho, A].$$

Inserting $A = H + k_B T \log \rho$ exactly gives the Hamiltonian part in (4). The quantum-classical coupling of (1)–(4) is generated by an Onsager operator, i.e., there exists a positive, symmetric $\mathbb{K}_{\text{coupling}}(n, p, \rho)$ such that

$$\left(S_n, S_p, \mathcal{D}\right)^T = \mathbb{K}_{\text{coupling}}(n, p, \rho) \cdot D\mathcal{F}(n, p, \rho).$$

The Onsager operator $\mathbb{K}(\rho)$ was originally introduced in [4], where it was shown that every Lindblad master equation satisfying detailed balance is a damped Hamiltonian system in the sense of GENERIC. The operator $\mathbb{K}(\rho)$ defines a transport metric on the space of density matrices and generates a non-commutative analogue of optimal transport distances for probability distributions.

Application

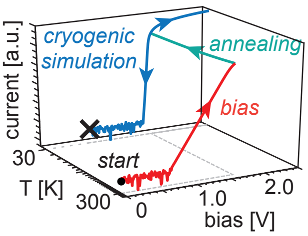

Fig. 6: *Annealing scheme for the numerical simulation of carrier transport at cryogenic temperatures [5]*

The system (1)–(4) is applied to the numerical simulation of an electrically driven single-photon source shown in Figure 7(a), where a single QD is embedded in the intrinsic region of a p-i-n diode. In the case of a leaky resonator, the light-matter interaction is weak, and the quantum system can be described by a purely electronic Hamiltonian. We consider a QD that can be occupied by up to two electrons and two holes, such that the model comprises several multi-particle states including bright and dark excitons and the biexciton. The device geometry, transport parameters, capture rate models, and further details can be found in [3]. The extremely low operation temperatures of quantum light sources cause severe convergence issues for standard numerical routines that can be handled by using the annealing technique [5] illustrated in Figure 6. The simulation results for a pulsed excitation of the device show a biexciton cascade leading to a single-photon emission from the bright exciton state on the order of nanoseconds after the excitation pulse; see Figure 7(b). The numerical results are found to be in good agreement with experimental observations.

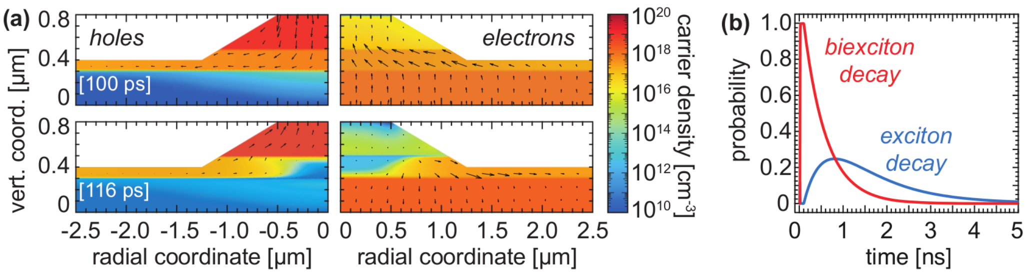

Fig. 7: *The pulsed electrical excitation of the device leads to the emission of non-classical light via the biexciton cascade*

Conclusion

By combining classical device physics with microscopic models from semiconductor quantum optics, we obtained a hybrid quantum-classical model system that can be applied to the simulation of electrically driven quantum light sources. The well-behaved thermodynamic properties of the combined model system are reflected by the underlying mathematical structure.

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1.2 Models and Numerical Methods for Electroosmotic Flows

Jürgen Fuhrmann, Clemens Guhlke, Alexander Linke, Christian Merdon, and Rüdiger Müller

Introduction

Liquid electrolytes are fluids containing electrically charged ions. Many electrochemical energy conversion systems like fuel cells and batteries contain liquid electrolytes. In biological tissues, nanoscale pores in the cell membranes separate different types of ions inside the cell from those in the intercellular space. Nanopores between electrolyte reservoirs can be used for analytical applications in medicine. Water purification technologies like electrodialysis rely on the electrolytic flow properties.

This article gives an overview of recent contributions by WIAS researchers to the mathematical modeling and numerical simulation of coupled electrolyte flow and ion transport, referring the reader to the corresponding publications for the details.

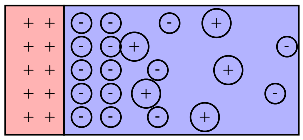


Fig. 1: *Accumulation of negative ions at positively charged electrode surface*

Improved continuum models

Electroosmotic flows are characterized by the presence of an electric field that excerts a net force on the fluid molecules in regions where the local net charge due to the present ions is nonzero. In addition to advection by the fluid, the dissolved ionic species molecules in electrolytes move relative to the barycentric fluid velocity due to diffusion induced by gradients of chemical potentials and due to applied electric fields. A counterforce to the motion of dissolved molecules is due to elastic interactions between the ions and the solvent.

Classical models for electrolytes rely on a *dilute solution* assumption. In this case, the ion-solvent interaction can be neglected, and the ion volume is set to zero. As a consequence, there is no mechanism to limit the accumulation inside narrow boundary layers that screen the electric field at electrodes or charged walls; see Figures 1, 2. The limitations of classical models are well known, and several remedies for these shortcomings have been suggested. In recent contributions [1, 2], WIAS scientists from RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* established a sound theoretical basis for improved continuum models for electrolytes, based on the second law of thermodynamics and consistent coupling of the transport equations to the momentum balance.

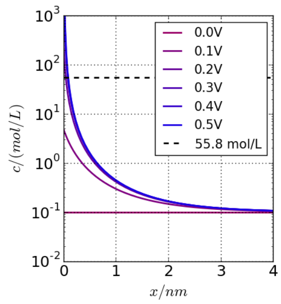


Fig. 2: *Already for moderate applied voltages, the classical Nernst–Planck model predicts unphysically high ion concentrations at an ideally polarizable electrode*

In a given bounded domain Ω, and with appropriate initial and boundary conditions, the system (1a)–(2c) on the following page describes the isothermal evolution of the concentration of N charged species $c_1 \dots c_N$ with charge numbers $z_1 \dots z_N$ dissolved in a solvent of concentration c_0. As a considerable simplification of the model, it is here assumed that the mass density of the solvent and all ionic species is equal. The electric field is described as the gradient of the electrostatic potential ϕ. The barycentric velocity of the mixture is denoted by $\vec{u}$, and p is the pressure. The following equations are considered:

$$-\nu\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \nabla p = q\nabla\phi\,, \tag{1a}$$

$$\nabla\cdot\vec{u} = 0\,, \tag{1b}$$

$$\partial_t c_i + \nabla\cdot(\mathbf{N}_i + c_i\vec{u}) = 0 \qquad (i = 1\dots N)\,, \tag{1c}$$

$$-\nabla\cdot(\varepsilon\nabla\phi) = F\sum_{i=1}^{N} z_i c_i = q. \tag{1d}$$

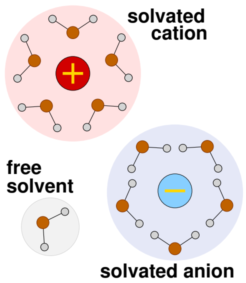


Fig. 3: *Constituents of the liquid electrolyte are the free solvent molecules and solvated ions, i.e., larger complexes that are built from a center ion and a solvation shell of bounded polar solvent molecules*

Equation (1a) together with (1b) comprise the incompressible Navier–Stokes equations for a fluid of viscosity ν and constant density ρ. In the general case, where molar volumes and molar masses are not equal, ρ will depend on the local composition of the electrolyte. In regions where the space charge $q = F\sum_{i=1}^{N} z_i c_i$ (F being the Faraday constant) is nonzero, the electric field $\nabla\phi$ becomes a driving force of the flow. The partial mass balance equations (1c) describe the redistribution of species concentrations due to advection in the velocity field $\vec{u}$ and molar diffusion fluxes $\mathbf{N}_i$. The Poisson equation (1d) describes the distribution of the electrostatic potential ϕ under a given configuration of the space charge. The constant ε is the dielectric permittivity of the medium.

The fluxes $\mathbf{N}_i$, the chemical potentials μ_i, and the incompressibility constraint for a liquid electrolyte are given by

$$\mathbf{N}_i = -\frac{D_i}{RT}c_i\left(\nabla\mu_i - \nabla\mu_0 + z_i F\nabla\phi\right) \qquad (i = 1\dots N)\,, \tag{2a}$$

$$\mu_i = \frac{1}{\bar{c}}(p - p^\circ) + RT\ln\frac{c_i}{\bar{c}} \qquad (i = 0\dots N)\,, \tag{2b}$$

$$1 = v_0 c_0 + \sum_{i=1}^{N}(\kappa_i + 1)v_0 c_i. \tag{2c}$$

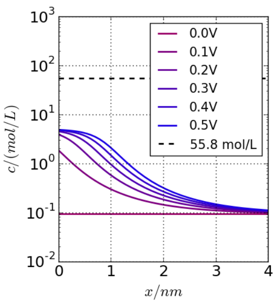


Fig. 4: *Physically reasonable ion concentrations at an ideally polarizable electrode in equilibrium for the generalized Nernst–Planck flux (2a)*

The generalized Nernst–Planck flux (2a) combines the gradients of the species chemical potential μ_i, the solvent chemical potential μ_0, and the electric field $\nabla\phi$ as driving forces. In this equation, D_i are the diffusion coefficients, R is the molar gas constant, and T is the temperature. Equation (2b) is a constitutive relation for the chemical potential μ_i depending on the local pressure and concentration. Here, p° is a reference pressure, and $\bar{c} = \sum_{i=0}^{N} c_i$ is the summary species concentration. In (2c), a simple model for solvated ions is applied. In polar solvents like water, ions carry a shell of electrically attracted solvent molecules; see Figure 3. Given the molar volume v_0 of the solvent, the volume of the solvated ion with κ_i solvent molecules in the solvation shell is set to $(\kappa_i + 1)v_0$. The resulting model limits the accumulation of ions in the polarization boundary layer to physically reasonable values; see Figure 4.

Comparing the constitutive equations (2a)–(2c) to the classical Nernst–Planck flux

$$\mathbf{N}_i = -D_i\left(\nabla c_i + z_i c_i\frac{F}{RT}\nabla\phi\right) \qquad (i = 1\dots N), \tag{3}$$

we observe that in (3) the ion-solvent interaction due to the difference $\mu_i - \mu_0$ is missing. Moreover, in (3) a material model is implicitly assumed that neglects the pressure dependence of μ_i, which is inappropriate in charged boundary layers.

Numerical methods

The numerical solution of the coupled system uses a fixed-point iteration scheme that is based on discretization methods for the subproblems recently developed by WIAS researchers of the RG 3 *Numerical Mathematics and Scientific Computing*.

A two-point flux finite volume method on boundary-conforming Delaunay meshes is used to approximate the Nernst–Planck–Poisson part of the problem. It was inspired by the successful Scharfetter–Gummel box method for the solution of charge transport problems in semiconductors. For a recent overview of this method, see [3]. The method was initially developed for drift-diffusion problems in non-degenerate semiconductors whose fluxes are structurally equivalent to (3).

In order to adapt the Scharfetter–Gummel scheme to take into account the displacement of the solvent, the generalized Nernst–Planck flux (2a) is reformulated in terms of activities $a_i = \exp\left(\frac{\mu_i - \mu_0}{RT}\right)$ [4]

$$\mathbf{N}_i = -D_i \frac{1}{\gamma_i}\left(\nabla a_i + a_i z_i \frac{F}{RT}\nabla\phi\right) \qquad i = 1\dots N. \tag{4}$$

The quantities $\gamma_i = \frac{a_i}{c_i}$ are the activity coefficients. They fulfil a nonlinear system of equations depending on species activities and pressure that can be obtained by an algebraic manipulation of (2b) and (2c). The modification of the Scharfetter–Gummel scheme is based on the similarity of the expressions (4) and (3); see Figure 5.

The resulting time-discrete finite volume scheme guarantees positivity of discrete solutions and exact zero fluxes under thermodynamic equilibrium conditions. It leads to large nonlinear discrete systems that are solved by Newton's method.

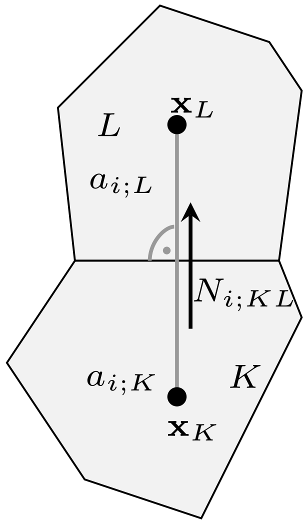


Fig. 5: *The modified Scharfetter–Gummel scheme: Neighboring finite control volumes K, L with collocation points $\mathbf{x}_K, \mathbf{x}_L$ hold activity values a_K, a_L defining the normal flux $N_{KL} = \frac{D}{\gamma_{KL}}\frac{B(-\delta_{kl})a_K - B(\delta_{kl})a_{i,L}}{|\mathbf{x}_K - \mathbf{x}_L|}$, where γ_{KL} is an average of the activity coefficients, and $\delta_{KL} = \frac{zF}{DRT}(\phi_K - \phi_L)$ is proportional to the local electric force. $B(\xi) = \frac{\xi}{e^\xi - 1}$ is the Bernoulli function.*

Pressure-robust, divergence-free finite elements for fluid flow. A fundamental property of the Stokes and Navier–Stokes equations consists in the fact that — under appropriate boundary conditions — the addition of a gradient force to the body force on the right-hand side of the momentum balance (1a) leaves the velocity unchanged, since it can just be compensated by a change in the pressure. Classical mixed finite element methods for the Navier–Stokes equations do not preserve this property. As a consequence, the corresponding error estimates for the velocity depend on the pressure. Moreover, the divergence constraint of the discrete solution is fulfilled only in a certain discrete finite element sense. This behavior causes problems when coupling the flow simulation to a transport simulation using finite volume methods, because the maximum principle for the species concentration is directly linked to the divergence constraint in a finite volume sense [5].

Pressure-robust mixed methods, first introduced in [6], are based on the introduction of a divergence-free velocity reconstruction Π into the discrete weak formulation of the flow problem. Assuming an inf-sup stable pair of velocity ansatz space V_h and pressure ansatz space Q_h, the discretization of the Stokes equation (provided here for simplicity) reads as: find $(\vec{u}_h, p_h) \in V_h \times Q_h$

such that

$$\int_\Omega \nu \nabla \vec{u_h} : \nabla \vec{v_h} dx + \int_\Omega p \nabla \cdot \vec{v_h} dx = \int_\Omega \vec{f} \cdot (\Pi \vec{v_h}) dx \quad \text{for all } \vec{v_h} \in V_h ,$$
$$\int_\Omega q_h \nabla \cdot \vec{u_h} \, dx = 0 \quad \text{for all } q_h \in Q_h .$$

This formulation differs from that of the classical mixed methods only in the introduction of a *reconstruction operator* Π with the properties
(i): $||\Pi \vec{v}_h - \vec{v}_h||$ small in a certain norm,
(ii): $\vec{w}_h$ discretely divergence free $\left(\int_\Omega q_h \nabla \cdot \vec{w}_h \, dx = 0 \text{ for all } q_h \in Q_h\right) \quad \Rightarrow \quad \nabla \cdot (\Pi \vec{w}_h) = 0 .$

From (i) it follows that the error introduced into the method by the use of the reconstruction operator does not disturb the asymptotic convergence rate of the method. Property (ii) states that the reconstruction of the discretely divergence-free solution u_h is pointwise divergence free, which is the prerequisite for mass conservative coupling of fluid flow and species transport guaranteeing positivity and maximum principle of species concentrations. Furthermore, the resulting velocity error estimate is independent of the pressure. Hence, even for a complicated structure of the pressure as in the case of electrolyte flows, a good velocity approximation can be obtained without the need to resort to high-order pressure approximations. This leads to a significant reduction of degrees of freedom numbers necessary to obtain a given accuracy of the velocity. The action of Π on a discrete velocity field can be calculated locally, on elements or element patches. Therefore, its implementation leads to low overhead in calculations.

For an overview of this method, and the role of the divergence constraint in flow discretizations, see the survey article [7].

Coupling strategy. The coupling approach between the Navier–Stokes solver and the Nernst–Planck–Poisson solver is currently based on a fixed-point iteration strategy:

Set $\vec{u_h}, p_h$ to zero, calculate initial solution for (1d)–(2c);
while *not converged* **do**
  Provide ϕ_h, q_h to Navier–Stokes solver;
  Solve (1a)–(1b) for $\vec{u_h}, p_h$;
  Project $\Pi \vec{u_h}, p_h$ to the Poisson–Nernst–Planck solver;
  Solve (1d)–(2c);
end

The projection of $\Pi \vec{u}$ to the finite volume solver includes an integration over interfaces between neighboring control volumes of the finite volume method [5]. Sufficient accuracy of this step guarantees that the projected velocity is divergence free in the sense of the finite volume approximation. As a consequence, in the case of electroneutral inert transported species, the maximum principle for species concentrations is guaranteed.

Simulation results

The discretization methods and the coupling strategy introduced above are implemented in the framework of the toolbox `pdelib` that is developed at WIAS.

We consider a straight nanopore with negatively charged walls. When a potential difference in longitudinal direction is imposed, there is an electroosmotic flow in a binary electrolyte of monovalent ions. The charged walls attract positive ions and repel the negative ones, creating a boundary layer in the vicinity of the walls where the space charge q is nonzero. According to the momentum balance (1a), the electric force acts only in these boundary layers, driving the fluid through the pore. If the pore is wide enough, the electrolyte is locally electroneutral in the center of the pore. Then, no force is present in the center region, leading to a velocity profile similar to a plug flow (Figure 6).

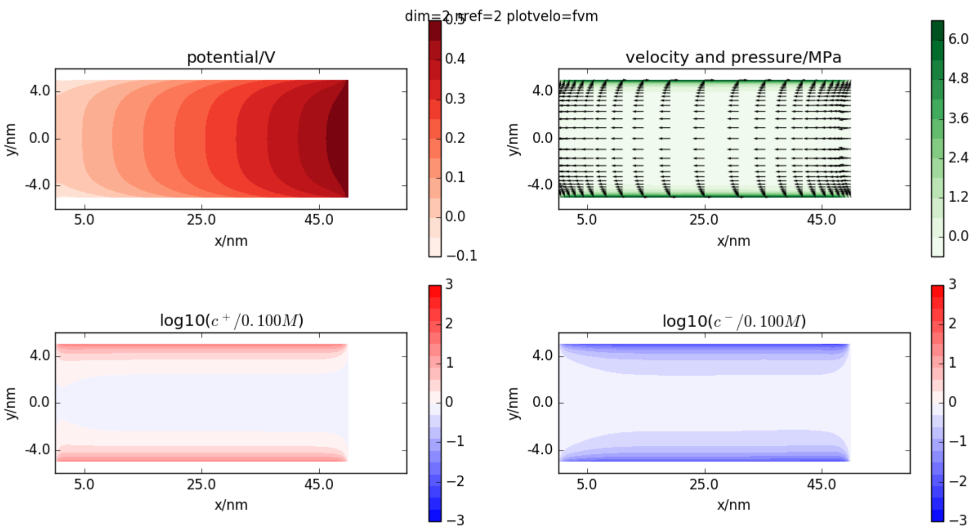
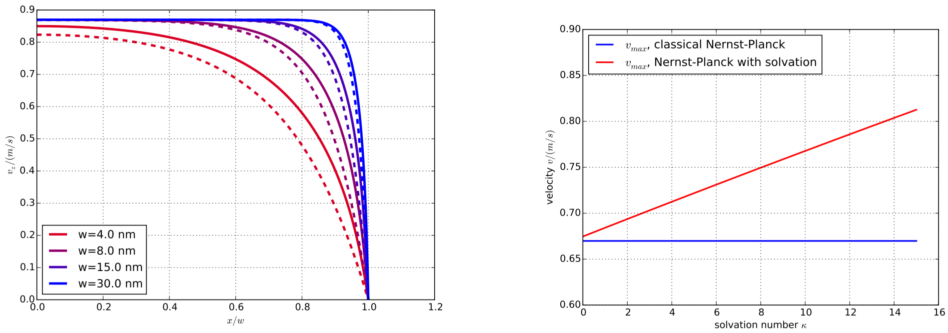


Fig. 6: *Electroosmotic flow through a straight nanopore with charged walls for an imposed potential difference of 0.5 V in longitudinal direction. Top left: distribution of the electrostatic potential. Top right: velocity field (arrows) and pressure (color). Bottom row: positive resp. negative ion concentration.*

For the considered problem, the classical Helmholtz–Smoluchowski theory predicts the electroosmotic velocity in a sufficiently wide pore as $v_{eo} = -\frac{\varepsilon E_x}{\eta}\zeta$, where $E_x = \partial_x \phi$ is the longitudinal component of the electric field on the center line of the pore, and ζ is the zeta potential. In the present case, the zeta potential is defined as the potential difference between the electroneutral region in the center of the pore and the pore wall. It depends on the surface charge of the wall and the boundary layer structure and is not given by the Helmholtz–Smoluchowski theory itself. Figure 7(a) on the following page demonstrates how, for increased pore width, the numerically calculated velocity approaches the predicted value.

The influence of the solvation effect in the improved model is demonstrated in Figure 7(b). Increased values of the solvation number κ lead to a widening of the space charge regions (as visible as well in Figure 4), and also to an increase of the zeta potential. As a consequence, the electroosmotic velocity increases proportionally with the solvation number.



(a) Velocity profile: numerical solution (lines) vs. Helmholtz–Smoluchowski approximation (dashed) for different pore widths w

(b) Flow velocity in the center line over solvation number for a pore of width $w = 10$ nm

Fig. 7: *Left: comparison of simulation results with the classical asymptotic Helmholtz–Smoluchowski theory. Right: An increase of the solvation number κ widens the boundary layers where the electric force acts and thereby increases the flow velocity in the center of the pore.*

Acknowledgement

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1.3 Mathematical Modeling, Simulation, and Optimization using the Example of Gas Networks

Holger Heitsch and Nikolai Strogies

Introduction

The question for the *capacity* of a given gas network, i.e., determining the maximal amount of gas that can be transported by a given network, appears as an essential question that network operators and political administrations are regularly faced with. Discussing the capacity of gas transport networks obviously involves the fact that all nodes are connected. Indeed, if one changes the pressure of some inflow or outflow, then this change can affect large parts of the network. This is due to the fact that there is usually no isolated capacity of a pipeline within the network. These two issues (capacity and connectivity) arise because of the interdependency between gas flow and pressure. This integral behavior makes the main difference between gas networks and other networks, as for example, telecommunication networks, in which there is a certain bandwidth available for each link. As a consequence, classical network flow theory does not suffice to describe the behavior of gas networks. Figure 1 shows the H-gas (high-calorific) and L-gas (low-calorific) network system of Germany, owned by Open Grid Europe (OGE).

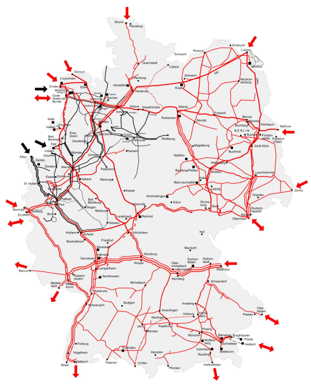

Fig. 1: *German H-gas (red) and L-gas (black) network system. The arrows indicate entry and exit nodes. (Source: OGE)*

In the context of the liberalization paradigm for gas markets, regulatory authorities have separated the natural gas transmission from production and services. Accordingly, network operators are solely responsible for the transportation of gas, and gas traders only need to specify or nominate where they want to inject gas, at so-called *entry points*, or extract gas (demands), at so-called *exit points*. An efficient handling of gas transportation induces a number of technical and regulatory problems, also in the context of coupling to other energy carriers. As an example, energy transporters are required by law to provide evidence that within the given capacities all contracts defining the market are physically and technically feasible. Given the amount of data and the potential of stochastic effects (such as random demand and uncertain friction along the pipes), this is a formidable task by itself, regardless of the actual process of distributing the proper amount of gas of the required quality to the customer.

Network operation under uncertainty

Presently, the reliability of the gas network operation depends on the accuracy of calculating the transport capacity and on the security of supply. This concern is called *nomination validation*, i.e., the determination whether given nominations of all entry and exit flows are technically and physically feasible with the available infrastructure (see [4]). This challenge is further complicated by the uncertainty in the feasibility check due to the coverage of future demand. When ensuring security of gas supply for end consumers, network operators have to quantify the coverage of uncertain future demand. The amount of gas that enters the network depends on volatile prices, and the amount of gas that exits the network is influenced by ambient temperature changes. Figure 2 displays two types of typical behavior of the gas exit flow demand with respect to temperature variation. The data was provided by OGE based on historical observations for one decade.

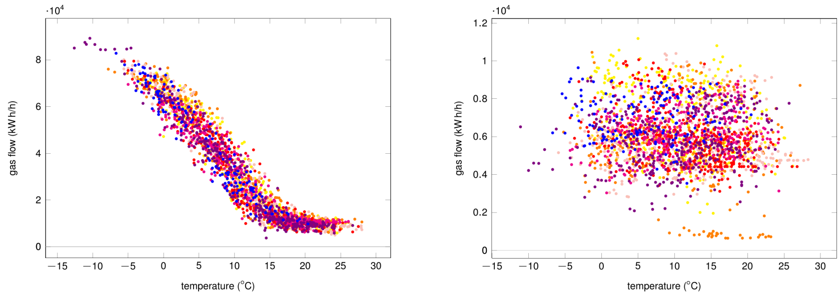

Fig. 2: *Left: typical sigmoidal relation between exit gas demand and temperature. Right: uniform-like distribution, i.e., almost no temperature dependency at all.*

Such historical measurements are useful for a statistical fitting that allows to represent future demand by means of stochastic distributions. In [4, Chapter 13], a detailed description was given for estimating continuous distributions (e.g., normal and normal-like distribution) from empirical observations based on the *Kolmogorov distance*. Therefore, temperature classes of intervals were identified, small enough to neglect the temperature dependence of demands within the interval.

Algebraic model for passive networks. Flow and pressure in gas grids are essentially governed by physical conservation laws. Adopting stationarity, these laws can be modeled by linear and non-linear equations, derived from Kirchhoff's first and second laws and resulting in equality systems given by multivariate polynomials of degree of at most 2.

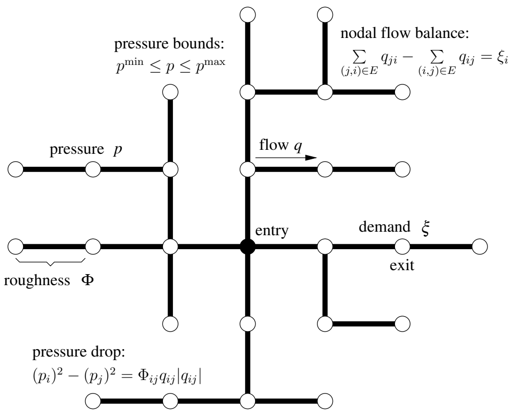

Fig. 3: *Kirchoff's laws (mass flow and momentum conservation) as well as limiting conditions in a passive network:*

p *- pressure variables*
q *- flow variables*
ξ *- demand vector*
Φ *- roughness coefficients*

In a passive gas network, feasibility of a nomination is equivalent to the existence of a pressure-flow profile fulfilling Kirchhoff's laws and meeting nodal bounds on the pressure. In [2], it is shown that pressure and flow variables can be eliminated. For a general characterization of the set of all capacities that can be realized, a mix of explicit and implicit conditions is considered where the implicit indeterminates correspond to the number of fundamental cycles in the network. On the other hand, if the network topology is represented by just a tree, then only explicit feasibility constraints remain. What follows is that in the tree case the check, whether a nomination vector ξ is feasibility or not, corresponds to verifying an explicit system of inequalities. Therefore, all network parameters, namely the pressure limits and roughness coefficients Φ, must be given.

The latter typically depend on *friction coefficients* λ as well as on the geometry of the pipe, the Reynolds number of the gas, and even on pressure. Unfortunately, in some situations the friction of the pipe must be viewed as uncertain as well. But in contrast to the demand, the uncertainty is of different nature as statistical information is hardly available directly. The next section is therefore concerned with an approach for estimating friction coefficients in gas pipelines.

Obtaining statistical information on the friction coefficients

The main problem concerning measurements of operating pipelines is the fact that distributed information on parameters at fixed times, like the volume flow or the friction coefficient at every position along the pipe, are typically not available. The natural remedy for such problems is to focus on quantities that are measure- or observable and to draw conclusions about the quantity that one is actually interested in. This so-called *inverse problem* was dealt with in [6] and aims at identifying the friction coefficient based on measurements of pressure or volume flow at the in- and outlets of a network.

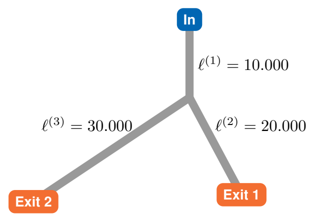

Fig. 4: *Sketch of a basic passive network*

In order to identify, instead of merely pipe-wise constant coefficients, even distributed information on this parameter, the consideration of time-dependent models for the transport of natural gas becomes relevant. Within a single pipe, the dynamic transport of natural gas can be modeled by a system of balance laws and associated initial and boundary conditions given by

$$\begin{aligned} &\rho_t + q_x = 0, && \rho(0,x) = \rho_0(x),\ q(0,x) = q(x), \\ &q_t + a^2 \rho_x = -\lambda \frac{q|q|}{\rho}, && q(t,x_L) = q_L(t),\ q(t,x_R) = q_R(t), \end{aligned}$$

while for networks the coupling conditions from Figure 3 have to be considered as well. Here ρ, q, p denote density, volume flow, and pressure of the pipe, and x_L, x_R refer to its left and right ends. The system represents a simplification of the compressible Euler equations and provides a useful time-dependent description of the underlying physical process. Moreover, it is strongly related to the questions of capacity maximization, since steady *broad solutions* of the latter model form the solutions to the time-independent problems [5].

Considering a minimum-least-squares formulation of the identification problem of the pipe-wise constant friction coefficients in small networks as depicted in Figure 4, suitable numerical methods can be employed to estimate it computationally (see [6]).

Besides the sole identification of the friction coefficient, associated statistical information is of particular interest in applications of optimization subject to probabilistic constraints. Since the friction coefficient is the result of a technical process, it can not be considered to be a common property of every pipeline. Instead, the friction coefficient is assumed to be distributed according to some probability distribution. While producers provide an estimate of this distribution called *prior*, Bayes' theorem and measurements of quantities that allow for an identification of the friction coefficient make these initial guesses more precise. In the particular example of pipe-wise constant friction coefficients and density being measured at the outlets of a network at a finite number of times, this so-called *Bayes inversion* is based on

$$\pi_{Posterior}(\lambda|\rho^d) \propto \pi_{DataLikelihood}(\mathcal{O}(\lambda) - \rho^d)\pi_{Prior}(\lambda).$$

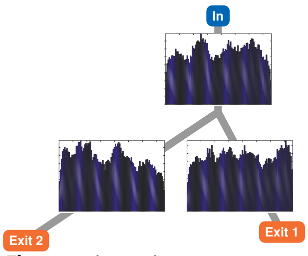

Fig. 5: *Pipe-wise constant: histogram of the samples from a Markov chain Monte Carlo sampling for a truncated normally distributed prior and normally distributed measurement error*

For given measured data ρ^d, the probability distribution of the friction coefficient is proportional to the product of the measurement error $\pi_{DataLikelihood}$, also referred to as *data likelihood*, and the initial guess how λ is distributed in different pipes $\pi_{Prior}(\lambda)$. The observation operator $\mathcal{O}(\lambda)$ represents the evaluation of solutions to the state system associated with λ at points and/or times that correspond to the measured data and can be chosen in a problem-dependent fashion. In case of distributed friction coefficients that are elements of some function space, the probabilities π have to be replaced by associated measures and, by Bayes' theorem, the Radon–Nikodym density $\frac{d\pi_{Posterior}}{d\pi_{Prior}}(\lambda)$ is proportional to $\pi_{DataLikelihood}(\mathcal{O}(\lambda) - \rho^d)$. In order to circumvent the evaluation of the proportionality factor, numerical methods like the Markov chain Monte Carlo method are employed to sample from the posterior distribution $\pi_{Posterior}$, essentially describing the probability distribution adjusted for the measured data with known measurement error. In particular, for a distributed λ, this was investigated in [5]. Figures 5 and 6 provide information on such distributions. They display histograms of values for λ obtained via realizations sampled from $\pi_{Posterior}$ in case of a passive network with friction coefficients that are assumed to be pipe-wise constant and realizations of friction coefficients sampled from $\pi_{Posterior}$ in case of a single pipe with distributed λ, respectively.

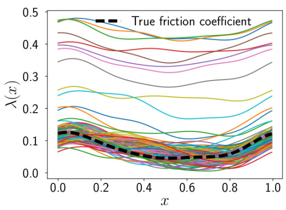

Fig. 6: *Distributed: histogram of the samples from a Markov chain Monte Carlo sampling for a uniformly distributed prior and normally distributed measurement error*

Formulation of optimization problems using probabilistic constraints

Having the stochastic and non-stochastic parameters of the gas network identified, a couple of highly relevant optimization problems can be formulated. In particular, from the network operator's point of view, the uncertainty quantification of nomination feasibility with respect to random demand, the network design problem of minimizing the upper pressure limits while maintaining a reliable network operation (see [1]), as well as the problem of maximizing network capacities (see next paragraph) should be mentioned here. Due to the stochastic nature, the problems are formulated as stochastic optimization problems with probabilistic (or chance) constraints in the form

$$\min\{f(x)\,|\,\varphi(x) \geq \alpha\} \qquad \text{and} \qquad \varphi(x) := \mathbb{P}(g(x,\xi) \leq 0),$$

where $\alpha \in [0,1]$ is a fixed probability level that should be chosen reasonably high, $\varphi(x)$ is the so-called *probability function*, that is the probability of decision x being feasible with respect to the given probabilistic constraints $g(\cdot,\cdot)$. Moreover, $f(\cdot)$ denotes a cost function, and ξ is a random vector in $\mathbb{R}^n$ with probability distribution $\mathbb{P}$.

Function evaluations. The computational challenge of probabilistic constraints arises from the absence of analytical representations for the probability function in general. However, in the Gaussian case, if $\xi \sim \mathcal{N}(0,\Sigma)$, we can represent the probability function by transformation via spheric-radial decomposition as integral over the unique sphere in the form

$$\varphi(x) = \int\limits_{v \in \mathbb{S}^{n-1}} \chi_{\mathrm{cdf}}(\rho(x,v))\,d\mu_\eta(v),$$

where $\mathbb{S}^{n-1}$ denotes the unique sphere in $\mathbb{R}^n$, η is the law of uniform distribution on it, and $\chi_{\text{cdf}}(\cdot)$ denotes the cumulative probability function of the χ-distribution with n degrees of freedom. In the convex case, the function $\rho(x, v)$ is the maximal radius r satisfying $g(x, rLv) \leq 0$ (see Figure 7), where L is such that the covariance matrix Σ decomposes into $\Sigma = LL^\top$. The motivation to consider the spheric-radial approach for representing the probability function is due to two reasons. First, even if the integral cannot be resolved analytically in many situations, the integral can be computed efficiently by applying specialized Quasi-Monte Carlo (QMC) sampling schemes on the unique sphere. A substantial variance reduction can be obtained when comparing with crude sampling (see Figure 8). Secondly, gradient formulae can be derived on the basis of the same sampling scheme.

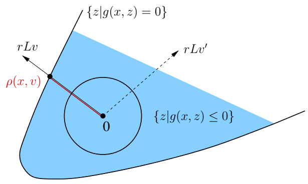

Fig. 7: *Spheric-radial decomposition: radius function $\rho(x, v)$ to compute the probability function*

Gradient formula. Like efficient function evaluations, also gradient information for the probability function should be available when dealing with numerical solutions of the above optimization problem. But computations that record difference quotients are numerically not practical due to the fact that, because of the absence of analytical representations, function evaluations can not be performed with high accuracy. As shown in Figure 9, an attempt to approximate the derivatives in this way is hopeless. The example shows that no step width can be identified for a reasonably good approximation of the involved partial derivatives. A remedy is to derive a similar formula as before that allows to compute even gradients with high accuracy. Under some regularity conditions, and if we assume convexity and smoothness of the constraint mapping $g(\cdot, \cdot)$, then we have that

$$\nabla\varphi(x) = \int_{v\in\mathbb{S}^{n-1}} -\frac{\chi_{\text{pdf}}(\rho(x, v))}{\langle \nabla_\xi g(x, \rho(x, v)Lv), Lv\rangle} \nabla_x g(x, \rho(x, v)Lv)\, d\mu_\eta(v)\,,$$

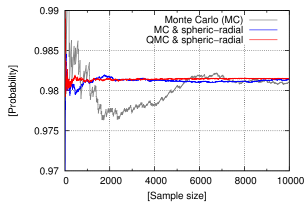

Fig. 8: *Comparison of sampling methods in order to compute the probability of technical feasibility in a gas network with random demand*

where $\chi_{\text{pdf}}(\cdot)$ denotes the χ-probability density function. In general, unfortunately, the probability function needs not to be differentiable at all. But as shown in [7], under additional assumptions, derivatives are available as sub-differentials in terms of Clarke or Mordukhovich. However, the main advantage of the above gradient formula is that the most expensive parts within calculations are (a) computing the sample scheme on the unique sphere and (b) computing the radius function $\rho(x, v)$ for each sample $v \in \mathbb{S}^{n-1}$. But both have to be done only once when computing function and gradient evaluations of a given probability function.

Application. Finally, we are going to take a brief look at the results of two example problems that follow the approach of probabilistic constraints in the context of optimization in stationary gas networks. The first example aims to assist gas network operators in managing uncertainty of friction along the pipes, while maintaining reliability of transmission and supply. The probability constraints are used to maximize shape parameters of uncertainty sets with respect to friction in a mixed probabilistic/robust model [3]. The shape parameter is fitted such that the probability of the technical feasibility for arbitrary Gaussian random demand is at least α. For example, such shape parameter could be the radius of balls around some nominal friction. Clearly, an increase of the shape parameter and, hence, of the uncertainty set, will result in a stronger condition and, thus, in a decrease of the probability. With this setup, we get access to the maximum amount of uncertainty for the friction coefficients which still allows us to technically satisfy the random demands for all

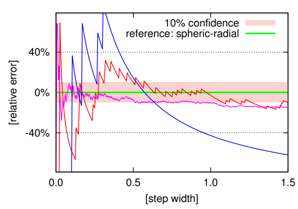

Fig. 9: *Relative error of partial derivatives of an example probability function computed via difference quotients and varying step width*

uncertain friction coefficients with a given probability. The solution of that optimization problem may provide the network operator with an idea with what precision the friction coefficients need to be known in the context of safe network operation (see Figure 10). Such information could be used to roughly estimate these coefficients by expensive indirect measurements as described before or in order to just identify critical parts of the network where it is more important to do so than in others.

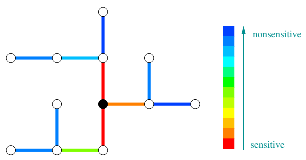

Fig. 10: *Sensitivity analysis with respect to the impact of uncertain friction in a stationary gas network*

Our second example addresses the maximization of free booked capacities. In fact, exit points can nominate their demands only according to given booked capacities. In principle, the network owner has to make sure that all nominations complying with the booked capacities can be satisfied by a feasible flow through the network. Since several nomination patterns may turn out to be highly unlikely, the operator may accept guaranteeing this feasibility only with a certain high probability level α, being aware that rare infeasibilities in the stationary model can be compensated for by appropriate measures in the dispatch mode such as exploiting interruptible contracts. This probabilistic relaxation of an originally worst-case-type requirement for feasibility gives the network owner the chance of offering significantly larger booked capacities. This degree of freedom can then be used to extend the currently booked capacities by a value that still allows one to keep the desired probability level α, no matter what additional nominations in the extended range have been chosen. Figure 11 displays the solution of the underlying optimization problem in a medium-sized gas network with Gaussian exit demand.

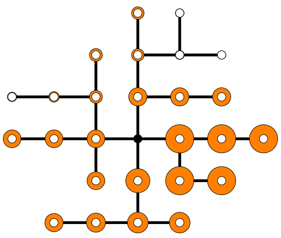

Fig. 11: *Solution illustration of maximizing booking capacities on the exit side within a stationary gas network*

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1.4 Probabilistic Methods for Mobile Ad-hoc Networks

Benedikt Jahnel and Wolfgang König

Wireless multihop ad-hoc communication systems

Since the 1960s, the idea of a wireless ad-hoc communication system has been around, in which messages are transmitted without the help of additional infrastructure like base stations. Instead, in such systems, the devices (transmitters and receivers) also carry a functionality as relays and forward messages. Such a system has all chances to lead to a higher performance. Indeed, if the messages do not have to jump in one hop to one particular base station, but can instead travel in many separate hops from device to device, then the amount of messages that the system can cope with is potentially larger, the number of trajectories of a given message is higher (which leads to a higher stability against transmission failures), and the number of necessary (expensive!) base stations is much lower. On the other hand, the transmission of each message might suffer from time delays (hence we are not talking about real-time transmission, but about down- or uploading, e.g.), and the high amount of message trajectories leads to additional logistic problems, like routing questions or the need for algorithms to forward messages in a given relay.

There is a lack of theoretical knowledge even about the most important properties of such systems in typical real-world situations. These properties are *connectivity* and *capacity*, i.e., the questions whether or not a message can be successfully forwarded via the existing relays, and whether or not the relays can cope with all the messages, that is, that they are not overloaded. The first question depends in a decisive manner on the location of every device at the time of the transmission of the messages considered. Certainly, there are many detailed effects that strongly influence these two basic questions, like *interference* that makes transmission impossible if too many messages concentrate in a given region, and details of the *environment*, i.e., the location of streets, houses, fences, trees and so on, which may hamper the transmission.

Probabilistic models: stochastic geometry

The mathematical analysis of wireless ad-hoc communication systems is often based on *probabilistic spatial models*. Here, the locations of the devices are modeled by a random Poisson point process X in a communication area $W \subset \mathbb{R}^d$ governed by a measure $\lambda\mu(\mathrm{d}x)$ on W, where $\lambda \in (0,\infty)$ is the *intensity* of the devices process. We connect each two of these locations if a direct transmission between them is possible, which depends mainly on their distance. In this way, we obtain a random graph, a geometric network. The question of connectivity is intimately related to the question of *percolation*, i.e., the question whether or not messages can travel unboundedly far on the graph via hops from device to device. This is closely connected with typical questions in *stochastic geometry*, more precisely, in continuum percolation theory, like the one about a *phase transition* in the parameter λ: Is the connectivity in the network dramatically improved if λ is pushed beyond a certain *critical threshold* λ_c? The knowledge of its value is vital for network operators, as it approximates a lower bound for the number of devices necessary for a good quality of service.

However, to be useful for the analysis of ad-hoc systems, the model has to be adapted to real situations in various ways, and additional structures must be introduced, like interference and congestion in the presence of many message trajectories, or environment details like streets, and capacity constraints. Our main investigations concern the quality of service (measured in terms of connectivity and capacity) in average situations or in extremely bad situations (by estimating probabilities of bad service), or the shape of the main flow of the message trajectories. For this, we derive analytical approximations in various limiting regimes (for example, the high-density limit $\lambda \to \infty$) and deduce general principles about the functionality of the system from that. Probabilistic theories are employed like weak convergence of point clouds, percolation theory, stochastic processes on random graphs, large deviations, and more.

Projects at Weierstrass Institute

At the Weierstrass Institute, a rich amount of research in several directions has been done since 2014. Here we report on some of these directions that were brought to a preliminary conclusion in 2017:

- *Random message routing.* In [4] and [5], we study the family of many random message trajectories from all the devices to one single base station in a model where this family has a tendency to minimize its interference and congestion.
- *Random street system.* In [1], we add to the communication area $W = \mathbb{R}^d$ a random street system and assume that the devices are placed only on the streets. We study large-distance connectivity properties.
- *Capacity constraints.* In [3] and [2], we study the effect of a hampering by exceedance of the capacity of the relays under the rule "first come – first serve". Here, we introduce a time dependence and analyze the probability of an unlikely bad quality of service.

Random message routing

In this line of research, we consider a fixed compact communication area $W \subset \mathbb{R}^d$, which contains one single base station, and a large cloud $X \subset W$ of randomly distributed devices in that area with intensity $\lambda \in (0, \infty)$. We assume that each device sends out a message that is supposed to arrive at the base station after some hops via the other devices. For each message, there are, of course, many possible trajectories. We study here the family of all possible such trajectories and give a joint distribution to it. This distribution is in the spirit of a *Gibbs measure*, i.e., the messages are *a priori* uniformly and independently distributed, and the probability of each trajectory is exponentially weighted with two terms: a term that favors low interference of the system, and a term that suppresses congestion, i.e., the appearance of too many hops at any relay. Interference is often — and also here — measured in terms of the *signal-to-interference ratio (SIR)* for a hop from a site x

to a site y if messages are sent out from any site of X, given by

$$SIR(x,y,X) = \frac{\ell(|x-y|)}{\sum_{z\in X\setminus\{x,y\}} \ell(|z-x|)}, \qquad x,y\in W,$$

where $\ell\colon (0,\infty)\to[0,\infty)$ is the *path-loss function*, which gives the strength of the transmitted signal at a given distance. Typical choices are $\ell(r)=\min\{1,r^{-\alpha}\}$ or $\ell(r)=(1+r)^{-\alpha}$ for some $\alpha\in(d,\infty)$. Then, our trajectory measure gives a weight $\exp(-\gamma\, SIR(x,y,X)^{-1})$ to any hop of a message from x to y of any of the message trajectories, where $\gamma\in(0,\infty)$ is a strength parameter, and an additional term of the same form for each pair of hops that use the same relay.

We study the resulting message trajectory distribution conditional on the point cloud X of users in the limit $\lambda\to\infty$ of high spatial density of the devices in the area W, i.e., we look at approximations of the main flow of all the trajectories in the situation in which extremely many devices are present in W. For simplicity, we do not introduce a time dependence and assume that all the many messages are present at the same instance, but we adapt the parameter γ to the exploding amount of interference that we have in this situation. In this limit, we obtain, using a large-deviation analysis for dense point clouds, an analytic characterization of the main flow of all the messages as the minimizers of a characteristic variational formula, which has two "energetic" terms describing interference and congestion and one "entropic" term describing probability.

In a second step, we analyze geometric properties of this flow in various asymptotic regimes, like a large area W and large number of hops, high strength γ of interference punishment, and existence of local regions of particularly high density of devices in W. We show that the "typical" trajectory approaches, in the first two regimes, a straight line and characterize the "typical" hop size. See Figure 1 and Figure 2 for simulations of the densities of the one-hop and the two-hop trajectories in a one-dimensional system.

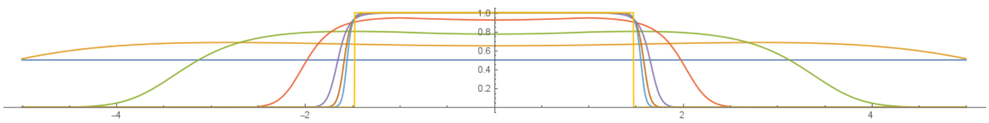

Fig. 1: *A one-dimensional picture: the density of the set of sites from which the typical message jumps directly to the base station without relaying hop*

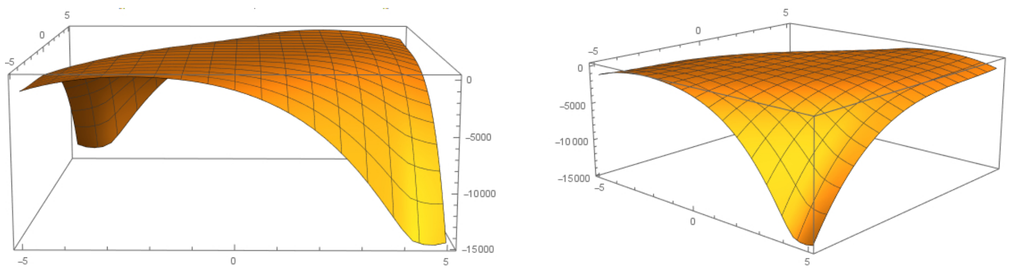

Fig. 2: *The logarithm of the joint distribution of the starting site and the first relaying hop for the same one-dimensional simulation, seen from two different sides*

In the last regime, we demonstrate that the high-density region has a suppressing effect on the number of relaying hops, both globally and locally.

Random street system

In this line of research, we consider a random cloud of devices X in the infinite space $W = \mathbb{R}^d$. They form a random graph by putting an edge between any two of them if their distance is not larger than r, the *reach*. The interesting feature here is that the intensity measure $\lambda\mu(\mathrm{d}x)$ of X is based on a *random* measure μ, for example, the Hausdorff measure on a given random street system. See Figure 3 for examples of such systems and Figure 4 for a model of devices and additional relays on one of these street systems.

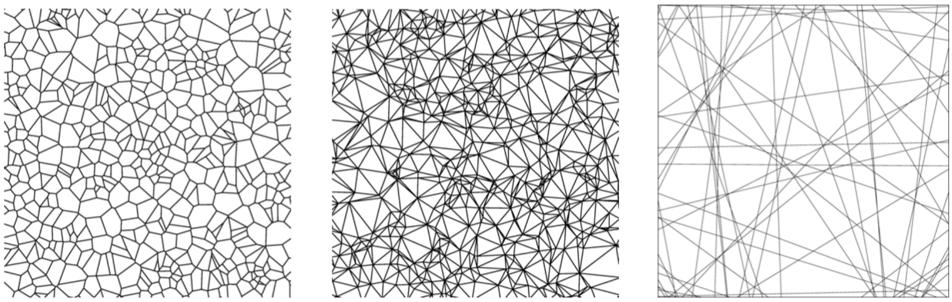

Fig. 3: *Street system models given by Poisson–Voronoi tessellation (left), Poisson–Delaunay tessellation (middle) or Poisson line tessellation (right)*

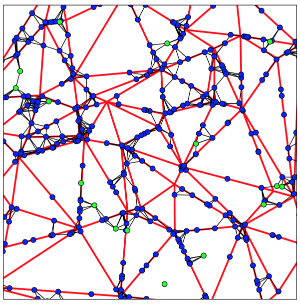

Fig. 4: *Connectivity network of devices (blue) and boxes (green) where devices are confined to be positioned on streets (red)*

We are interested in phase transitions in the global connectivity and in more detailed information about the probability of long-distance communications. A first rough criterion for the quality of the network is the existence of infinite clusters in our network, i.e., the occurrence of *percolation* beyond a critical threshold λ_c. This critical intensity, of course, depends in a non-trivial way on the underlying street system.

We also provide more detailed information about the probability that a typical device is connected to another device far away. This probability is encoded in the *percolation probability* θ that, under the Palm version of the distribution, the origin is connected to infinity. In our project, we investigate the asymptotic behavior of θ in a variety of limiting regimes. For example, we show that in the limit $\lambda \to \infty$ of a large device intensity, θ approaches 1 exponentially fast, and the exponential rate of convergence depends delicately on the local probabilistic properties of the random street system. On the other hand, in the limit $\lambda \downarrow 0$ of sparse devices, when at the same time the reach r tends to infinity, θ approaches a universal limit given by the percolation probability of the corresponding Boolean model (i.e., the network without confinement to streets).

Capacity constraints

We consider a Poisson point process of transmitters $X = \{X_i : i \in I\}$ in a compact area $W \subset \mathbb{R}^d$, with intensity measure $\lambda\mu(\mathrm{d}x)$ under the high-density limit as $\lambda \to \infty$. Additionally, there is a deterministic point cloud $Y \subset W$ of relays, which approaches a density $\nu(\mathrm{d}x)$. Every transmitter $X_i \in X$ comes with two independent random times S_i and T_i at which it starts and ends its transmission in a finite time interval $[0, \tau]$. When the transmission starts, X_i randomly chooses a relay $Y_i \in Y$ according to some preference kernel

$$\kappa(Y_i|X_i) = \frac{\kappa(X_i, Y_i)}{\sum_{y \in Y} \kappa(X_i, y)}.$$

Now, every relay is assumed to have a limited capacity of 1, in other words, it can only serve one transmitter at a time. Consequently, from the perspective of the relay, only the first connection attempted by a transmitter X_i is successful and subsequent attempts are in vain during the time interval $[S_i, T_i]$, but again possible afterwards.

We are interested in the normalized empirical measure of frustrated transmitters and their transmission intervals,

$$\Gamma = \frac{1}{\lambda} \sum_{i \in I:\, Y_i = \text{occupied at time } S_i} \delta_{(S_i, T_i, X_i)},$$

in other words, of those transmitters that are unable to establish a connection to their selected relay and their individual time interval of transmission. We analyze the situation where Γ is away from its expected behavior. In that sense, we investigate the bottleneck properties of a system where, for example, too many users are disconnected. Let us mention that bottlenecks can appear for different reasons, for example, due to spatial concentration of transmitters or too long transmission times. But not all these options are equally likely to be the reason for the undesired system behavior.

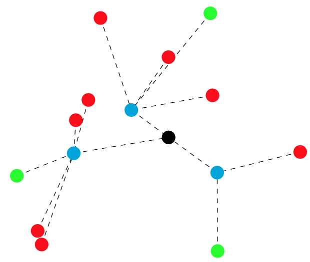

Fig. 5: *Three relays (cyan) are connected to the base station (black). Green transmitters have successfully established a connection, red ones not*

Mathematically, we perform a large deviation analysis for the set of frustrated transmitters in the limit $\lambda \to \infty$ of more and more transmitters in W. Similarly to the above project on random message routing, the resulting variational formula for the exponential rate of decay takes the form of an entropy–energy minimization problem and can be used to determine the most likely behavior of the system in the frustration event.

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1.5 Statistical Inference for Barycenters

Vladimir Spokoiny and Alexandra Suvorikova

Many applications in modern statistics go beyond the scope of classic setting and deal with data that lie on certain manifolds: statistics on shape space, computer vision, medical image analysis, bioinformatics. Most of these problems have a common feature; namely, they are closely related to the detection of *patterns*. Pattern is a very general concept that describes some (unknown and hidden) structure in the data, which has to be revealed. For instance, the problem of classification of neuro-cognitive states of mind is associated with the detection of brain activity patterns in functional magnetic resonance imaging. Another example comes from bioinformatics, namely, from computational epigenetic, that aims to detect common patterns in gene expression regulation, which is supposed to be one of the crucial aspects of morphogenesis. Pattern can also be interpreted in a more specific way as a "typical" geometric shape inherent to all observed items. One can define shape as whatever remains after proper normalization of the object (i.e., rotations, dilations, and shifts are factored out). As a toy example, one can think of cursive letter practice, where kids aim to follow some template, but sometimes fail to repeat it exactly due to lack of experience. So, given only letters written by several children, we are interested in the recovery of the true template that was provided to them by the teacher. As a problem of the same flavor, one can consider an estimation of a typical spatial configuration of protein backbones. Basically, this setting appears in problems where the data is subjected to deformations through a random warping procedure. Such problems are also common for image analysis and shape analysis.

Another interesting application arises in the context of Big Data in connection with *data fusion* problems, which deal with the growing use of distributed or parallelized calculations. Massive data sets are collected and treated by different units, since their large number makes the analysis on a single machine not feasible. Yet the homogeneity of the distribution of the data corresponding to each unit is not true. So the task consists in aggregating all the different results and defining a consensus result between all these processes. The problem appears to be closely related to the problem of pattern extraction.

Of data and averaging

The most natural way of factoring out the noise from a given sample goes to the time of Gerolamo Cardano (1501–1576), who suggested that the accuracy of the empirical mean improves with the growth of the sample size. Now the principle is known as the *Law of Large Numbers*. However, a problem of definition of a mean might not be as straightforward as one might think: The first question at stake is about the possibility to introduce a mean that preserves the inner structure or the pattern that is inherent to all observed items. Figure 1 explains the idea.

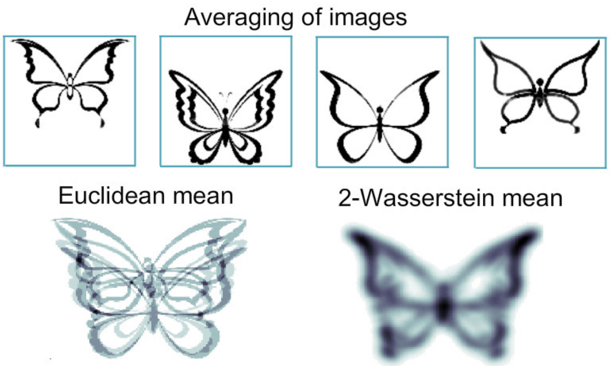

***Fig. 1:** Euclidean mean vs. 2 -Wasserstein mean*

The top panel contains four geometric shapes, while the images below depict two different approaches to averaging. The left-bottom one corresponds to the "classical" Euclidean mean, i.e., all shapes are considered as vectors in a high-dimensional Euclidean space endowed with 2 -norm. The right-bottom shape is a Fréchet mean, computed in 2 -Wasserstein space.

Thus, a suitable way of constructing averages leads immediately to the extraction of the inner structure of interest. The left column of Figure 2 contains random sub-samples from the US-American Modified National Institute of Standards and Technology (MNIST) database (i.e., digits written by different persons), while the right column depicts the typical patterns of writing the digits "3" and "5" among all respondents in the database (average of all handwritten "3" and "5", respectively).

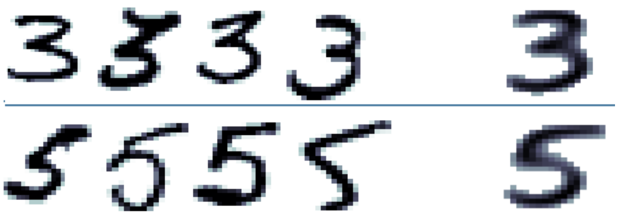

***Fig. 2:** Averaging over the MNIST database*

The key takeaway message is that the usual mean is not suitably representative of a collection of points on an arbitrary manifold, since the natural distance between these objects is not the Euclidean one. Indeed, much of statistical methodology is deeply rooted in methods resting upon linearity, in the sense that they exploit the vector structure of the ambient space in a fundamental way. And this is not the case any more when dealing with objects having some inner geometric structure. Now we are coming to the main question of this section: "What is a nice way to average butterflies?"

How to average on a manifold. In what follows, we consider a probabilistic setting. Let (X, ρ) be some general metric space and $\mathbb{P}$ a Borel measure on it. The straightforward generalization of the least-square estimator leads to the concept of the Fréchet mean, that is, the (set of) global minima of the $\mathbb{P}$-variance

$$\mu^* \subseteq arg \min_{\mu \in X} \int_X \rho^2(\mu, \nu)\mathbb{P}(d\nu),$$

where μ^* is referred to as *the population Fréchet mean* and is not necessarily unique.

Further, we assume that $\mathbb{P}$ and X are such that μ^* is unique and is considered as a pattern, generated by the distribution $\mathbb{P}$. Given an independent and identically distributed (iid) sample

$\{\nu_1, ..., \nu_n\}$ s.t. $\nu_i \backsim \mathbb{P}$, one can build its empirical mean

$$\mu_n := arg \min_{\mu \in X} \frac{1}{n} \sum_{i=1}^{n} \rho^2(\mu, \nu_i),$$

which is referred to as an *empirical barycenter*.

How to capture the geometry. A good choice for extracting the underlying geometry is to take the 2-Wasserstein space as the underlying space. Let X be a set of all probability measures supported on $\mathbb{R}^d$ with finite second moment, $X = \mathcal{P}_2(\mathbb{R}^d)$. Note that many images and signals can be considered as points in $\mathcal{P}_2(\mathbb{R}^d)$ up to a normalization; so, from now on without loss of generality we refer to observed objects as *measures*. The space is endowed with the 2-Wasserstein distance W_2; see [1]. For any μ and ν ($\text{supp}(\mu), \text{supp}(\nu) \subseteq \mathbb{R}^d$) that belong to $\mathcal{P}_2(\mathbb{R}^d)$ it is defined as

$$W_2^2(\mu, \nu) = \inf_{\pi} \int \|x - y\|^2 d\pi(x, y),$$

with π ranging in the set of probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ and ν. The 2-Wasserstein distance is a particular case of the Earth Mover Distance (EMD): The distributions μ and ν are considered as two different ways of piling up a certain amount of ground over the region in $\mathbb{R}^d$, and the EMD is the minimum cost of turning one pile into the other. The overall transportation cost is calculated as the amount of ground moved multiplied by the distance by which it is moved.

Further, we refer to the Fréchet mean in Wasserstein space as the *Wasserstein barycenter*; see [2]. Thus, the population barycenter μ^* and its empirical estimator μ_n, which is built using an observed iid sample $\{\nu_1, ..., \nu_n\}$, are defined as

$$\mu^* := arg \min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\mu, \nu) \mathbb{P}(d\nu), \tag{1}$$

$$\mu_n := arg \min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^{n} W_2^2(\mu, \nu_i). \tag{2}$$

It is a well-known fact that μ_n is a good (consistent) estimator of μ^*; see [3]:

$$W_2(\mu_n, \mu^*) \longrightarrow 0, \text{ as } n \to \infty. \tag{3}$$

In other words, with the growth of the size of an observed sample n, the estimator tends to be closer to the object of interest. All aforementioned naturally leads to the problem formulation.

Problem statement. Let $\mathbb{P}$ be some unknown distribution on a space of measures $\mathcal{P}_2(\mathbb{R}^d)$: $\text{supp}(\mathbb{P}) \subseteq \mathcal{P}_2(\mathbb{R}^d)$. And let μ^* be the induced template object, defined in (1). Instead of observing μ^* itself, we are given its *deformed* or *noisy* counterparts $\{\nu_1, ..., \nu_n\}$, $\nu_i \backsim \mathbb{P}$. A possible consistent *estimator* of μ^* is μ_n, defined in (2). Apart from consistency, this estimator captures the underlying geometry of μ^*. An example is presented in Figure 3.

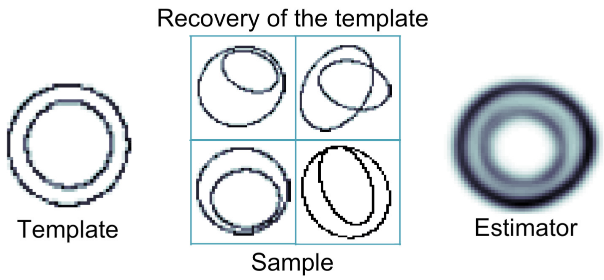

Fig. 3: *Recovery of the template object*

An *observed* set of deformed nested circles $\{\nu_1, \nu_2, \nu_3, \nu_4\}$ is placed in the center, and a *recovered* shape μ_4 is to the right. The object of interest μ^*, which is not known in real-life problems, is depicted on the left-hand side of the box.

The information about *asymptotic convergence* properties is not enough for many practical applications. From an engineering point of view, it is very important to know how large the observed sample should be to be able to approximate μ^* with the desirable precision and how fast the convergence of μ_n is. These two questions were addressed in our work [4].

Reliability matters

The ability to extract important geometric information leads us to the problem of validation of the quality and precision of the shape recovery procedure, described above. In statistical inference, this is usually done by the construction of *confidence sets*. First, we briefly recall the concept.

Confidence sets. As before, let μ_n be an estimator, constructed from a random sample $\{\nu_1, ..., \nu_n\}$ of size n. We aim to recover radii of a ball $\mathcal{B}_r(\mu_n)$, centred around μ_n, which contains the template μ^* with a fixed probability $1-\alpha$:

$$\mathcal{B}_r(\mu_n) := \left\{\text{all } \mu \in \mathcal{P}_2(\mathbb{R}^d) : \; W_2(\mu_n, \mu) \le r\right\}, \tag{4}$$

$$r_n(\alpha) := arg \min_{r>0} \left\{\mathbb{P}\Big(\mu^* \notin \mathcal{B}_r(\mu_n)\Big) \le \alpha\right\}.$$

The quantity $r_n(\alpha)$ is referred to as α*-quantile*. In many real-world problems, the confidence level is set to $95\,\%$, i.e., $\alpha = 0.05$. However, in real life, $\mathbb{P}$ is usually not known and a given training sample is not large enough to construct its empirical counterpart. Thus, the direct estimation of $r_n(\alpha)$ using classical resampling techniques, e.g., Monte Carlo-like methods, is not possible. A plausible alternative in this case is the *multiplier bootstrap* technique, which allows to replace $r_n(\alpha)$ with some computable counterpart $r_n^\flat(\alpha)$; see [5].

Method in a nutshell

Multiplier boostrap. The idea of multiplier bootstrap consists in inducing some additional randomness, which, nevertheless, can be controlled. It is done by generating random weights and the reweighting of summands in (2). Namely, let $\{\nu_1, ..., \nu_n\}$, $\nu_i \backsim \mathbb{P}$, be an iid training set. The weights $\{u_1, ..., u_n\}$ are also iid, generated from $u_i \backsim \mathbb{P}^\flat$. For instance, one may choose a Poisson distribution with parameter 1, $\mathbb{P}^\flat = \mathrm{Po}(1)$. Now we are ready to construct a new reweighted barycenter

$$\mu_n^\flat := arg \min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \sum_{i=1}^n W_2^2(\mu, \nu_i) u_i,$$

which differs from (2) by additional multipliers u_i. However, this does the trick: Now all the randomness is controlled by a procedure of weight generation. One can easily estimate $r_n^\flat(\alpha)$

$$r_n^\flat(\alpha) := arg \min_{r>0} \left\{ \mathbb{P}^\flat \left(\mu_n \notin \mathcal{B}_r(\mu_n^\flat) \right) \leq \alpha \right\}.$$

Under some technical conditions, see [4], it appears to be a valid replacement for $r_n(\alpha)$ with high probability

$$\left| \mathbb{P}(\mu^* \notin \mathcal{B}_{r_n^\flat(\alpha)}(\mu_n)) - \alpha \right| \leq \mathcal{C}/\sqrt{n},$$

where $\mathcal{C}$ is some generic constant.

Rate of convergence. The obtained rate of convergence of the estimator μ_n to the true point μ^* is of order $1/\sqrt{n}$. With high $\mathbb{P}$-probability, it holds

$$W_2(\mu_n, \mu^*) \leq \mathcal{C}/\sqrt{n},$$

where $\mathcal{C}$ is again some generic constant.

Conclusions. Wasserstein barycenters or Wasserstein variations are complicated random variables whose asymptotic distribution relies on the initial distribution of admissible deformations $\mathbb{P}$. Multiplier bootstrap proves to be helpful to estimate variance error bounds in their estimations, enabling the construction of confidence sets, given a relatively small training set. And this appears to be very useful in many practical applications. The next step in this research is to define the limiting distribution of the approximation error in (3).

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1.6 Gradient Structure for Flows of Concentrated Suspensions

Dirk Peschka, Marita Thomas, and Barbara Wagner

Introduction: From dilute to dense suspensions

Mixtures of solid particles and viscous liquids are omnipresent in nature and everyday life. An example for such a suspension is the mixture of sand particles with water, also known as mud or slurry. The fraction of volume occupied by solid particles $0 \le \phi_s \le 1$ relative to the liquid content, as indicated in Figure 1, strongly affects the suspension flow. For $0 < \phi_s \ll 1$ the suspension is dilute, and particles are transported almost passively with the liquid, whereas when the density approaches a critical volume fraction $\phi_s \to \phi_{\text{crit}}$ depending on particle shape and distribution, the suspension undergoes a jamming transition where the solid part becomes rigid and the fluid flow is in a Darcy regime.

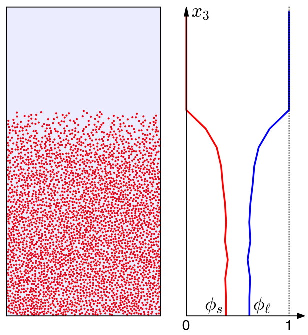


Fig. 1: *Particle distribution and corresponding volume fractions ϕ_s, ϕ_ℓ. Left: characteristic functions of particles $P_s : \Omega \to \{0,1\}$; right: volume fractions $\phi_s = \langle P_s \rangle$ defined by a suitable average.*

Suspension flows are involved in a plethora of technological processes such as in the food, pharmaceutical, printing, or oil industries. Predictive models on the length scale of these applications need to combine the interactions of the liquid and solid particles among each other on the microscale with a description of the dynamics of the liquid and solid phase on the continuum scale. On the continuum scale, such a two-phase model operates on averaged flow quantities such as volume fraction ϕ_s, velocities $\mathbf{u}$, or effective viscosity μ_{eff} relating shear stress τ and shear rate $\mathbb{D}\mathbf{u}$ via $\tau = 2\mu_{\text{eff}}\mathbb{D}\mathbf{u}$. For dilute suspensions of Newtonian liquids with viscosity μ and spherical particles Einstein (1905) derived an effective viscosity

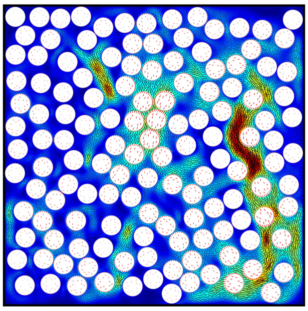
$$\frac{\mu_{\text{eff}}}{\mu} = 1 + \frac{5}{2}\phi_s. \tag{1}$$

However, for most problems suspensions are not dilute and exhibit the formation of aggregates, dense sedimentation layers, and shear-induced phase separation into highly concentrated and dilute regions. In fact, for any suspension where the liquid evaporates, Einstein's result (1) will eventually fail.

For many decades a great number of experimental and theoretical studies have been devoted to the extension of Einstein's law to the regime of concentrated suspensions. It has been observed experimentally that, as the suspension attains a solid-like state, it undergoes a jamming transition and develops further distinct phases, reflecting how particles interact and form large-scale networked patterns. They show a direct dependence on the microscopic properties, such as particle shape or interparticle forces. In fact, the transitions towards a concentrated suspension can be viewed as a paradigm for studying nonlinear rheological behavior of complex liquids.

In a ground-breaking experimental study by Cassar et al. [1], it was found that a dense suspension on an inclined plane sheared at a rate $\mathbb{D}\mathbf{u}$ under a confining pressure p_{p} can be characterized by a single dimensionless control parameter, the *viscous number*

$$I_{\text{v}} = \frac{2\mu|\mathbb{D}\mathbf{u}|}{p_{\text{p}}}. \tag{2}$$



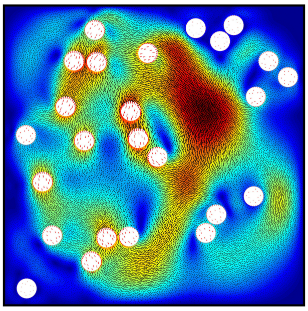


Fig. 2: *Sedimentation of discrete heavy particles in a box with a Stokes flow in* $\Omega \subset \mathbb{R}^2$ *showing flow fields. Top: dense suspension with* $\phi_s = 0.47$*; bottom: dilute suspension with* $\phi_s = 0.09$.

This result was taken up by Boyer et al. [2], where a new constitutive friction law combining the rheology for non-Brownian suspension and granular flow has been proposed, and for the first time offers to quantitatively capture the jamming transition. In Ahnert et al. [5], this new constitutive friction law was incorporated in the derivation of a new two-phase model for non-homogeneous shear flows. The derivation is based on an averaging of discrete particulate flows as in Figures 1 and 2 along the lines of Drew & Passman [4]. In Murisic et al. [3], models including particle interactions, i.e., shear induced migration, were used to predict the dynamics of a suspension on inclined planes. Also here, the limit $\phi_s \to \phi_{\text{crit}}$ was incorporated by letting $\mu_{\text{eff}} \to \infty$.

From a mathematical point of view, it is of interest to carry out the transition from a dilute to a concentrated suspension as a rigorous scaling limit. For this it is beneficial if models for the different regimes have a general mathematical structure in common, preferably of variational type, so that the limit passage can be pursued using variational convergence methods. This is, e.g., given when the models are of gradient-flow type, so that the evolution of the system is characterized in terms of an energy functional and a dissipation potential.

The topic of this contribution is twofold: Firstly, we discuss the modeling of two-phase flows from an energetic point of view to highlight that the general mathematical structure behind indeed is of gradient-flow type. Secondly, we present recent novelties in the modeling of concentrated suspensions and show that the deduced models fit into this general framework.

Modeling: Variational formulation via gradient flows

Moving domains and flow maps. We consider a liquid (index ℓ) and a solid (index s) phase at time $t \in [0,T]$, both located in a domain $\Omega(t) \subset \mathbb{R}^d$, $d = 2, 3$, with boundary $\Gamma(t)$. At each time t, each point in $\Omega(t)$ is occupied by a certain volume fraction $\phi_s(t,\cdot) : \Omega(t) \to \mathbb{R}$ of solid and $\phi_\ell(t,\cdot) : \Omega(t) \to \mathbb{R}$ of liquid, so that

$$0 \le \phi_s, \phi_\ell \le 1, \qquad \text{and} \qquad \phi_s + \phi_\ell = 1, \qquad \text{in} \quad [0,T] \times \Omega(t). \tag{3}$$

Each of the two phases $i \in \{s, \ell\}$ is transported by a velocity field $\mathbf{u}_i(t,\cdot) : \Omega(t) \to \mathbb{R}^d$

$$\partial_t \phi_i + \nabla \cdot (\phi_i \mathbf{u}_i) = 0, \tag{4}$$

so that the total velocity $\mathbf{u} = \phi_\ell \mathbf{u}_\ell + \phi_s \mathbf{u}_s$ satisfies $\nabla \cdot \mathbf{u} = 0$. The basis for this construction are so-called *flow maps* $\mathbf{X}_i : [0,T] \times \Omega(0) \to \mathbb{R}^d$, which are defined on the reference domain $\Omega(0)$ and which describe the motion of the domain at any time $t \in [0,T]$ by the kinematic condition for the current domain $\Omega(t) = \{\mathbf{x} = \mathbf{X}_s(t,\mathbf{X}),\ \mathbf{X} \in \Omega(0)\} \stackrel{!}{=} \{\mathbf{x} = \mathbf{X}_\ell(t,\mathbf{X}),\ \mathbf{X} \in \Omega(0)\}$. Hence, a function $\phi_i^0 : \Omega(0) \to \mathbb{R}$ given in the reference domain $\Omega(0)$ is transformed to the current domain $\Omega(t)$ in the following way: $\phi_i(t,\mathbf{x}) = \det(\nabla_{\mathbf{X}} \mathbf{X}_i(t,\mathbf{X}))^{-1} \phi_i^0(\mathbf{X})$. The velocities are $\mathbf{u}_i(t,\mathbf{x}) = \partial_t \mathbf{X}_i(t,\mathbf{X})$, so that (4) holds automatically. On the free boundary $\Gamma(t)$ between the two phases, we claim $\mathbf{u}_s = \mathbf{u}_\ell$. Alternatively, one can set $(\mathbf{u}_s - \mathbf{u}_\ell) \cdot \mathbf{n} = 0$ and generate an additional boundary condition.

Energy and dissipation functionals. For given phase indicators $q = (\phi_s, \phi_\ell) \simeq (\mathbf{X}_s, \mathbf{X}_\ell)$ and any pair of velocities $\dot q = (\mathbf{u}_s, \mathbf{u}_\ell) \in V$ satisfying $\nabla\cdot\mathbf{u} = 0$, we assign the dissipation potential

$$\begin{aligned}\mathcal{D}(\dot q, q) &= \int_{\Omega(t)} \phi_s \tilde\mu_s |\mathbb{D}\mathbf{u}_s|^2 + \phi_\ell \tilde\mu_\ell |\mathbb{D}\mathbf{u}_\ell|^2 + \tfrac{M}{2}|\mathbf{u}_s - \mathbf{u}_\ell|^2 \,\mathrm{d}\mathbf{x}, \\ &\text{if } \phi_i, \mathbf{X}_i \text{ satisfy (3) \& (4), and } \mathcal{D}(\dot q, q) = \infty \text{ otherwise,}\end{aligned} \tag{5}$$

where the symmetrized gradient $\mathbb{D}\mathbf{u}_i := \frac{1}{2}[\nabla\mathbf{u}_i + (\nabla\mathbf{u}_i)^\top]$ is the shear rate of the material, and where $\tilde\mu_i, M$ are nonnegative functions depending on ϕ_s. For a Newtonian liquid we have the limit $\tilde\mu_\ell(\phi_\ell) \to \mu > 0$ as $\phi_\ell = (1-\phi_s) \to 1$. We further assume that the system stores energy as the sum of gravitational and surface energies $\mathcal{E}(q) = \mathcal{E}_{\text{grav}}(q) + \mathcal{E}_{\text{surf}}(q)$, where

$$\begin{aligned}&\mathcal{E}_{\text{grav}}(q) = \int_{\Omega(t)} \varepsilon(\phi_s, \phi_\ell)\,\mathrm{d}\mathbf{x} \quad \text{and} \quad \mathcal{E}_{\text{surf}}(q) = \int_{\Gamma(t)} \sigma \,\mathrm{d}\mathbf{a}, \\ &\text{if } \phi_i, \mathbf{X}_i \text{ satisfy (3) \& (4), and } \mathcal{E}_{\text{grav}}(q) = \infty, \text{ resp. } \mathcal{E}_{\text{surf}}(q) = \infty \text{ otherwise,}\end{aligned} \tag{6}$$

with the energy density $\varepsilon(\phi_s, \phi_\ell) = g x_3(\phi_s\rho_s + \phi_\ell\rho_\ell)$, earth's gravity g, mass densities ρ_s, ρ_ℓ of solid and liquid phase, and surface tension $\sigma > 0$.

Gradient flow and resulting PDE system. The gradient flow induced by $\mathcal{D}$ and $\mathcal{E}$ from (5) and (6) is formally equivalent to the Helmholtz–Rayleigh dissipation principle $\min \overset{!}{=} \mathcal{D}(\dot q, q) + \langle \mathrm{D}_q\mathcal{E}(q), \dot q\rangle$ over all possible velocities $\dot q$. As a result, the decay of energy

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}\big(q(t)\big) = -\langle \mathrm{D}_{\dot q}\mathcal{D}(\dot q, q), \dot q\rangle = -2\mathcal{D}(\dot q, q) \le 0 \tag{7}$$

is satisfied by definition for minimizers. Herein, the functional derivatives of $\mathcal{D}$ and $\mathcal{E}$ are obtained using Reynold's transport theorem, integration by parts, and the shape derivative of surface integrals, so that for all test velocities $\dot q_{\mathbf{v}} := (\mathbf{v}_s, \mathbf{v}_\ell) \in V$ with $\mathbf{v} = \phi_s\mathbf{v}_s + \phi_\ell\mathbf{v}_\ell$ it is

$$\begin{aligned}\langle \mathrm{D}_{\dot q}\mathcal{D}(\dot q_{\mathbf{u}}, q), \dot q_{\mathbf{v}}\rangle &= \int_{\Omega(t)} \big[-\nabla\cdot\tau_s(\mathbf{u}_s)\big]\cdot\mathbf{v}_s + \big[-\nabla\cdot\tau_\ell(\mathbf{u}_\ell)\big]\cdot\mathbf{v}_\ell + M(\mathbf{u}_s - \mathbf{u}_\ell)\cdot(\mathbf{v}_s - \mathbf{v}_\ell)\,\mathrm{d}\mathbf{x} \\ &\quad + \int_{\Gamma(t)} \mathbf{v}_s\cdot\big(\tau_s(\mathbf{u}_s)\cdot\mathbf{n}\big) + \mathbf{v}_\ell\cdot\big(\tau_\ell(\mathbf{u}_\ell)\cdot\mathbf{n}\big)\,\mathrm{d}\mathbf{a}, \quad \text{and} \\ \langle \mathrm{D}_q\mathcal{E}(q), \dot q_{\mathbf{v}}\rangle &= \int_{\Omega(t)} \sum_i [\mathbf{v}_i\cdot(\phi_i\nabla p_i)]\,\mathrm{d}\mathbf{x} + \int_{\Gamma(t)} \left[\sum_i(-\phi_i p_i)\mathbf{v}_i\cdot\mathbf{n}\right] + [\varepsilon - (d-1)\sigma\kappa]\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}\mathbf{a}\end{aligned}$$

with the pressure $p_i = \partial_{\phi_i}\varepsilon \equiv g x_3 \rho_i$, the shear stress as $\tau_i(\mathbf{u}_i) = 2\phi_i\tilde\mu_i\mathbb{D}\mathbf{u}_i$, κ the signed mean curvature of $\Gamma(t)$. A minimizer of the Helmholtz–Rayleigh dissipation principle satisfies $\langle \mathrm{D}_{\dot q}\mathcal{D}(\dot q_{\mathbf{u}}, q), \dot q_{\mathbf{v}}\rangle + \langle \mathrm{D}_q\mathcal{E}(q), \dot q_{\mathbf{v}}\rangle = 0$ for all test velocities $\dot q_{\mathbf{v}} \in V$ as above. This is the weak formulation of the following system of partial differential equations

$$\partial_t\phi_s + \nabla\cdot(\phi_s\mathbf{u}_s) = 0 \qquad \text{in } \Omega(t), \tag{8a}$$

$$\partial_t\phi_\ell + \nabla\cdot(\phi_\ell\mathbf{u}_\ell) = 0 \qquad \text{in } \Omega(t), \tag{8b}$$

$$-\nabla\cdot\tau_s + M(\mathbf{u}_s - \mathbf{u}_\ell) = -\phi_s\nabla\big(p + p_s\big) \qquad \text{on } \Gamma(t), \tag{8c}$$

$$-\nabla\cdot\tau_\ell - M(\mathbf{u}_s - \mathbf{u}_\ell) = -\phi_\ell\nabla\big(p + p_\ell\big) \qquad \text{on } \Gamma(t), \tag{8d}$$

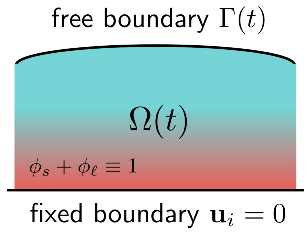


Fig. 3: *Sketch of moving domain $\Omega(t)$ and its free and fixed boundaries and particles represented with densities ϕ_s, ϕ_ℓ*

where the additional Lagrange multiplier p enforces the constraint $\nabla \cdot (\phi_s \mathbf{u}_s + \phi_\ell \mathbf{u}_\ell) = 0$. On fixed boundaries we have no-slip conditions $\mathbf{u}_s = \mathbf{u}_\ell = 0$, whereas on free boundaries $\Gamma(t)$, the formalism generates the boundary condition

$$(\tau_s + \tau_\ell)\mathbf{n} = \big[(d-1)\sigma\kappa + p\big]\mathbf{n} \quad \text{on } \Gamma(t), \tag{8e}$$

where we used $\phi_s p_{\mathrm{s}} + \phi_\ell p_\ell = \varepsilon$ and the essential boundary conditions $\mathbf{u}_s = \mathbf{u}_\ell$ at $\Gamma(t)$; see Figure 3. The proper behavior of the system for dilute or concentrated suspensions is encoded in the behavior of $\tilde{\mu}_{\mathrm{s}}, \tilde{\mu}_\ell, M$ as functions of ϕ_s as $\phi_s \to 0$ or $\phi_s \to \phi_{\text{crit}}$.

Rheology for concentrated suspensions

In Ahnert et al. [5], a model for dense suspension was derived by use of a systematic averaging procedure of particle characteristic functions $P_s : \Omega \to \{0,1\}$, so that $\phi_s = \langle P_s \rangle$; see also Figure 1. While the fluid momentum balance (8d) is unchanged, the specific choice of closure relations produces the slightly different form of the solid momentum balance

$$-\nabla \cdot \tau_s - M(\mathbf{u}_s - \mathbf{u}_\ell) = -\phi_s \nabla\big(p + p_s\big) + (p_\ell - p_s)\nabla\phi_s \quad \text{in } \Omega(t),$$

where the last term $(p_\ell - p_s)\nabla\phi_s$ additionally appears. Then, by defining $p_c := \phi_s(p_s - p_\ell)$, the so-called *contact pressure* [5] is added to the formulation. In order to turn either of these models into a model description for concentrated suspensions in the sense of [1, 2], one needs to make a specific choice for the coefficients: We set $M = \mathrm{Da}\frac{\phi_s^2}{\phi_\ell}$ with the Darcy number Da. While the liquid stress τ_ℓ can be assumed, for simplicity, to be purely Newtonian $\tau_\ell(\mathbf{u}_\ell) = 2\phi_\ell \mu \mathbb{D}\mathbf{u}_\ell$, a major issue is the modeling of the stress-strain relationship for the solid phase. It basically divides into two cases:

Case I: For $0 \le \phi_s < \phi_{\text{crit}}$ the solid shear stress is proportional to the shear stress and the contact pressure is proportional to the modulus of the shear rate

$$\tau_s = 2\phi_s \tilde{\mu}_s \mathbb{D}\mathbf{u}_s, \qquad p_c \equiv \phi_s(p_s - p_\ell) = 2\mu_n(\phi_s)|\mathbb{D}\mathbf{u}_s|, \tag{9}$$

with $\tilde{\mu}_s = \mu\eta_s(\phi_s)$ and $\mu_n = \mu\eta_n(\phi_s)$ defined using

$$\eta_s(\phi_s) = 1 + \frac{5}{2}\frac{\phi_{\text{crit}}}{\phi_{\text{crit}} - \phi_s} + \eta_c(\phi_s)\frac{\phi_s}{(\phi_{\text{crit}} - \phi_s)^2}, \tag{10}$$

$$\eta_n(\phi_s) = \left(\frac{\phi_s}{\phi_{\text{crit}} - \phi_s}\right)^2, \tag{11}$$

where we additionally introduced $\eta_c(\phi_s) = \eta_1 + (\eta_2 - \eta_1)/(1 + I_0\phi_s^2(\phi_{\text{crit}} - \phi_s)^{-2})$. The functions η_s, η_n have contributions from Einstein's for dilute suspensions and a contribution for dense suspensions. For the constitutive law, it is important to note that η_n and η_s exhibit a quadratic singularity, when ϕ_s approaches the critical volume fraction ϕ_{crit}.

This has the following implications: For a positive contact pressure p_c, as the shear rate $\mathbb{D}\mathbf{u}_s$ goes to zero, η_n has to go to infinity. Hence, η_s has to go to infinity at the same rate and, therefore, the modulus of τ_s has to go to a positive value. This turns out to be $\mu_1 p_c/\phi_s$, with $\mu_1 = 0.32$,

$\mu_2 = 0.7$, and $I_0 = 0.005$ (experimentally fitted) and is a yield stress threshold below which we are in Case II, where the shear rate is zero and the particles are jammed.

Case II: Here, $\phi_s = \phi_{\text{crit}}$ and, therefore, $\mathbb{D}\mathbf{u}_s = 0$ and $|\tau_s| \leq \mu_1 p_c/\phi_s$. Jammed regions are separated from regions where $|\mathbb{D}\mathbf{u}_s| > 0$ by yield surfaces across which ϕ_s, $\mathbf{u}_\ell$, $\mathbf{u}_s$, $(-p_\ell \mathbf{I} + \tau_\ell)\cdot\mathbf{n}$, $(-p_s\mathbf{I} + \tau_s)\cdot\mathbf{n}$, $\mathbb{D}\mathbf{u}_s$ are continuous. Fluid transport still takes place in the jammed state, which for small particles $\mathrm{Da} \gg 1$ is described by Darcy's law.

For some simple flow geometries such as channel flow, phase-space analysis showed that there is a critical value ϕ_{crit} of the volume fraction where the flow separates into two regions, a jammed one in the middle of the channel and a dilute outer region, and captured for the first time the experimentally found results. Moreover, reduced drift-flux models were asymptotically derived and numerically solved to show the evolution towards this stationary state. Some first studies [6] on the stability of these solutions show a wealth of structure even for this simple flow geometry.

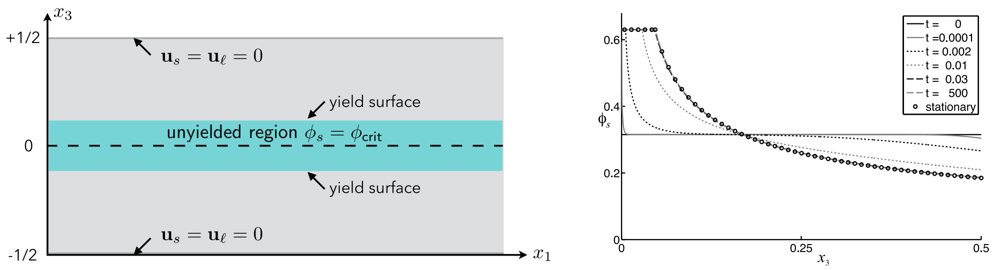


Fig. 4: Left: sketch of plug flow region in a channel; right: time evolution of solid volume fraction using the drift-flux approximation for the parameters with $\mu_1 = \mu_2$ and $p_1 = -10$, starting from an initial uniform profile of $\phi(0, x_3) = \phi_{\text{crit}}/2$. The profile first changes near the channel center and wall. The volume fraction increases near the center until maximum packing is reached, which spawns an unyielded region. This unyielded region then grows so that the yield surface approaches a stationary value.

Further mathematical insight into the structure of these equations will be necessary to treat complex liquid problems, in particular, with free surfaces. Here, the concept of gradient structures will be highly valuable to produce well-posed models for dense suspensions.

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[5] T. Ahnert, A. Münch, B. Wagner, *Models for the two-phase flow of concentrated suspensions*, Eur. J. Appl. Math, published online on 04.06.2018, https://doi.org/10.1017/S095679251800030X.

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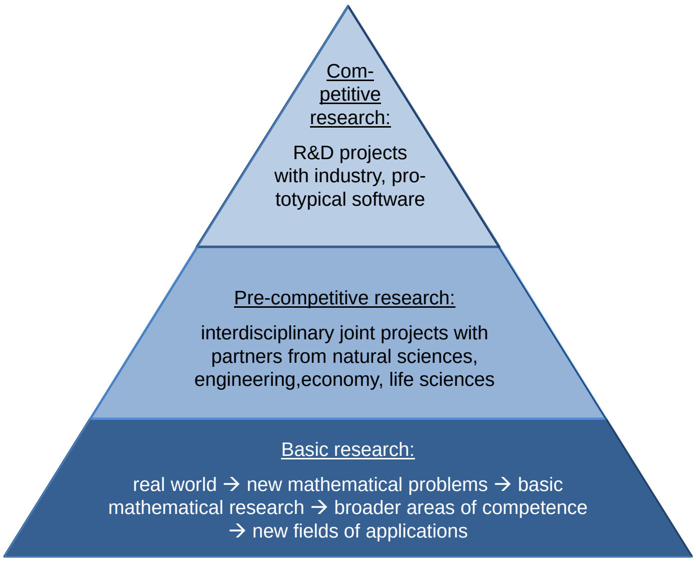
2 WIAS in 2017

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

2.1 Profile

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



The mission of WIAS is to carry out *project-oriented* research in applied mathematics. WIAS contributes to the solution of complex economic, scientific, and technological problems of transregional interest. Its research is interdisciplinary and covers the entire process of problem solution, from mathematical modeling to the theoretical study of the models using analytical and stochastic methods, to the development and implementation of efficient and robust algorithms, and the simulation of technological processes. In its field of competence, WIAS plays a leading role in Germany and worldwide. WIAS's successful research concept is based on the above pyramid-shaped structure: Right at the bottom, basic mathematical research dedicated to new mathematical problems resulting from real-world issues as well as research for broadening mathematical areas of competence for developing new, strategically important fields of application. Based on this foundation, precompetitive research, where WIAS cooperates in interdisciplinary joint projects with partners from the natural sciences, engineering, economy, and life sciences. On top, cooperations with industry in R&D projects and the development of prototypical software. Close cooperations with companies and the transfer of knowledge to industry are key issues for WIAS. This is also reflected by the fact that Prof. Dietmar Hömberg, head of a research group at WIAS, has become the President of the *European Consortium for Mathematics in Industry (ECMI)* for the period 2016–2017.

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

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

WIAS promotes the international collaboration in applied mathematics by organizing workshops and running guest and postdoc programs. The institute is embedded in a dense network of scientific partners. In particular, it maintains various connections with Leibniz institutes and actively takes part in the forming and development of strategic networks in its fields. Thus, WIAS coordinates the Leibniz Network "Mathematical Modeling and Simulation (MMS)" connecting twenty-eight partners from all sections of the Leibniz Association. Modern methods of MMS are imperative for progress in science and technology in many research areas. In 2017, WIAS received 100,000 euros from the Strategic Fund of the Leibniz Association for 24 months to organize the network. The "2nd Leibniz MMS Days" took place from February 22 to 24, 2017, in Hanover; see page 118.

Fig. 1: *The President of the Leibniz Association, Prof. Kleiner, opened the "2nd Leibniz MMS Days"*

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

2.2 Structure and Scientific Organization

2.2.1 Structure

In 2017, WIAS was organized into the following divisions for fulfilling its mission: Eight research groups, one Leibniz and one Weierstrass group, and one Focus Platform[1], form the scientific body of the institute. In their mission, they are supported by the departments for technical and administrative services. The Secretariat of the International Mathematical Union (IMU, see page 56), hosted by WIAS, is a supportive institution for the international mathematical community. Moreover, WIAS hosts the German Mathematics Association DMV and the Society of Didactics of Mathematics GDM.

Research Groups:

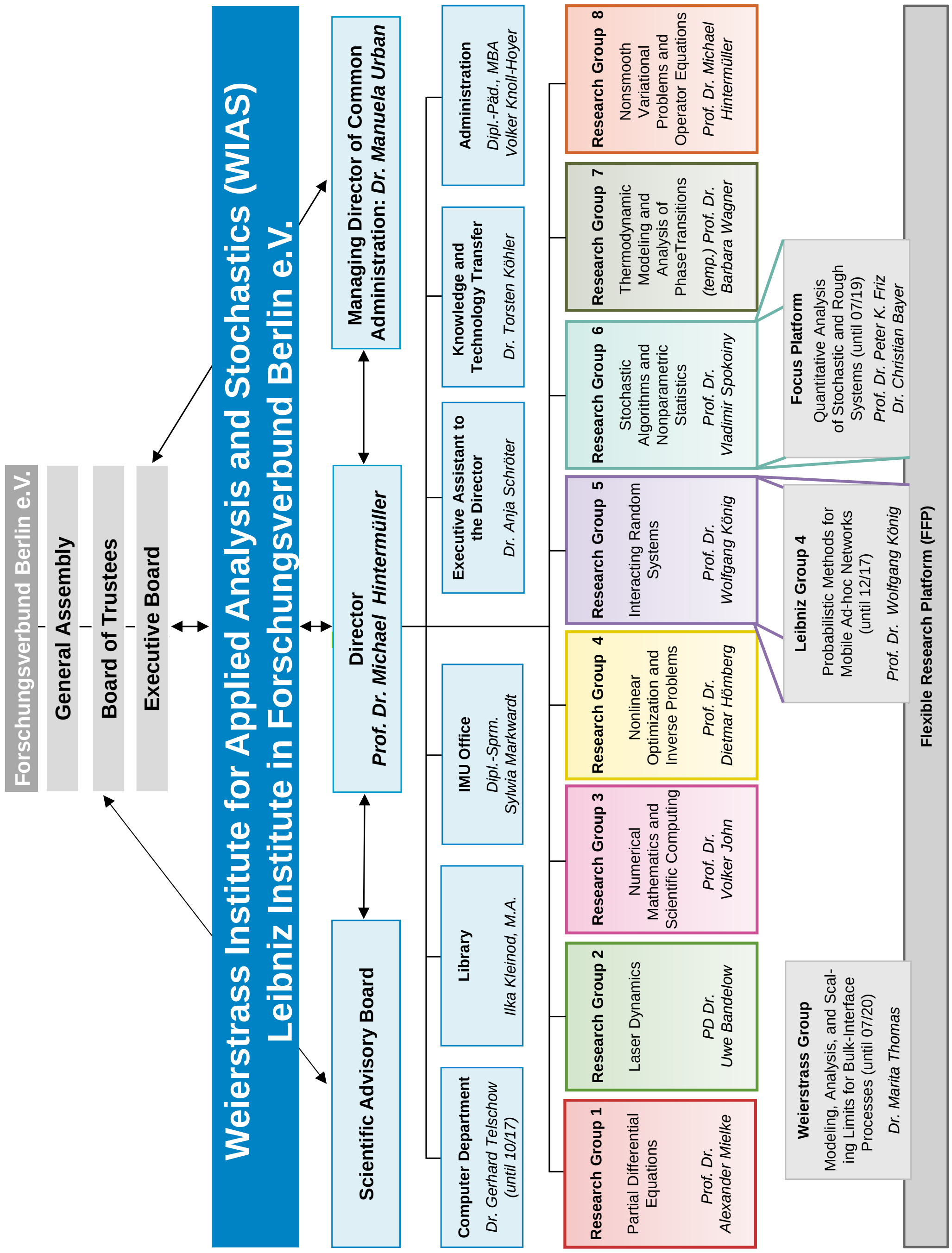
RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing
RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase Transitions
RG 8. Nonsmooth Variational Problems and Operator Equations

Flexible Research Platform:

LG 4. Probabilistic Methods for Mobile Ad-hoc Networks
WG 1. Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes
FP 1. Quantitative Analysis of Stochastic and Rough Systems

The organization chart on the following page gives an overview of the organizational structure of WIAS in 2017.

[1] In the following, the terms “research group” will often be abbreviated by “RG”, “Leibniz group” by “LG”, Weierstrass group by “WG”, and Focus Platform by “FP”.


Forschungsverbund Berlin e.V.
General Assembly
Board of Trustees
Executive Board
Weierstrass Institute for Applied Analysis and Stochastics (WIAS)
Leibniz Institute in Forschungsverbund Berlin e.V.
Scientific Advisory Board
Director
Prof. Dr. Michael Hintermüller
Managing Director of Common Administration: Dr. Manuela Urban
Computer Department
Dr. Gerhard Telschow
(until 10/17)
Library
Ilka Kleinod, M.A.
IMU Office
Dipl.-Sprm.
Sylwia Markwardt
Executive Assistant to the Director
Dr. Anja Schröter
Knowledge and Technology Transfer
Dr. Torsten Köhler
Administration
Dipl.-Päd., MBA
Volker Knoll-Hoyer
Research Group 1
Partial Differential Equations
Prof. Dr.
Alexander Mielke
Research Group 2
Laser Dynamics
PD Dr.
Uwe Bandelow
Research Group 3
Numerical Mathematics and Scientific Computing
Prof. Dr.
Volker John
Research Group 4
Nonlinear Optimization and Inverse Problems
Prof. Dr.
Dietmar Hömberg
Research Group 5
Interacting Random Systems
Prof. Dr.
Wolfgang König
Research Group 6
Stochastic Algorithms and Nonparametric Statistics
Prof. Dr.
Vladimir Spokoiny
Research Group 7
Thermodynamic Modeling and Analysis of PhaseTransitions
(temp.) Prof. Dr.
Barbara Wagner
Research Group 8
Nonsmooth Variational Problems and Operator Equations
Prof. Dr. Michael
Hintermüller
Weierstrass Group
Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes (until 07/20)
Dr. Marita Thomas
Leibniz Group 4
Probabilistic Methods for Mobile Ad-hoc Networks (until 12/17)
Prof. Dr. Wolfgang König
Focus Platform
Quantitative Analysis of Stochastic and Rough Systems (until 07/19)
Prof. Dr. Peter K. Friz
Dr. Christian Bayer
Flexible Research Platform (FFP)

2.2.2 Main Application Areas

The research at WIAS focused in 2017 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

- **Conversion, Storage, and Distribution of Energy**
- **Flow and Transport**
- **Materials Modeling**
- **Nano- and Optoelectronics**
- **Optimization and Control in Technology and Economy**
- **Quantitative Biomedicine**

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

2.2.3 Contributions of the Groups

The eight Research Groups, the Leibniz Group, and the Weierstrass Group form the institute's basis to fully bring to bear and develop the scope and depth of its scientific expertise. A Focus Platform, on the other hand, represents an interesting topical focus area in its own right and operates under the umbrella of one or more Research Groups. 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 a prerequisite to enter new fields of applications, calling for a well-directed long-term *basic research in mathematics*.

The table gives an overview of the main application areas to which the groups contributed in 2017 in the interdisciplinary solution process described above.

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

In the following, special research topics are listed that were addressed in 2017 within the general framework of the main application areas.

Conversion, Storage and Distribution of Energy

This main application area takes account of an economic use of energetic resources based on mathematical modeling and optimization. With regard to future developments, sustainability and aspects of electro-mobility play a major role. Lithium-ion batteries belong to the key technologies for storing renewable energy. Charging time and capacity of such batteries are decisively determined by stochastic processes within multi-particle electrodes as well as by transportation processes in the electrolyte and on the electrodes surface. The modeling and stochastic analysis of multi-particle electrodes is realized by a cooperation of RG 6 and RG 7. RG 3 and RG 7 cooperate in modeling the transport processes and their evaluation by simulations. A further focus is put on the phase-field modeling of the liquid phase crystallization of silicon in order to develop optimized thin-film solar cells in the framework of an interdisciplinary research project. Furthermore, RG 4 and RG 8 investigate aspects of uncertainty in energy management via stochastic optimization or uncertainty quantification, respectively. Here, the emphasis is put on gas networks and renewable energies with uncertain parameters given, e.g., by demand, precipitation, or technical coefficients. In this context, new perspectives in modeling and analyzing equilibria in energy markets with random parameters and when coupling markets with the underlying physical or continuum mechanical properties of the energy carrier in a power grid open up.

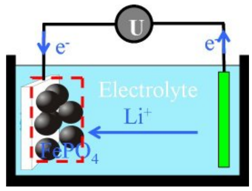


Fig. 1: *Sketch of a lithium-ion battery (LiFePO4)*

Core areas:

- Light-emitting diodes based on organic semiconductors (OLEDs; in RG 1 and RG 3)
- Modeling of experimental electrochemical cells for the investigation of catalytic reaction kinetics (in RG 3)
- Lithium-ion batteries (in RG 3 and RG 7)
- Modeling and analysis of coupled electrochemical processes (fuel cells, batteries, hydrogen storage, soot; in RG 1, RG 3, RG 5 (planned), and RG 7)
- Nonlinear chance constraints in problems of gas transportation (in RG 4)
- Parameter identification, sensor localization, and quantification of uncertainties in switched PDE systems (in RG 8)

Flow and Transport

Flow and transport of species are important in many processes in nature and industry. They are generally modeled by systems consisting of partial differential equations. Research groups at WIAS are working at the modeling of problems, at the development and analysis of discretizations for partial differential equations, at the development of scientific software platforms, and the simulation of problems from applications. Aspects of optimization, inverse problems (parameter estimation), and stochastic methods for flow problems become more and more important in the research of the institute.

Fig. 2: *Flow through an aortic arch*

Core areas:

- Thermodynamic models and numerical methods for electrochemical systems (in RG 1, RG 3, and RG 7)

- Development and analysis of physically consistent discretizations (in RG 3)
- Modeling and numerical methods for particle systems (in RG 1, RG 3, and RG 5)
- Modeling of nanostructures of thin films (in RG 7)
- Computational hemodynamics (in RG 3 and RG 8)
- Scientific software platforms `ParMooN` and `pdelib` (in RG 3)

Materials Modeling

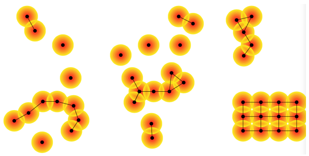


Fig. 3: *A realisation of a many-body system showing a small crystal in the lower right corner*

Modern materials increasingly show multi-functional capabilities and require precise and systematically derived material models on many scaling regimes. To include theories from the atomistic to the continuum description, multi-scale techniques are at the core in the derivation of efficient models that enable the design of new materials and processes and drive the development of new technologies. Combining stochastic and continuum modeling with numerical methods and the rigor of mathematical analysis to address some of today's most challenging technological problems is a unique characteristic of the WIAS.

Core areas:

- Homogenization and localization in random media (in RG 1 and RG 5)
- Models of condensation and crystallization in interacting many-particle systems to help understand metastability and ageing processes (in RG 3, RG 5, RG 6, and RG 7)
- Asymptotic analysis of nano- and microstructured interfaces (including their interaction with volume effects; in RG 7 and WG 1)
- Dynamical processes in nonhomogeneous media (in RG 6 and RG 7)
- Material models with stochastic coefficients (in RG 1, RG 3, RG 4, RG 5, and RG 7)
- Modeling, analysis, and simulation of gas-solid and liquid-solid transitions (phase separation with thermomechanical diffusion; in RG 7 and RG 5)
- Thermodynamically consistent electrochemical models of lithium-ion batteries and fuel cells (in RG 3 and RG 7)
- Thermomechanical modeling of phase transitions in steels (in RG 4)
- Hysteresis effects (elastoplasticity, shape memory alloys, lithium batteries, hydrogen storage; in RG 1 and RG 7)
- Modeling of elastoplastic and phase-separating materials including damage and fracture processes (RG 1, RG 7, and WG 1)
- Analysis of local and nonlocal phase field models and their sharp-interface limits (applied to thin-film solar cells and lithium-ion batteries; in RG 1, RG 7, and WG 1)
- Stochastic modeling of phase transitions (in RG 5)

Nano- and Optoelectronics

Optical technologies count among the most important future-oriented industries of the 21st century, contributing significantly to technological progress. They facilitate innovative infrastructures, which are indispensable for the further digitalization of industry, science, and society.

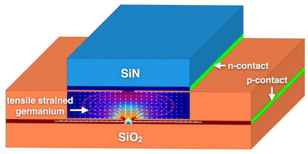


Fig. 4: *Cross section through an edge-emitting germanium microstrip, showing hole currents (color and arrows) and optical mode (red isolines) in the optically active germanium region under tensile strain*

Mathematical modeling, numerical simulation, as well as theoretical understanding of the occurring effects are important contributions of WIAS to today's technological challenges. A central topic is the modeling and mathematical analysis of the governing equations and the simulation of semiconductor devices.

Core areas:

- 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 2 and 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, RG 2, and RG 3)
- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in RG 2)
- Photovoltaics, OLED lighting, and organic transistors (in RG 1, RG 3, and RG 7)
- Mathematical modeling, analysis, and optimization of strained germanium microbridges (in RG 1 and RG 8)

Optimization and Control in Technology and Economy

For planning and reconfiguration of complex production chains as they are considered in the Industry 4.0 paradigm as well as for innovative concepts combining economic market models and the underlying physical processes, e.g., in energy networks, modern methods of algorithmic optimal control are indispensable. In many of these problems different spatial and temporal scales can be distinguished, and the regularity properties of admissible sets plays an important role.

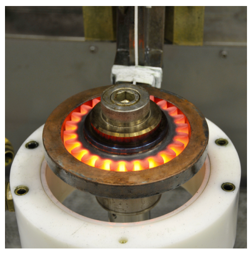


Fig. 5: *Induction heat treatment of a gear*

Applications may range from basic production processes such as welding and hardening to the design of diffractive structures and simulation tasks in process engineering industry to optimal decision in financial environments such as financial (energy) derivatives, energy production, and storage.

Core areas:

- Simulation and control in process engineering (in RG 3, RG 4, and RG 6)
- Problems of optimal shape and topology design (in RG 4)
- Optimal control of multifield problems in continuum mechanics and biology (in RG 3, RG 4, and RG 7)

- Evaluation of the quality of ad-hoc telecommunication systems in view of connectivity, message routing, propagation of malware and capacity restrictions (in LG 4 and RG 5)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6)
- Realistic design of telecommunication models on street systems (in LG 4)
- Optimal control of multiphase fluids and droplets (in RG 8)

Quantitative Biomedicine

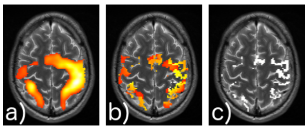


Fig. 6: *Signal detection in a single-subject finger-tapping experiment using (left to right) (a) standard Gaussian filter, (b) structural adaptive smoothing and Random field theory (RFT), (c) structural adaptive segmentation*

Quantitative Biomedicine is concerned with the modeling, analysis, simulation, or optimization of various highly relevant processes in clinical practice. Not only the modeling of cellular, biochemical, and biomolecular processes, but also applications in medical engineering, such as the modeling, simulation, and optimization of prostheses or contributions to the area of imaging diagnostics, are major focus topics.

At WIAS, mathematical models for a better understanding of haemodynamic processes are developed, analyzed, and simulated. These models are then employed for the prognosis or optimization after medical interventions, using, e.g., model reduction and optimization techniques with partial differential equations. Other foci are the modeling and analysis of time-based systems, e.g., cartilage reconstruction, calcium release, or medical image and signal processing. In the latter, classical tasks of image processing like registration, denoising, equalization, and segmentation, but also (low-rank/sparse) data decomposition and functional correlations, e.g., in neurological processes, are studied. These processes typically lead to complex, nonlinear, or nonsmooth inverse problems where often also statistical aspects play a central part.

Core areas:

- Numerical methods for biofluids and biological tissues (in RG 3 and RG 8)
- Branching processes in random media (in RG 5)
- Genetic evolution (in RG 5)
- Image processing (in RG 6 and RG 8)
- Dynamics of learning processes in the neurosciences (in RG 6)
- Modeling of high-resolution magnetic resonance experiments (in RG 6)
- Methods of diagnosis of neurodegenerative diseases (in RG 6)
- Free boundary models for actin filament networks (in RG 7)
- Modeling of a nanopore for the analysis of DNA-type macromolecules (in RG 7)

2.3 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 2017, WIAS successfully renewed the *berufundfamilie audit certificate* in a re-auditing process for three years. With the certificate, the institute documents its commitment to a family-friendly personnel policy, adapted to the various life stages. The new agreement on objectives is aiming to optimize the already high standards in family-friendly arrangements. A cooperation with the family service agency *benefit@work* was established and will be further adapted to meet the needs of WIAS's staff. For organizing the work in a family-conscious way, the project management tool *JIRA* was introduced in the directorate, in the administration, and among scientific staff. Especially for staff members interactive presentations on various focal topics held by external experts are offered regularly.

Zertifikat seit 2013
audit beruf**und**familie

Fig. 1: *Prof. Dietmar Hömberg, in charge in 2017 of the field of family and work in the directorate of WIAS (upper row, third from left), at the Certificate Conferment Ceremony of the* audit berufundfamilie *in Berlin*

In December 2017, WIAS's equal opportunities officer and her substitute held the second women's assembly. They gave the female employees a report on their work during the year and answered questions. As a part of the audit berufundfamilie, WIAS's equal opportunities officer and her substitute carried out the 2017 staff survey. The results are currently being examined. On May 5, Franziska Flegel (RG 5) and Ilka Kleinod (equal opportunities officer) participated in the 2017 Female Ph.D. Students' Seminar of Forschungsverbund Berlin. The topic was "Communication and Conflict Management for Women". In April, WIAS again took part in the "Girls'Day – Mädchen Zukunftstag", an initiative of the German Federal Ministry of Family, Senior Citizens, Women and Youth in collaboration with the Federal Ministry of Education and Research. Four girls followed various lectures and asked many questions, mentored by scientists from WIAS.

2.4 Grants

The raising of grants under scientific competition is one of the main indicators of scientific excellence and thus plays an important role in the efforts of WIAS. In this task, WIAS was very successful in 2017, having raised a total of 3.053 million euros, from which 50 additional researchers (+ 7 outside WIAS; Dec. 31, 2017) were financed. In total in 2017, 24.25 percent of the total budget of WIAS and 43.2[2] 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 108ff.

2.5 Participation in Structured Graduation Programs

Graduate School *Berlin Mathematical School (BMS)*

Berlin Mathematical School

Berlin's mathematicians are proud that, after its successful installation in 2006, a second funding period was granted to this graduate school in Summer 2012 for 2013–2017, for the excellent work done since its inception. The BMS is jointly run by the three major Berlin universities within the framework of the German Initiative for Excellence. The BMS is funded with more than one million euros per year to attract excellent young Ph.D. students from all over the world to the city. Many members of WIAS are contributing to the operations of the BMS.

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

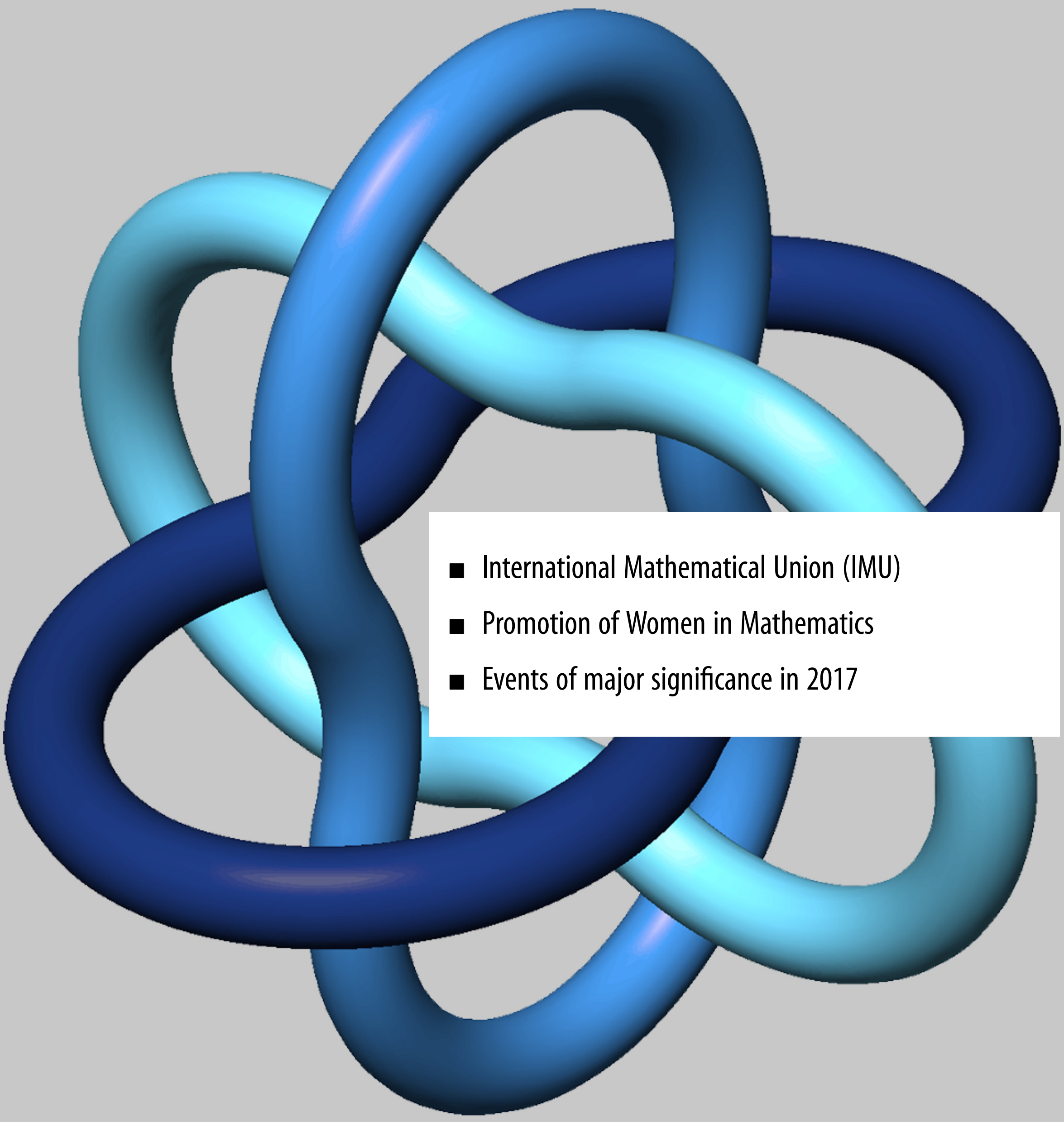
In October 2013, this International Research Training Group took up its work for 4.5 years. The faculty consists of internationally renowned scholars from Humboldt-Universität zu Berlin, WIAS (RG 6), Freie Universität Berlin, the German Institute for Economic Research (DIW), and Xiamen University in China. In December 2017, the IRTG was prolongated until September 2022.

2.6 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 183ff. for a list of software packages that WIAS makes available. Licensing models depend on the specifics of the corresponding projects. Codes are offered under open source and proprietary licenses as well as combinations thereof.

[2] With scholarship holders.

3 IMU@WIAS



- International Mathematical Union (IMU)
- Promotion of Women in Mathematics
- Events of major significance in 2017

3.1 International Mathematical Union (IMU)

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.

Staff members:

Alexander Mielke, *Head of the Secretariat and IMU Treasurer*. A. Mielke is a professor at Humboldt-Universität zu Berlin, Deputy Director of WIAS, and head of Research Group 1 at WIAS. In his function as the head of the secretariat, he is responsible for the IMU Secretariat as a separate unit within WIAS. He was appointed as IMU Treasurer by the IMU Executive Committee and is responsible for all financial aspects, including collecting dues, financial reports, and drafting the budget of IMU.

Sylwia Markwardt, *Manager of the Secretariat*. S. Markwardt's responsibilities include to head and supervise all administrative operations of the secretariat and actively participate in the implementation of the decisions and duties of the IMU Executive Committee and the IMU General Assembly, which is done in close cooperation with the IMU Secretary. She communicates with the IMU member countries, drafts written materials, writes minutes and reports, and supervises the IMU website. 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.

TBA, *IMU Accountant*. The IMU Accountant 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.

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

Ramona Fischer, *Project Assistant*. R. Fischer is on leave.

Theresa Loske, *Project Assistant*. T. Loske's task is to support the administrative work of the IMU Secretariat, in particular, to assist in the organization and wrap-up of the International Congress of Mathematicians in 2018 and the initialization of new CDC programs.

The IMU Secretary

Helge Holden is the IMU Secretary. He holds a professorship at the Norwegian University of Science and Technology, Trondheim, and at the Center of Mathematics for Applications, University of Oslo, Norway. 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 Promotion of Women in Mathematics

Marie-Françoise Roy (CWM)

Women mathematicians are increasingly visible in the mathematical community. The 2014 International Congress of Mathematicians played a special role in this process when Maryam Mirzakhani became the first woman ever to be awarded the Fields Medal.

The IMU Committee for Women in Mathematics (CWM), created in 2015, is the only committee whose main concern is the issues for women in mathematics at the world level. As such, it has an important role and responsibility. Change takes generations: There are gradual improvements, but with each step forward come new challenges. Networking, both inside the mathematical community and more globally, seems to be key to driving change.

Communicating through CWM website and CWM ambassadors. CWM's website `http://www.mathunion.org/cwm/` plays a central role in CWM's work. Launched in August 2014 by the

IMU following an initiative of its President Ingrid Daubechies, its aim is to provide an internationally based resource for women mathematicians. It is a crucial means of communication and is kept updated and enriched by the committee.

CWM has also established about 100 ambassadors worldwide, each of whom disseminates information such as CWM funding calls, and keeps CWM informed about relevant activities or initiatives.

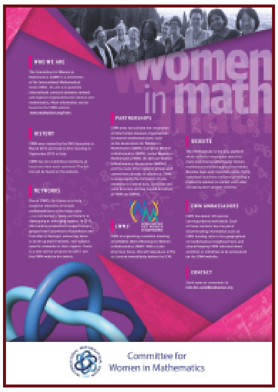


Fig. 1: *CWM Poster*

Supporting networks through the CWM annual call. The main initial goal set by CWM was to help establish and foster networks of women mathematicians especially in Asia, Latin America, and Africa. To this end, it has made three calls offering sponsorship, in 2016, 2017, and 2018.

The 2018 call elicited 55 applications, of which 10 were approved. Most grants are devoted to the above aims. Many of the initiatives take the form of a meeting with both a mathematical and a career development part. This is the case for two regional meetings of the African Women in Mathematics Association (AWMA), one in Addis Ababa (Ethiopia) for East Africa and one in Ibadan (Nigeria) for West Africa, and also for the second Central Asia Women in Mathematics Association meeting in Uzbekistan. Support for the Indian Women in Mathematics Association will enable the participation of women from the South Asian Association for Regional Co-operation at the IWM meeting at Shiv Nadar University in Uttar Pradesh. The first workshop of "*Women in Mathematics in the Balkan Region*" taking place in Skopje (Macedonia) will involve several neighboring countries. A workshop in El Salvador (supported by the Vice Minister of Science and Technology and the ICSU Regional Office of Latin America and the Caribbean) entitled "*Why Mathematics?: Encouraging Girls to Pursue the Dream of Becoming Teachers or Researchers in this Discipline*" will be focussed on less developed Central American countries such as Guatemala, Honduras, Nicaragua, the Dominican Republic, El Salvador, and Panama. An activity inspired by the series of meetings "*Women in . . .*" (see for example "*Women in Numbers*") held at the Banff International Research Station, is planned for the first time in South America, in Uruguay.

The African Women in Mathematics Association will design portraits of African women mathematicians to be used for promoting mathematics among young African women. The portraits will be posted on the AWMA website and published as a booklet.

Two further events are taking place in Europe, an Abdus Salam International Centre for Theoretical Physics (ICTP) school in Trieste (Italy) on Dynamical Systems, with all-female organizers and lecturers, and the European Women in Mathematics General Meeting in Graz (Austria). In both cases, the CWM grant will be used to support the attendance of women from developing countries.

Fig. 2: *Left: CWM meeting in Cortona 2015. Right: Gender Gap in Science project in Paris 2017*

Leading a pluridisciplinary project on the Gender Gap in Science. In 2016, the International Council for Science (ICSU) announced a new grant program to address long-standing priorities for ICSU members in developing science education, outreach, and public engagement activities, and to mobilize resources for international scientific collaboration.

The IMU is leading the project "A Global Approach to the Gender Gap in Mathematical, Computing and Natural Sciences: How to Measure It, How to Reduce It?", one of the three projects approved by ICSU. Its coordinator is Marie-Françoise Roy, CWM chair. There are ten partner organizations: six ICSU members (International Union of Pure and Applied Chemistry, International Union of Pure and Applied Physics, International Astronomical Union, International Union of Biological Sciences, International Council for Industrial and Applied Mathematics, and International Union for History and Philosophy of Science and Technology), UNESCO, as well as Gender in Science, Innovation, Technology and Engineering, the Organization for Women in Science in the Developing World, and the Association for Computing Machinery.

The motivation for the project comes from the persistence of a significant gender gap at all levels. Barriers to achievement by women persist, especially in developing countries, despite mathematical, computing, and natural sciences having long and honorable traditions of participation by highly creative female contributors.

The project will produce sound data, including trends (since the situation for women continues to change around the world, with some negative developments), to support the choices of interventions which ICSU and member unions can feasibly undertake. It will provide evidence for informed decisions and provide easy access to materials proven to be useful in encouraging girls and young women in these fields. Regional information about careers, jobs, and salaries will be included.

A Joint Global Survey is planned to reach 45,000 respondents in more than 130 countries using at least 10 languages, while a Joint Study on Publication Patterns will analyze comprehensive metadata sources corresponding to publications of more than 500,000 scientists since 1970. Contrasts and common ground across regions and cultures, less developed and highly developed countries, men and women, mathematical and natural sciences, will be highlighted.

Fig. 3: Logo of the World Meeting for Women in Mathematics

Organizing the first World Meeting for Women in Mathematics (WM)^2. CWM is organizing the first World Meeting for Women in Mathematics – (WM)^2, a satellite event of the International Congress of Mathematicians (ICM) 2018, Rio de Janeiro. It will bring together female mathematicians from all over the world with a strong focus on Latin America. Although there is currently no formal network for women mathematicians in Latin America, several initiatives have taken place from 2015–2017, in Brazil, Mexico, Chile, and Colombia, most with the encouragement of CWM. It is anticipated that (WM)^2 will lead to better coordination of activities for women mathematicians in this part of the world. The program includes research talks, group discussions about gender issues in mathematics, a panel discussion, and poster presentations. There will also be a tribute to Maryam Mirzakhani whose premature death in July 2017 saddened us all.

3.3 Events of major significance in 2017

Grants

IMU won ICSU grant 2017–2019. IMU's application to ICSU (International Council for Science) was successful. The project proposal "A Global Approach to the Gender Gap in Mathematical, Computing and Natural Sciences: How to Measure It, How to Reduce It?", jointly led by IMU's committee CWM and IUPAC (International Union of Pure and Applied Chemistry), won a grant of 100,000 euros per annum for three years. The adminstration of the grants funds is supported by the IMU Secretariat.

Meetings

CWM meeting. The Committee for Women in Mathematics of the IMU met in the IMU Secretariat from May 29–30, 2017.

IPC meeting ICMI Study 24. The International Program Committee for the ICMI Study 24 volume met in the IMU Secretariat from November 13–15, 2017.

Events

WIAS Days 2017. The IMU Secretariat contributed to the program in the form of a presentation and a poster informing on the responsibilities of the Secretariat.

Visit of the FVB Board of Trustees at the IMU Secretariat. On June 14, 2017, the Board of Trustees of Forschungsverbund Berlin e.V. (FVB) held its meeting at WIAS. An item of the agenda was the visit to the IMU Secretariat in order to present to the Board the activities and services provided by the office for the international scientific community.

WIAS Evaluation 2017. The IMU Secretariat contributed a survey poster presenting the International Mathematical Union (IMU), the support of the Secretariat to the IMU and IMU's Commissions and Committees, as well as the interaction of WIAS and IMU.

Heidelberg Laureate Forum. The fifth Heidelberg Laureate Forum (HLF) took place from September 24–29, 2017, 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 is a partner of the HLF. Among the participating laureates at the HLF 2017 who had been awardees of the Fields Medal (FM) or the Nevanlinna Prize (NP) were: Sir Michael Francis Atiyah (FM), Martin Hairer (FM), Shigefumi Mori (FM), Stephen Smale (FM), Daniel Spielman (NP), Madhu Sudan (NP), Robert Endre Tarjan (NP), Leslie Valiant (NP), and Efim Zelmanov (FM).

Relaunch of the website of the IMU and IMU's Commissions and Committees. After months of intense work on redesigning and restructuring the web presentation of the IMU, the revamped website went live on December 7, 2017.

Fig. 4: *New website of the IMU*

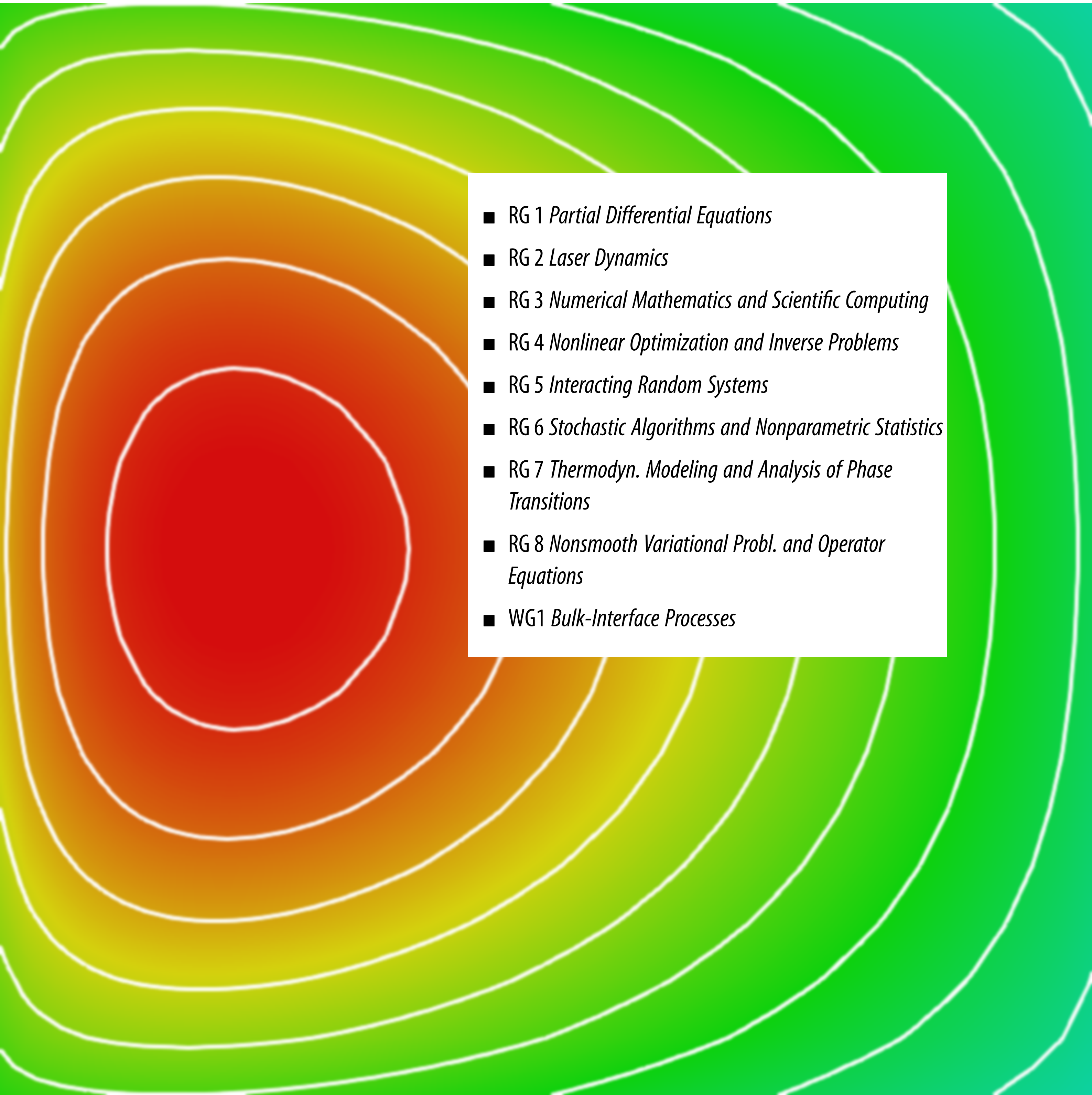
Participation of IMU Secretariat members in international events.

- IMU Executive Committee meeting, London, UK (S. Markwardt, A. Mielke)
- CDC meeting, Sussex, UK (L. Koch)
- Site visit General Assembly and ICM 2018, São Paulo and Rio de Janeiro, Brazil (S. Markwardt)
- ICMI Executive Committee meeting, Geneva, Switzerland (L. Koch)
- Heidelberg Laureate Forum, Heidelberg, Germany (S. Markwardt)

List of guests at the IMU Secretariat

Date	Guests	Event
May 29 – 30	Carolina Araujo, Brazil; Bill Barton, New Zealand; Petra Bonfert-Taylor, USA; Ari Laptev, Sweden; Neela Nataraj, India; Marie Francoise Quedrago, Burkina Faso; Ami Radunskaya, USA; Sujatha Ramdorai, Canada; Marie-Françoise Roy, France; Caroline Series, UK; Noh Sunsook, Republic of Korea; Betul Tanbay, Turkey; John Toland, UK	CWM
June 14	Stefan Eisebitt, Germany; Peter A. Frensch, Germany; Mark Gessner, Germany; Peter Gottstein, Germany; Rainer Hammerschmidt, Germany; Michael Heuken, Germany; Barbara Kaltenbacher, Austria; Ulrich Krafft, Germany; Andreas Offenhäusser, Germany; Joachim Wieland, Germany; Thomas Zettler, Germany	Individual visit
July 6	Konrad Fiedler, Austria; Peter Heil, Germany; Claudia Herok, Germany; Barbara Kaltenbacher, Austria; Bernd Lietzau, Germany; Frank Reifers, Germany; Hans-Peter Seidel, Germany; Brigitte Voit, Germany; Jonas Wirth, Germany; Frank Wolf, Germany	Individual visit
Oct 31 – Nov 5	Bernard Hodgson, Canada	ICMI Archive
Nov 6	Bernard Hodgson, Canada; Ragni Piene, Norway; John Toland, UK; Wendelin Werner, Switzerland	IMU Office Committee
Nov 13 – 15	Jill Adler, South Africa; Abraham Arcavi, Israel; Ferdinando Arzarello, Italy; Marianna Bosch, Spain; Angel Ruiz, Costa Rica; Yoshinori Shimizu, Japan; Renuka Vital, South Africa; Yan Zhu, China	ICMI Study 24

4 Research Groups' Essentials



- RG 1 *Partial Differential Equations*
- RG 2 *Laser Dynamics*
- RG 3 *Numerical Mathematics and Scientific Computing*
- RG 4 *Nonlinear Optimization and Inverse Problems*
- RG 5 *Interacting Random Systems*
- RG 6 *Stochastic Algorithms and Nonparametric Statistics*
- RG 7 *Thermodyn. Modeling and Analysis of Phase Transitions*
- RG 8 *Nonsmooth Variational Probl. and Operator Equations*
- WG1 *Bulk-Interface Processes*

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 the sciences and in engineering. The theory is developed in connection with well-chosen problems in applications, mainly in the following areas:

- Modeling of semiconductors; in particular, organic semiconductors and optoelectronic devices
- Reaction-diffusion systems, also including temperature coupling
- Multifunctional materials and elastoplasticity

The methods involve topics from pure functional analysis, mathematical physics, pure and applied analysis, calculus of variations, and numerical analysis:

- Qualitative methods for Hamiltonian systems, gradient flows, or consistently coupled systems
- Multiscale methods for deriving effective large-scale models from models on smaller scales, including models derived from stochastic particle systems
- Existence, uniqueness, and regularity theory for initial and boundary value problems in nonsmooth domains and with nonsmooth coefficients, thereby also including nonlocal effects

European Research Council
Established by the European Commission

The qualitative study of partial differential equations provides a deeper understanding of the underlying processes and is decisive for the construction of efficient numerical algorithms. Corresponding scientific software tools are developed in cooperation with other research groups.

General methods for evolutionary systems

ERC project. The ERC-Advanced Grant *Analysis of Multiscale Systems Driven by Functionals* (AnaMultiScale) started in April 2011 and concluded in March 2017. The project group, which was embedded in RG 1, involved about 5 researchers, whose task was to study evolutionary systems driven by energy or entropy and to derive effective models for multiscale problems, e.g., via evolutionary Gamma-convergence. The applications had their focus in material modeling and optoelectronics.

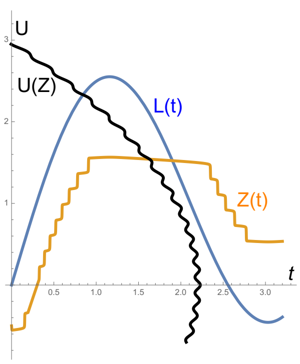


Fig. 1: *A wiggly energy $U(z)$ and a smooth loading $L(t)$ lead to a stick-slip response $Z(t)$*

A major achievement emanated from joint work with researchers from Pavia and concerned the development of a general existence theory for generalized gradient systems based on De Giorgi's energy-dissipation principle (EDP). This includes the definition of *balanced-viscosity solutions* and the understanding of the jump behavior for systems in the limit of vanishing viscosity, which settled a long-standing problem in treating vanishing-viscosity limits for rate-independent systems.

For such generalized gradient systems different notions of *evolutionary Gamma-convergence* were developed to give a proper meaning to what it means that a family of gradient systems converges to an effective gradient system. This led to the notion of EDP-convergence, and most recently to relaxed EDP-convergence for wiggly-energy gradient systems; see Figure 1. Moreover, in collaboration with RG 5 *Interacting Random Systems*, a relation between generalized gradient structures and large-deviation principles for the underlying stochastic processes was discovered.

For applications in nanophotonics a new gradient structure for dissipative quantum master equations was developed in [4]. It provides a thermodynamically consistent coupling mechanism for the development of hybrid models combining classical drift-diffusion for charge carriers and quantum dots; see the Scientific Highlights article on page 10.

During the running time of the ERC project AnaMultiScale, in addition to the PI and several WIAS members, 14 different researchers were employed for a total of 223 months; and the research is documented in one research monograph and about 60 papers in peer-reviewed journals.

Hellinger–Kantorovich distance. The concept of entropy transport problems is a natural generalization of the theory of optimal transport problems. While the latter is restricted to probability measures, the former applies to arbitrary non-negative and finite Borel measures of possibly unequal total mass. This theory was successfully developed in [3]. As a special case of this class of problems, the Hellinger–Kantorovich distance, which can be seen as an interpolation between the Kantorovich–Wasserstein distance and the Hellinger–Kakutani distance, and its geometry were characterized. In particular, new geometric properties for the Hellinger–Kantorovich space were obtained, including a two-parameter rescaling and reparametrization of the geodesics, local angle condition, and some partial K-semiconcavity of the squared distance, that will be useful for proving the existence of metric gradient flows. The latter will provide new analytical results for classes of scalar reaction-diffusion equations.

Oberwolfach Workshop. Together with Mark Peletier (Eindhoven) and Dejan Slepcev (Pittsburgh), Alexander Mielke organized the Workshop "Variational Methods for Evolution" (November 12–18) in the Mathematical Research Institute in Oberwolfach (MFO). The event brought together a broad spectrum of researchers from calculus of variations, partial differential equations, metric geometry, and stochastics, as well as applied and computational scientists. It focused on variational tools, such as incremental minimization approximations, Gamma-convergence, optimal transport, gradient flows, and large-deviation principles for time-continuous Markov processes.

Fig. 2: *Photo by Petra Lein, Copyright: MFO*

Advances in parabolic regularity theory. In continuation of the joint work with A.F.M. ter Elst (Auckland) on maximal parabolic regularity for non-autonomous problems, a theory was developed where not only the integrability power in the Lebesgue space L^q deviates from 2 but also the index of differentiability differs from 1. The motivation for the analysis are models for semiconductors with avalanche generation, where the nonlinearities depend on the gradient ∇u of the densities as in

$$\partial_t u - \operatorname{div}\big(\mu_t \nabla u\big) = |\nabla u|^2, \quad u(0) = u_0.$$

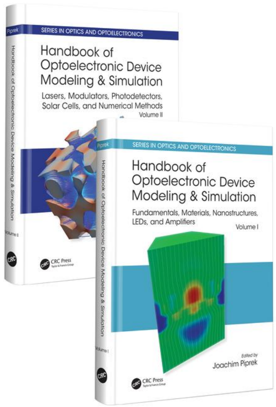
The extra challenge arises from the heterogeneities of the material, i.e., discontinuities of μ, and from mixed boundary conditions, excluding the application of classical regularity theories.

By developing a suitable elliptic regularity theory for the divergence operator with heterogeneities and exploiting Sneiberg's extrapolation theorem, it was possible to show that the nonlinearities are still locally Lipschitz functions in suitable interpolation spaces, like Bessel potential spaces $H^{\theta,q}_{\mathrm{Dir}}$. In the former broad geometric context with heterogeneities, such interpolation results only existed in the case $q = 2$.

Semiconductors

In this field, the group profits from a strong cooperation with RG 2 *Laser Dynamics* and RG 3 *Numerical Mathematics and Scientific Computing*.

Funded by the Einstein Center for Mathematics Berlin (ECMath), the MATHEON subprojects D-OT1 and D-SE2 run until May 2017, and two new subprojects D-OT7 (together with RG 6 *Stochastic Algorithms and Nonparametric Statistics*) and D-SE18 started in June 2017. Moreover, the group is involved in the DFG Collaborative Research Center CRC 787 *Semiconductor Nanophotonics: Materials, Models, Devices* via subproject B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters" (jointly with research group RG 2 and Zuse Institute Berlin). Here, the coupling of the van Roosbroeck system with a dissipative quantum master equation in Lindblad form led to a novel hybrid quantum-classical modeling approach that enables a comprehensive description of quantum-dot devices on multiple scales; see the Scientific Highlights article on page 10 and the report of RG 2.



The high competence in the field of semiconductors is expressed by the fact that group members contributed two extended chapters to the "Handbook of Optoelectronic Device Modeling & Simulation" [5]: Chapter 12 deals with nanowires, and Chapter 50 provides up-to-date numerical methods for drift-diffusion semiconductor models. Progress in the numerics for semiconductors with non-Boltzmann statistics as well as in the development of the semiconductor device simulation tool `ddfermi` is illustrated in detail in the research report of RG 3.

ECMath subproject D-SE2 "Electrothermal modeling of large-area organic light-emitting diodes" studies organic semiconductor devices in close collaboration with the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) at TU Dresden. A thermistor model for the complex electrothermal behavior of organic LEDs was established, where the balance equation for the total current flow of $p(x)$-Laplacian type is coupled to a heat flow balance where the right-hand side is only in L^1. Besides analytical investigations concerning existence and regularity of solutions, a structure-preserving hybrid finite-volume/finite-element scheme was derived that respects the maximum principle for the current flow equation and the positivity of temperature.

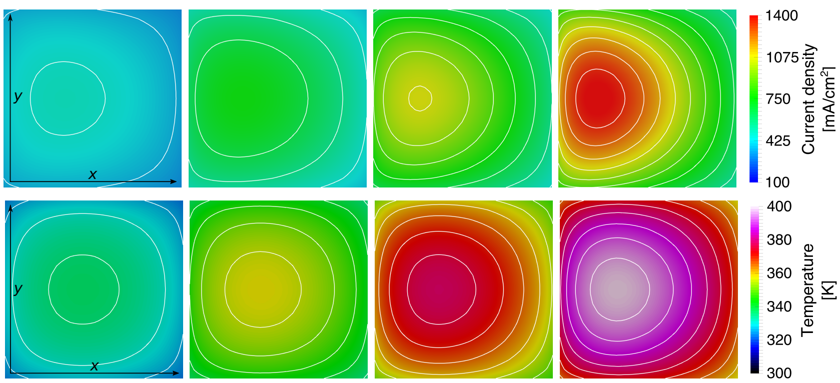


Fig. 3: *Simulated current densities and temperature distribution in an OLED for different applied voltages*

By extending the model to multiple layers with parallel nonlinear conductivity laws, which also take into account diode-like behavior in recombination zones, and additionally using a path-following technique, the developed simulation tool is able to reproduce the experimentally observed electrothermal behavior of organic LEDs; see [2]. Figure 3 shows spatial distributions, and Figure 4 displays typical S-shaped current-voltage relations.

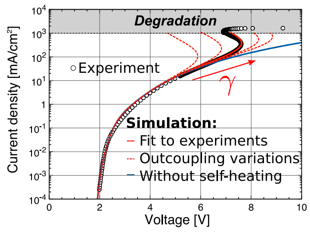


Fig. 4: *Simulated S-shaped current-voltage relations for different thermal outcoupling*

The subproject D-SE18 “Models for heat and charge-carrier flow in organic electronics” started in June 2017 and is concerned with a more detailed description of the specific features of organic semiconductor devices. Within the device simulation tool `ddfermi`, the van Roosbroeck system is generalized via Gauss–Fermi statistics and incorporates new charge-carrier mobility functions that result from a numerical solution of the master equation for hopping transport in a disordered energy landscape with a Gaussian density of state.

Material modeling

The research in this field was done in cooperation with RG 5 and the WG *Modeling, Analysis and Scaling Limits for Bulk-Interface Processes* and was driven by subprojects of the DFG Collaborative Research Centers CRC 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application* and CRC 1114 *Scaling Cascades in Complex Systems*. One special highlight was the Workshop “Homogenization Theory and Applications” (HomTAp, October 4–6), which focused on periodic and stochastic homogenization and on numerical methods for multiscale problems. Another highlight was the CRC 1114 Spring School “Methods for Particle Systems with Multiple Scales” (May 29 – June 2) at WIAS, which was organized by Alexander Mielke and Michel Renger (RG 5) and which gathered 30 young researchers.

Multiscale problems. Subproject C05 “Effective models for interfaces with many scales” of CRC 1114 deals with evolution equations having a gradient structure and describing problems with two or more interacting physical scales. The focus lies on the development of mathematical tools that help to capture the influence of microscopic effects on the macroscopic level of observation. A major field of application are problems from geoscience. Here, the scales range from tiny cracks on the level of 10^{-3} m to large faults on the level of 10^{3} km including virtually all sizes of faults in between. While rock is an elastic medium, so-called *stick-slip motion* along the cracks is observed, which is basically driven by shear forces and friction.

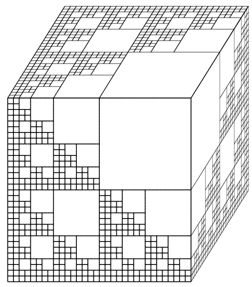


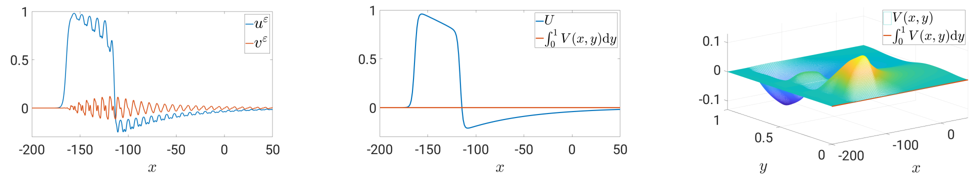
Fig. 5: *Cantor set of order 5 as model for geological network of faults and cracks*

Clearly, numerical methods cannot resolve the geometrical structures over the whole range of scales, which differ by a factor of 10^9. Due to the continuum of scales, classical methods fail for the analytical study of multiscale problems. In C05, an ansatz called *fractal homogenization* was proposed that allows one to show that the influence of small scales diminishes exponentially. Numerical experiments by Ralf Kornhuber and Joscha Podlesny (FU Berlin) show that the analytical results indeed provide good approximations. A suitable mathematical model for the geometric setting are Cantor-like sets with a fractal structure such as sketched in Figure 5.

SFB 910

Traveling waves in periodic media. Within subproject A5 “Pattern formation in systems with multiple scales” of CRC 910 and in cooperation with Pavel Gurevich (FU Berlin), traveling pulse solutions were studied in FitzHugh–Nagumo systems with rapidly oscillating coefficients [1]. Based on previous results, a two-scale limit system was identified in the vicinity of vanishing period lengths. It was then proved that existence and stability of the corresponding two-scale pulse solutions follow via an explicit representation from well-known results on FitzHugh–Nagumo systems with constant coefficients. For certain parameter regimes, it was possible to show that pulses, i.e., the excitation and relaxation of the activator u, can still propagate, although the inhibitor V changes sign and vanishes on average; see Figure 6.

Fig. 6: *Left: solution* $(u^\varepsilon, v^\varepsilon)$ *of original system. Center: two-scale pulse solution* (u, V) *of the limit system with averaged inhibitor* V. *Right:* V*-component in two-scale space.*



Jointly with subproject B5 in CRC 910 (Physikalisch-Technische Bundesanstalt), anti-symmetrically coupled Swift–Hohenberg equations were investigated. With the help of amplitude equations, it was possible to find local controls for globally competing patterns, namely left and right traveling waves, as well as Turing patterns.

Mathematical models as research data

Mathematical modeling and simulation (MMS) has now been acknowledged as an essential part of the scientific work in many disciplines, which is reflected in the fact that the Leibniz Association has established the "Leibniz Network MMS". In general, simulations in MMS are characterized by possibly huge amounts of data and software used for the relevant research. In order to ensure the reproducibility as well as the re-usability of scientific results, the long-term storage and accessibility of the involved research data are required. Repositories and information services for *numerical data* such as `DataCite` exist or are emerging. Recently, also *software* is categorized as research data, and information services on mathematical software, like `swMath`, have been developed. However, data and software alone are not enough to fully characterize the research data for scientific results: They can only be correctly interpreted and used if the corresponding *mathematical models* are treated as a third pillar and are explicitly linked to both; see Figure 7.

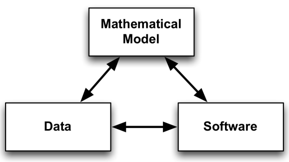


Fig. 7: *Components of research data in modeling and simulation:*
☐ *mathematical models,*
☐ *simulation software, and*
☐ *numerical data*

Finding appropriate representations for models is far less obvious than for data and software. Currently, model description occurs in scientific publications via a mixture of formulae and text, which is rigorous but informal, creates ambiguity and potential incompleteness, is less reproducible, and often leads to duplication of existing work. The aim is to find a representation that is suited for creating a "model repository" in analogy to those for data and software. In collaboration with RG 6, FAU Erlangen-Nürnberg (Michael Kohlhase) and FIZ Karlsruhe (Wolfram Sperber), a new machine-actionable, but human-understandable representation of mathematical models based on *Model Pathway Diagrams* (MPD) was developed; see [6]. MPDs specify the physical quantities and the relations between them and can be represented in a special machine-readable description language for mathematical documents. This enables the unique identification of mathematical models, the automatic derivation of relationships between them, and the modular creation of new models from existing ones, as well as the development of semantic services for them.

Further highlights of 2017

Foundation of the Weierstrass Group (WG). As one form of the new flexible research platforms at WIAS, the WG *Modeling, Analysis and Scaling Limits for Bulk-Interface Processes* was established on April 1, 2017. It is headed by Marita Thomas, a former member of RG 1.

Habilitation. Karoline Disser was awarded her habilitation for the thesis "Optimal elliptic and maximal parabolic regularity in non-smooth settings and applications to bulk-interface processes", on October 18, 2017, at Humboldt-Universität zu Berlin.

Gesellschaft für Angewandte Mathematik und Mechanik (GAMM). Marita Thomas and Maria Neuss-Radu (Erlangen) jointly organized the Section "Applied Analysis" at the Annual GAMM conference in Weimar, March 19–23, 2017. Moreover, Markus Mittnenzweig was elected GAMM Junior for a period of three years.

Research internship. The Iranian bachelor student Shima Aflatounian from Toosi University of Technology was supervised by Oliver Marquardt in the DAAD exchange program IAESTE (International Association for the Exchange of Students for Technical Experience). She carried out model studies for semiconductor nanostructures.

Representative for disabled employees. Hans-Christoph Kaiser was elected deputy spokesman of the representative body for disabled employees of the Leibniz Association.

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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 2017 within the Research Center MATHEON (subproject D-OT2 "Turbulence and extreme events in nonlinear optics"), the DFG Collaborative Research Center 787 *Semiconductor Nanophotonics: Materials, Models, Devices* (subprojects B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters", jointly with RG 1 *Partial Differential Equations* and Zuse Institute Berlin, and B5 "Effective models, simulation and analysis of the dynamics in quantum-dot devices"), as well as the DFG Collaborative Research Center 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application* (subproject A3 "Activity patterns in delay-coupled systems", jointly with Serhiy Yanchuk, TU Berlin). Furthermore, RG 2 established a close collaboration with industry in the framework of the BMBF funding measure "Efficient high-performance laser beam sources" (EffiLAS), as a subcontractor of Ferdinand Braun Institute for High Frequency Technology (FBH) in the projects HoTLas (on high-performance efficient and brilliant broad-area diode lasers for high ambient temperatures) and PLUS (on pulse lasers and scanners for LiDAR applications – automotive, consumer, robotic), as a partner in the EU framework EUROSTARS project E!10524 "High Power Composites of Edge Emitting Semiconductor Lasers" (HIP-Lasers), as well as in direct industry collaborations with TRUMPF Laser GmbH and others.

Dynamics of semiconductor lasers

The group intensified its acitivties in the modeling, simulation, and analysis of high-power broad-area edge-emitting semiconductor lasers (BA lasers), which resulted in the further development of the software kit BALaser. In particular, the modeling and efficient implementation of models for inhomogeneous current spreading in BA lasers was performed in close collaboration with FBH, RG 1 *Partial Differential Equations*, and RG 3 *Numerical Mathematics and Scientific Computing*, within project HoTLas; see Figure 1 on the next page. Furthermore, heating-induced inhomogeneous refractive index effects in BA lasers were studied in close collaboration with FBH and TRUMPF Laser GmbH. Within the project PLUS, nonlinear effects in pulsed high-power BA distributed Bragg reflector (DBR) lasers, as two-photon absorption and gain compression, were implemented, simulated, and analyzed. Within the EUROSTARS HIP-Lasers project, the modeling, implementation, simulation, and analysis of high-power laser systems consisting of BA lasers with photonical crystal external cavities were performed in collaboration with Monocrom (Vilanova, Spain), Femtika (Vilnius, Lithuania), UPC (Barcelona, Spain), Raab-Photonik GmbH (Potsdam) and RG 4 *Nonlinear Optimization and Inverse Problems*. On the basis of further developments of the software package LDSL-tool, simulation and analysis of multisection semiconductor lasers and coupled laser systems, including different configurations of DBR lasers and ring lasers with several branches of filtered optical feedback, were performed (collaboration with TU Moldova, FBH, and VU Brussels). A highlight was the appearance of the book chapter [1].

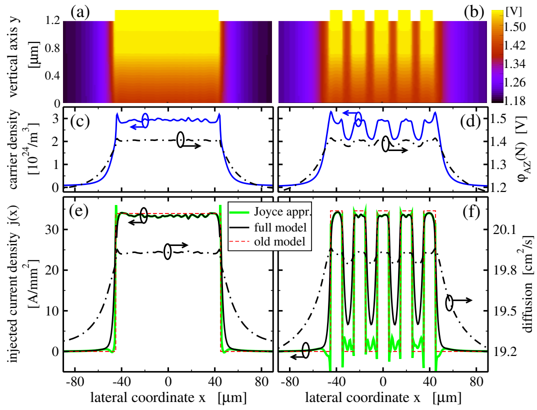

Fig. 1: *Current spreading in two different BA lasers (left, right). Top: Fermi potential along the p-doped regions. Middle panels: Carrier density and Fermi potential in the active zone ($y = 0$). Lower panels: Inhomogeneous carrier diffusion and current density according to different modeling approaches. From* RADZIUNAS ET AL., *Efficient coupling of the inhomogeneous current spreading model to the dynamic electro-optical solver for broad-area edge-emitting semiconductor devices, Opt. Quantum Electron., 49 (2017), pp. 332/1–332/8.*

A distributed delay differential equations model that incorporates the effect of dispersion in multimode lasers was proposed and applied to study long-cavity lasers that operate in the Fourier domain mode-locked regime [2]. It was demonstrated that while in the normal dispersion regime both the experiment and the theory show a stable operation, a modulation instability can lead to the degradation of the output characteristics of the laser in the anomalous dispersion regime.

Dynamics of arrays of nearest-neighbor coupled mode-locked lasers, each generating a periodic sequence of short pulses, were studied using a set of coupled delay differential equations. Regimes with sequences of clusters of closely packed pulses were found on that basis, which occur due to a balance of attraction and repulsion between them; see Figure 2. These regimes are different from the pulse bound states reported earlier in different laser, plasma, chemical, and biological systems. A simplified analytical description was developed based on the derivation and analysis of reduced pulse interaction equations.

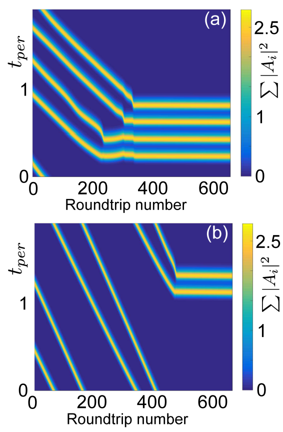

Fig. 2: *Space-time diagram of the bound pulse train regimes in a four-laser (a) and a two-laser (b) array*

Electrically driven quantum light sources based on semiconductor quantum dots are key elements for applications in quantum communication and quantum information science. The design of electrically driven quantum light sources, such as single-photon emitters and sources of entangled photon pairs, asks for novel modeling approaches that combine classical device physics with models from cavity quantum electrodynamics. Within the framework of the CRC 787 *Semiconductor Nanophotonics*, a hybrid-quantum classical modeling approach was developed that self-consistently couples the van Roosbroeck system for macroscopic charge transport with a Markovian quantum master equation in Lindblad form that describes the dynamics of a quantum mechanical many-body problem [3]. The approach allows to compute the decisive quantum-optical figures of merit, such as, e.g., the second-order intensity correlation function, along with the spatially resolved charge transport in a unified framework. A particular strength of the hybrid model is its consistency with fundamental axioms of (non-)equilibrium thermodynamics; see the Scientific Highlights article on page 10 for details.

Pulses in nonlinear optical media

Pulses in optical fibers are subject to degradation, due to, e.g., dispersion and attenuation. An attractive nondestructive compensation of this unwanted degradation is to support these pulses by an additional pump wave, which offers a way to all-optical pulse control. Pump parameters can be used to remove the negative effect, providing a suitable interaction between these pulses. The compensation, however, may turn out to be unstable, as shown in Figure 3 (left).

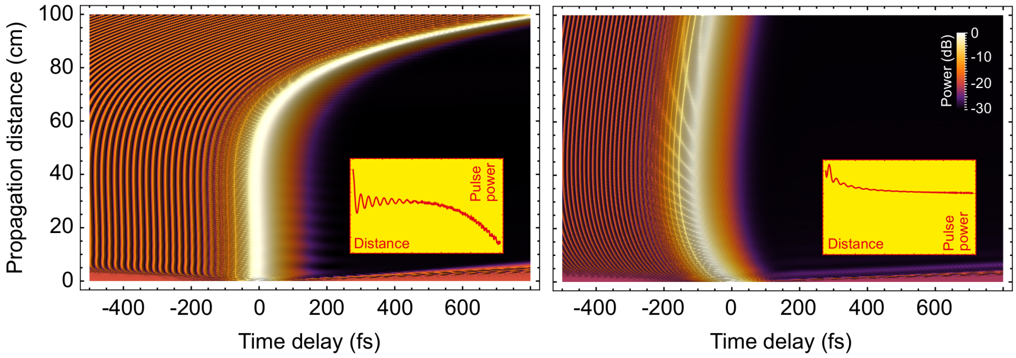

Fig. 3: *Left: An instability develops, resulting in sudden changes in the pulse amplitude and trajectory. Right: The soliton is captured by the pump wave in a stable manner.*

Reference [4] describes interactions like in Figure 3, by introducing a reduced dynamical system for the soliton parameters. An optical pulse, which propagates without changes, corresponds to an equilibrium state of the reduced system. This circumstance greatly simplifies both the stability analysis and the search for pump waves that support pulses in a stable manner, as shown in Figure 3 (right). The proposed theory shows large agreement with numerical simulations of the full model.

The efficient generation and detection of radiation in the terahertz regime of the electromagnetic spectrum remains a technological challenge to date. Significant progress in this direction could recently be achieved by exploiting the nonlinear interaction of intense, two-color laser pulses with gases. These pulses induce pronounced sub-cycle electron dynamics, with the corresponding emission of a strong THz signal. In [5], a novel mechanism for inducing sub-cycle electron dynamics and THz emission, based on the excitation of atomic resonances between the ground state and Rydberg states, was theoretically devised in collaboration with Max Born Institute Berlin, the Institute of Quantum Optics in Hanover, and Lomonosov Moscow State University.

Theory of dynamical systems

The research in the field of dynamical systems aims to provide the mathematical background for the applied research on semiconductor lasers and optical fibers and contributes to the fields of self-organized patterns and dynamics in delay-differential equations and coupled oscillator systems.

For the control of localized structures, a control scheme that was developed for coupled oscillator systems was successfully transferred to a classical problem in fluid dynamics. Together with Yohann Duguet (Paris) and Ashley Willis (Sheffield), a proportional control scheme was applied for the efficient computation of so-called *edge states* in several configurations of cylindrical pipe flow. These unstable dynamical states establish the boundary in phase space between the stable laminar flow and the coexisting fully turbulent regime. Using the control scheme, they can be efficiently and dynamically stabilized, and found directly, by a simple run of a slightly modified computational fluid dynamics (CFD) simulation, thus providing an enormous gain in computational efficiency [6].

Moreover, the dynamical regime of mode-locking, which is a long-standing topic in the research group's activities in the field of semiconductor laser dynamics, was found in the context of coupled phase oscillator systems.

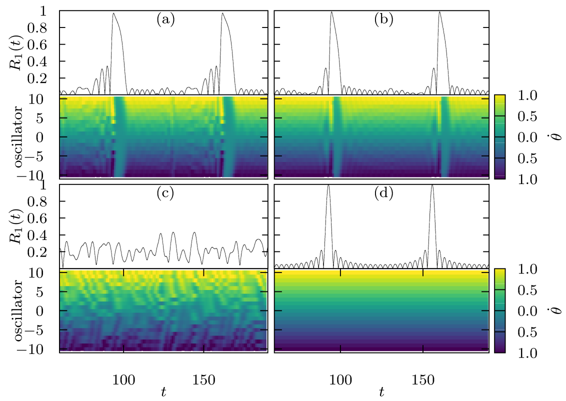

Fig. 4: *Phase velocities and self-organized pulses in the mean field of a globally coupled system of phase oscillators; (a), (b) – stable mode-locking; (c) – phase turbulence; (d) – linear mode-locking by superposition of oscillations with equidistant frequencies*

A further highlight was the *Focus Issue: Time delay dynamics* within the journal Chaos: An Interdisciplinary Journal of Nonlinear Science, where Matthias Wolfrum was a guest editor together with Serhiy Yanchuk (TU Berlin), Thomas Erneux (Université Libre de Bruxelles), and Julien Javaloyes (Universitat de les Illes Balears); see http://aip.scitation.org/doi/full/10.1063/1.5011354.

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

RG 3 studies the development of numerical methods, their numerical analysis, and it works at implementing software for the numerical solution of partial differential equations. Many of the research topics have been inspired by problems from applications. Below, a selection of topics of the group is briefly described. Further topics include discretizations of convection-diffusion equations, which are at the same time accurate, efficient, and free of unphysical oscillations, and conservation law preserving finite element methods for equations from fluid mechanics. Research software based on the developed methods is used in applications like semi-conductor device simulation (in collaboration with RG 1 *Partial Differential Equations* and RG 2 *Laser Dynamics* (`https://www.wias-berlin.de/software/ddfermi`)), the simulation of problems from hemodynamics and cancer growth, of electrolytes and electrochemical systems (in collaboration with RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*); see also the Scientific Highlights article on page 15, and the development of algorithms for reduced-order modeling.

A novel coupled simulation method for stochastic particle systems

Stochastic particle systems can be modeled by population balance systems (PBS). PBSs are encountered in chemical engineering, meteorology, oceanography, or biomedicine. The type of particles depends on the application area. In chemical engineering, particles are, e.g., crystals, in meteorology, atmospheric pollutants, or in oceanography, sediment particles that are transported by marine currents. PBSs describe the development of the particle population itself, as well as of the surrounding flow field, its temperature, and the concentration of transported dissolved species. Thus, PBSs comprise multiple interaction phenomena, and they pose several numerical challenges; see, e.g., [5].

Fig. 1: *Snapshot of the mass of crystalline aspirin in a flow tube crystallizer, due to attachment growth of dissolved aspirin from the surrounding fluid. The flow is from left to right, the upper boundary is a solid wall, and the lower boundary is the symmetry axis.*

Together with RG 5 *Interacting Random Systems*, stochastic-deterministic methods for the solution of PBSs were developed. The temperature, concentration, and flow fields are modeled with partial differential equations, using advanced finite element methods for their simulation. Highly developed stochastic methods (kinetic Monte Carlo methods) are utilized for simulating the particle population. The coupled simulation method is based on a suitable splitting strategy for PBSs and on using two specialized in-house research codes: ParMooN (finite element fluid dynamics, RG 3) and `Brush` (stochastic particle methods, RG 5). An interface between these codes was implemented, interchanging information like velocity, particle positions, or particle properties. An efficient communication between both codes was achieved.

In the first step, an application from chemical engineering was studied: a flow crystallizer for the production of aspirin. The considered problem can be modeled with an axisymmetric setup; see Figure 1. In an experimental paper, well-controlled setups are reported, exploiting surface growth and particle collision growth. These particle interaction phenomena entered the stochastic simulation. A temperature and mass balance equation and the flow field were dealt with by the continuous part of the simulation. This combination of methods enabled good reproduction of the experimental results for four different setups, in reasonable computing time, compare Figure 2. The blue histogram shows the inlet crystal size distribution, i.e., the crystal fraction that was pumped into the crystallizer. The flatter, pink histogram is the simulation result, which shows distinctly the effect of particle growth in the tube crystallizer.

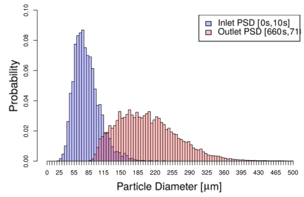

Fig. 2: *Particle size distribution of inlet and outlet crystal fraction of an aspirin flow crystallizer, computed with the new coupled simulation method*

The newly developed method is well suited for systems of particles with multiple inner coordinates. Simulations of applications with such particles are future work. In addition, the extension of the method to three dimensions and its implementation on parallel computers are planned.

Tetrahedral mesh improvement using moving mesh smoothing, lazy searching flips, and radial basis functions (RBF) for surface reconstruction

TetGen is a C++ program and library for generating tetrahedral meshes of 3D domains [4]. It is a long-term research project of WIAS. Its goals are to investigate the mathematical problems, to develop theoretically guaranteed algorithms, and to implement robust, efficient, and easy-to-use software. Recently, a new algorithm on mesh improvement was developed [2].

Given a tetrahedral mesh and objective functionals measuring the mesh quality, which take into account the shape, size, and orientation of the mesh elements, the aim is to improve the mesh quality as much as possible. In this new algorithm, the recently developed flipping and smoothing methods were combined into one mesh improvement scheme and applied in combination with a smooth boundary reconstruction via radial basis functions; see Figure 3.

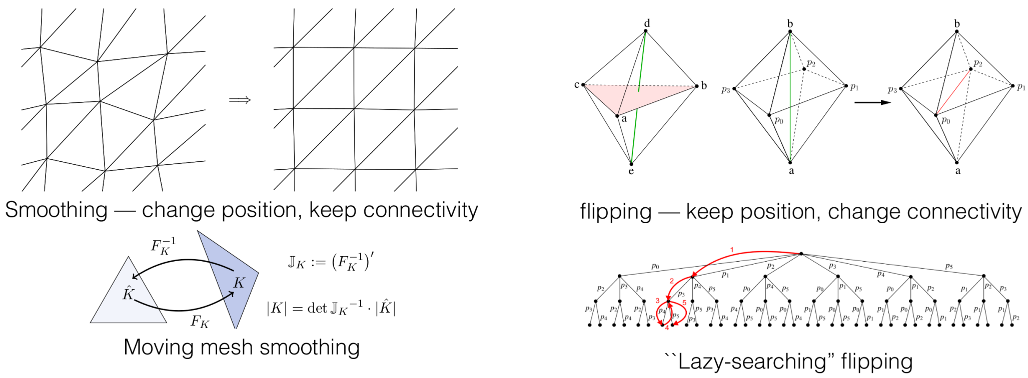

Fig. 3: *Mesh improvement operations*

Numerical studies show that the combination of these techniques into a mesh improvement framework achieves results that are comparable and even better than the previously reported ones; see examples in Figure 4.

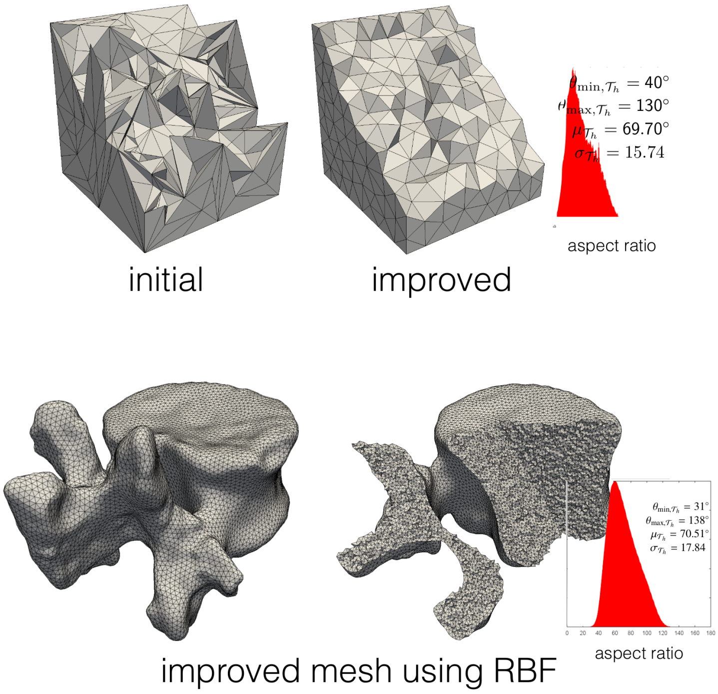

Fig. 4: *Numerical studies that show the improvement of the mesh quality with the new algorithm proposed in [2]*

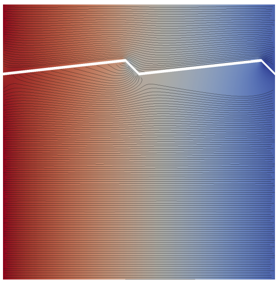

Fig. 5: *Solution to the Stokes–Darcy coupled problem for a "river bed" computed by* ParMooN

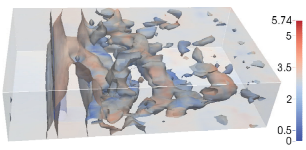

Fig. 6: *Pressure isosurfaces of a flow computed by* ParMooN

ParMooN – A software platform for problems from fluid dynamics

ParMooN is a flexible finite element package for the solution of steady-state and time-dependent convection-diffusion-reaction equations, incompressible Navier–Stokes equations, and coupled systems consisting of these types of equations, like population balance systems or systems coupling free flow and flows in porous media. ParMooN abbreviates *Parallel Mathematics and object oriented Numerics* and is developed in cooperation with the Computational Mathematics Group of Prof. Sashikumaar Ganesan at the Department of Computational and Data Sciences (Indian Institute of Science, Bangalore) and the group of Prof. Gunar Matthies (TU Dresden).

ParMooN is the successor of MooNMD, whose development started in 1996 in Magdeburg and whose reference paper has more than 100 citations. Starting in 2013, the parallelization for distributed memory systems and the re-implementation of large parts of the code base led to the new name ParMooN.

One of the main features of both is the clear separation of geometry and finite elements as one can find them in textbooks. Well over 100 finite elements are implemented in one, two, and three spatial dimensions, including conforming, non-conforming, discontinuous, higher-order, vector-valued, and isoparametric ones as well as finite elements with bubbles. A number of time stepping methods, such as θ-, diagonally implicit Runge–Kutta, and Rosenbrock–Wanner schemes, can be employed. A wide variety of spatial discretizations is available, especially many stabilizations for convection-dominated convection-diffusion-reaction equations and for finite element pairs for the Navier–Stokes equations that are not inf–sup stable. Furthermore, turbulence models can be used.

ParMooN has interfaces to external libraries to solve the resulting linear systems of equations. These include direct solvers (UMFPACK, PARDISO, MUMPS) as well as many iterative ones (through the portable, extensible toolkit for scientific computation PETSc). Additionally, ParMooN has built in a fully parallelized geometric multigrid solver/preconditioner. It outperformed external solvers in the context of incompressible Navier–Stokes equations by up to 24 processes; see [6]. And a very good speedup of the multigrid preconditioner for the heat equation was obtained up to 960 processes; see Figure 7 and [3].

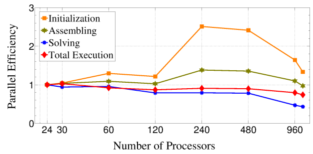

Fig. 7: *Parallel efficiency for the heat equation with 135,005,697 degrees of freedom*

The code is continually extended and revised to address both new software and architectural developments (for examples concerning the build system, compilers, and debugging tools), as well as new discretizations and stabilizations. There are, e.g., several solvers/preconditioners for incompressible flow simulations available in ParMooN that are quite different in nature. A study assessing a direct solver (UMFPACK) with the FGMRES method preconditioned with a coupled multigrid scheme or the least-squares commutator (LSC) method was conducted in [1]. None of these solvers was superior in all considered cases. In fact, the efficiency rather depends on the pair of inf-sup stable finite element spaces, the fineness of the spatial mesh, and the length of the time step. While direct solvers are feasible in two space dimensions for small to medium-size problems, in all other situations, iterative methods are the only option. It furthermore turned out that for steady-state problems a coupled multigrid preconditioner (using Vanka-type smoothers) was generally the most efficient approach; see Figure 8. The LSC preconditioner, on the other hand, was fastest whenever time-dependent problems were discretized with small time steps.

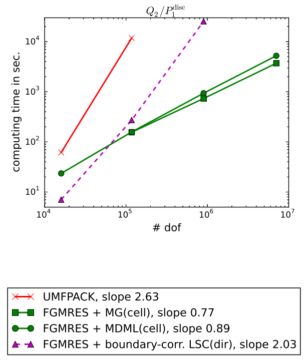

Fig. 8: *Different solvers for a steady-state flow around a cylinder in 3D: computing times and slope of best-fit line for* Q_2/P_1^{disc}

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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 nonsmooth data. Together with 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.

Fig. 1: *MIMESIS mid-term meeting, September 2017*

In 2017, the research group successfully completed its participation in the first phase of the DFG Transregio (TRR) 154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks* and now prepares itself for participating in a possible second phase.

Moreover, besides of the evaluation of WIAS by the Senate of the Leibniz Association, this year's work was marked by two further important events. Together with RG 6 and colleagues from TU Berlin, in September we organized the Workshop "Mathematics of Deep Learning", where more than 60 participants from different disciplines discussed approaches towards a mathematically rigorous understanding of deep learning architectures and their applications.

Later in September, the mid-term meeting of the Marie Skłodowska-Curie EID Project "MIMESIS" took place at WIAS. The academic and industrial supervisors from WIAS, University of Oulu, the industrial partners EFD Induction, SSAB and Outokumpu, and two representatives of the Research Executive Agency (REA) of the European Commission met in Berlin to discuss preliminary results of the project. The eight early stage researchers gave interesting presentations about their Ph.D. topics related to mathematics and steel production. With a very positive feedback from the REA representatives, the MIMESIS team continues highly motivated into the second period of its project.

In the following, selected scientific achievements of the research group in 2017 are detailed.

Stochastic and nonsmooth optimization

The group continued its intensive research on stochastic and nonsmooth optimization. The main driving force for the investigation of this topic is the work on 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*. The novel class of stochastic optimization problems subject to probust (probabilistic/robust) constraints, introduced earlier in this project, was analyzed in more detail in the context of gas networks [1]. As a particular application, the network owner's capacity maximization problem under random exit loads could be solved for arborescent networks (see Figure 2). A numerical solution algorithm for such problems was developed on the basis of gradient formulae for Gaussian probability functions related to smooth systems of random inequality constraints obtained in [2]. Another part of research in stochastic optimization was supported by the Gaspard Monge Program for Optimization and Operations Research funded by the Jacques Hadamard Mathematical Foundation and Electricité de France (EDF). Here, the investigation of structural properties of probabilistic constraints for dynamic models and different types of multivariate distributions was in the focus of considerations. The potential application behind that would be hydro power management. An implementation based on the sequential quadratic programming code SNOPT and the specialized code MVNDST for evaluating Gaussian probabilities of rectangles was realized and tested on several examples from EDF with a focus on robustness and precise estimates of confidence intervals for the optimal value. The research in nonsmooth optimization and variational analysis is partially of independent interest but also strongly related to stochastic optimization. First, it plays a significant role in analyzing (Lipschitz) continuity of probability functions and deriving subdifferential formulae. Second, it is an essential tool for deriving necessary optimality conditions (M-stationarity) for mathematical programs with equilibrium constraints (MPECs) already in a deterministic setting. This issue will play a central role in a possible second phase of the above-mentioned TRR project, where the general emphasis will be laid on stochastic and deterministic models for gas markets. Such models typically lead to MPECs. In a preparatory step, the role of the so-called *calmness* of perturbed generalized equations as a constraint qualification for stationarity conditions in MPECs was analyzed in detail.

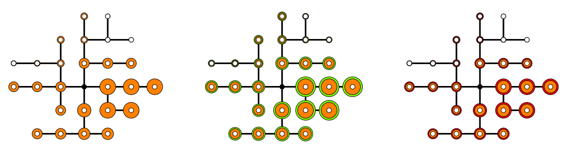

Fig. 2: *Solution of the capacity maximization problem for a gas network under random exit loads (left). Feasible (middle) and unfeasible (right) exit load scenario*

Inverse problems for stochastic data and reconstruction of stochastic surfaces

Application-related problems based on PDE models usually include a large number of parameters, e.g., determining stochastic coefficients and data, and/or inverse problem settings. The quality of their solution is restricted by limited storage capacity and computing time. To enable an efficient and accurate treatment, sparse representations of the functions and operators have to be exploited, especially by using adaptive discretizations and model order reduction approaches. Moreover, new algorithms have to be designed. In our research group, adaptive low-rank tensor methods were developed and applied to random PDEs, to parametric forward models, Bayesian inversion, and to topology optimization with uncertain data.

A new adaptive stochastic Galerkin finite element method (FEM) based on low-rank tensor methods was derived in [3]. As an extension, a novel approach to treat generic coefficient approximations in the tensor-train format was investigated. This theoretically derived and practically implemented method generalizes the framework of affine-uniform and log-normal coefficients in random PDEs and allows for a complete adaptive treatment of all discretization parameters in the solution process. It is the first numerical method for log-normal coefficients with reliable a posteriori error estimators.

The (statistical) determination of model parameters based on a finite set of measurements is a central task in UQ (uncertainty quantification) and of great practical relevance. Based on the adaptive stochastic Galerkin FEM, an explicit Bayesian inversion was developed, which extends the a posteriori adaptivity to the inversion process, leading to a functional representation of the posterior density [4].

In a collaborative project with industrial partners and the Leibniz-Institut für innovative Mikroelektronik (IHP Frankfurt/Oder) supported by the Central Innovation Programme (ZIM) of the Federal Ministry of Economics and Technology, the scatterometric measurement of surface geometries during plasma etching was investigated. For the control of such processes, a fast measurement technique is mandatory. Illuminating the surface of the workpieces by a light ray from above, measurement devices provide new spectral curves in time steps of a period between a half and two seconds. In the same time period, an inverse algorithm has to recover the geometry, e.g., the relevant parameters of a periodic structure, from the measured reflectance spectrum. This problem is severely ill posed, i.e., the size of the parameters to be reconstructed is beyond the diffraction limit. However, a suitable parametrization of the geometry leads to a regularized problem for which a gradient-based local minimization algorithm was developed, where the optimization functional is the deviation of the measured spectrum from the sparse-grid interpolation of the spectra simulated for different parameter values; see Figure 3.

To simulate acoustic waves scattered by a bounded elastic body, an algorithm coupling FEM and boundary elements was analyzed; see [6]. Different discretization schemes for the Dirichlet-to-Neumann map were derived and implemented. All this can be employed for the inverse algorithm developed at WIAS.

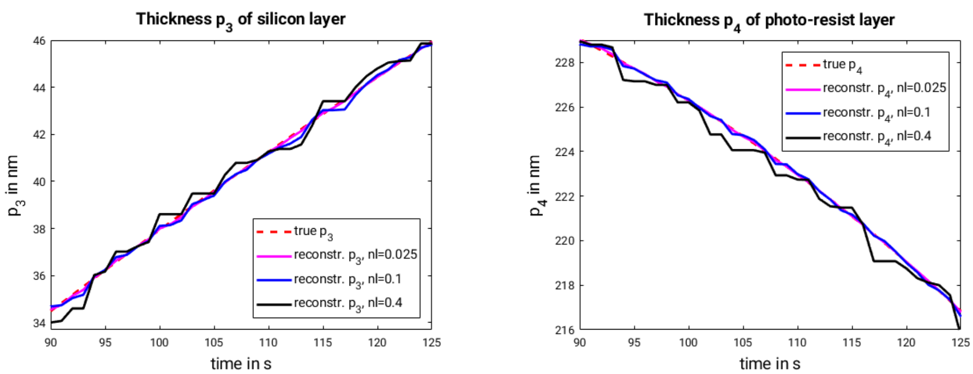

Fig. 3: *Reconstruction of periodic line-space structure for different noise levels nl: reconstructed height p_3 of the silicon layer (left), reconstructed height p_4 of the photo-resist layer (right)*

Optimal control of multifield and multiscale problems

Last year's work in this area was dominated by the European Industrial Doctorates (EID) project "MIMESIS", which is coordinated by our group. Three of the eight MIMESIS PhD students are supervised by the research group, another one by RG 3 *Numerical Mathematics and Scientific Computing*. The research topics cover modeling, simulation, and optimization of high-frequency induction welding, single- and multi-frequency induction hardening of helical and bevel gears, and inductive pre- and post-heating for the thermal cutting of steel plates. In all projects, the models consist of coupled, nonlinear systems of partial differential equations. Depending on the application, the equations involve the heat equation, Maxwell's equations to compute the magnetic field as source of the inductive heating, the equations of elasticity to account for structural deformations as consequence of thermal expansion and phase transition phenomena in steel, and a system of ordinary differential equations to describe the evolution of different phases in steel.

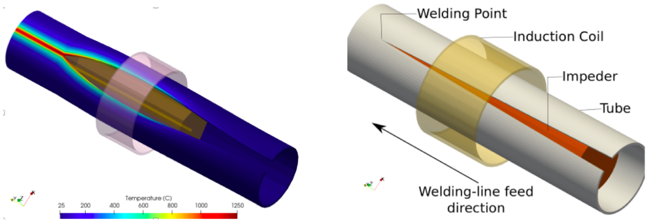

Fig. 4: *Temperature profile in tube (left), weld setup for electromagnetic heating (right)*

For a numerically efficient treatment of these electro-thermal problems in a time-domain setting, different time scales for Maxwell's equations and the energy balance have to be considered. To justify the chosen numerical approach, a model problem with two parabolic equations on different time scales was investigated. The modeling of phase transitions was considered in cooperation with the materials science Ph.D. topics in MIMESIS. And for the evolution of grain sizes, a new Fokker–Planck-type approach was developed [5].

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4.5 Research Group 5 "Interacting Random Systems"

In 2017, RG 5 continued its research on various topics in Probability and Statistical Mechanics, like (static and dynamic) interacting particle systems, random walk models in random media, concentration properties of spectra of random operators, on Gibbs measures and percolation. While all these mathematical topics have an origin in concrete applied questions, the most immediate connection with applications is present in the work of *Leibniz Group* LG 4 *Probabilistic Methods for Mobile Ad-hoc Networks*, which is embedded in RG 5. Within this work, a promising and flourishing collaboration with one of Europe's largest telecommunication companies was established. In this partnership, theoretical questions are investigated by the group, and their most interpretable and most applied results are delivered to the company.

The main subject of LG 4 is the probabilistic treatment of large spatial ad-hoc communication networks, a subject that has many facets and is under investigation in RG 5 in various additional programmes, like a Ph.D. project within the *Berlin Mathematical School* (BMS; project started in Summer 2016), a new Ph.D. project within the MATHEON (started in Summer 2017), and several master's theses. The combination of various tools from probability and analysis is characteristic for the research of RG 5 also in this field; the usage of models from Stochastic Geometry (interacting point processes, e.g.) is vital here. This part of the work of RG 5 will be detailed in the Scientific Highlights article on page 27.

Another strong concentration of the group is on the combination of tools from the theories of static and dynamic interacting particle systems, i.e., tools from large deviation theory for point processes and for clouds of many paths, parameter-dependent rate functions, many-body systems, Gibbs measures, etc. At several places, it turned out that some of these models can be employed both in telecommunication models and in the description of chemical processes. The investigation of the impact and reach of these cross-connections is in full swing within RG 5.

Two important schools were (co-)organized by RG 5 in 2017: Within the DFG Collaborative Research Center (CRC) 1114 *Scaling Cascades in Complex Systems*, jointly with RG 1 *Partial Differential Equations*, the group organized a Spring School on "Methods for Particle Systems with Multiple Scales", presenting three minicourses by worldwide experts, additional talks by members of the CRC and supplementary exercises. One of the two annual BMS Summer Schools was organized by the head of RG 5, Wolfgang König, at the Technische Universität Berlin on "Probabilistic and Statistical Methods for Networks", jointly with the Centre for Doctoral Training *SAMBa* of Bath University. There were two WIAS researchers among the eight minicourse speakers, one of which was from RG 5. The program comprised exercises and talks by the organizers and by the participants.

A particular highlight in the efforts of RG 5 to increase the popularity of mathematics in particular and of science in general was the involvement of the youngest member of RG 5, Franziska Flegel, in the organization of the conference "I, Scientist" at Freie Universität Berlin in Spring. The focus of this big conference was on gender, career planning, and networking in all the sciences; it featured a number of highly visible researchers and was a big success. Further activities of members of RG 5 consisted in public talks on occasions like the annual Day of Mathematics for Berlin pupils or the Girls'Day or talks in Urania Berlin.

In teaching, the head of RG 5, supported by some group members and some Ph.D. students, supervised again a very large quantity of bachelor's and master's theses at Technische Universität Berlin on various subjects in the scientific spectrum of his research group.

Please find below a closer description of some of the group's achievements in 2017.

Random walk on random walks

Random walk in dynamic random environment (RWDRE) is a model for the movement of a tracer particle in a disordered medium that evolves in a time scale comparable to the displacement of the tracer; an example is a pollutant moving in a turbulent fluid. To define the model, fix $d \in \mathbb{N}$ and let $\omega = (\omega_{x,t})_{x\in\mathbb{Z}^d, t\in\mathbb{N}_0}$ be a random collection of time-dependent probability measures on $\mathbb{Z}^d$, called *dynamic random enviroment*. Given a realization of ω, the RWDRE is defined as the Markov chain X on $\mathbb{Z}^d$ that, when at site x at time t, jumps at time $t+1$ to the site $x+y \in \mathbb{Z}^d$ with probability $\omega_{x,t}(y)$.

An important motivation in $d = 1$ comes in comparison with the static version of the model, where $\omega_{x,t} = \omega_{x,0}$ for all x, t. In this case, it is known since the seminal works of Solomon and Kesten, Kozlov and Spitzer in the 1970's that the model may exhibit *anomalous diffusion*, i.e., scaling limits different from the usual central limit theorem (CLT). This is related to the occurrence of *traps* in the lattice, which are regions where, due to atypical configurations of ω, the random walk tends to spend abnormally large amounts of time. In the dynamic setting, traps may disappear, hence the question is raised whether or not anomalous diffusion persists. So far, this question has only partially been answered in the literature, mostly by identifying regimes where the usual CLT holds.

In the works [1], [2], ω is a functional of a Poisson system of independent simple symmetric random walks in $\mathbb{Z}^d$, i.e., of a family of moving particles. This case is both interesting and challenging because of its conservation properties and poor space-time mixing properties. The group's analysis is perturbative around parameters for which the behavior is known; in particular, the random walk is always *ballistic*, i.e., has non-zero limiting velocity. The results include ballisticity conditions, laws of large numbers, CLTs and large deviation bounds under the annealed measure, i.e., the joint law of ω and X. The regimes considered are as follows: In [1], previous work is extended in the regime of high particle density to dimensions $d \geq 2$ and more general transition kernels. In [2], the group restricts to $d = 1$ and treats the regimes of low particle density and large local drift on particles; a surprising discontinuity in the velocity is observed depending on whether the environment particles are "permeable" to the random walk, roughly meaning that the latter may freely cross the former, or not.

Interaction clusters in rarefied gases

Connections between nonlinear kinetic equations and stochastic interacting particle systems have been studied in the group for many years. Particular application areas were the Boltzmann equation for rarefied gases and the Smoluchowski equation for coagulating systems. Recent results on interaction clusters are related to both of these areas.

Interaction clusters provide the decomposition of a particle system with localized interactions into groups of particles that influenced each other up to a given time. The evolution of interaction clusters in a frictionless elastic billiard model was studied in the literature. Based on numerical experiments, a phase transition in the cluster formation process was observed. Namely, at some critical time a sharp qualitative change occurs: There appears a distinct largest cluster, which creates a gap in the mass distribution between the largest cluster and the rest of the clusters.

In [5] the group studies a general stochastic particle model with binary interactions. The model covers the spatially homogeneous stochastic Boltzmann model, where the binary interactions are collisions of particles leading to a transformation of their velocities. The interaction clusters in the general model show an effect similar to that observed in the billiard model, namely, a distinct largest cluster forms in a finite time (see Figure 1).

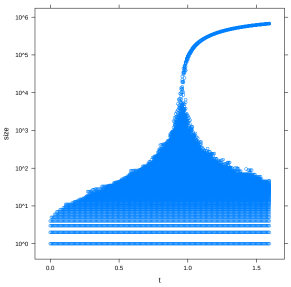

Fig. 1: *Sizes of all clusters of the system with* 10^6 *particles*

A kinetic equation for the asymptotic cluster distribution is established when the number of particles goes to infinity and the interaction rates are appropriately scaled. In terms of the kinetic equation, the phase transition corresponds to the solution becoming non-conservative. Specific results concern the following three issues:

- *Cluster distribution:* A recursive representation for the cluster distribution is found under some restrictions on the interaction kernel. Several explicit formulas for various cluster properties are obtained for particular choices of the interaction kernel, which include the Boltzmann model with a collision kernel of quadratic type.
- *Gelation time:* Upper and lower bounds for the formation time t_{gel} of the huge cluster are obtained. Using some of these estimates as well as several examples and numerical experiments, we obtain the conjecture $t_{\mathrm{gel}} \leq t_{\mathrm{mf}}$, where t_{mf} is the asymptotic mean free time (time between interactions) for one particle.
- *Numerics:* Numerical experiments are performed for the Boltzmann model. Both the explicit formulas for cluster properties and the conjecture concerning the gelation time are illustrated.

Gibbs measures under time evolution and their representations

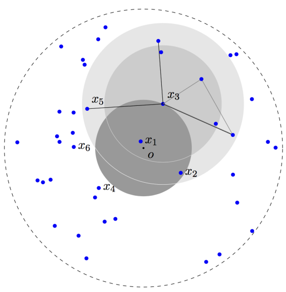

Fig. 2: *Absolutely summable hyperedge potentials for Gibbsian point processes via regrouping*

Since the work of Boltzmann and Gibbs, in the second half of the 19th century, it has been understood that microscopic phenomena in physics, which lead to macroscopic changes of the system under consideration, can effectively be modeled via a probabilistic approach. Here, the microscopic configurations of particles are drawn from Gibbs distributions, the thermodynamic equilibrium states of the system. A Gibbs distribution is a measure that balances two competing powers: the desire to minimize the mutual *energy* between particles, and *entropy* that drives the system towards some a priori measure.

To move beyond the equilibrium setting, transformations of Gibbs measures are a natural way to model, for example, a system of particles being heated up. It was observed that, in many situations, the transformed measures lose certain locality properties and thereby can not be represented as a Gibbs measure anymore. It is exactly this relation that is analyzed in [3] in the setting of Gibbsian point processes. Here, the transformed measure is locally given by a random field that is absolutely continuous with respect to the Poisson point process. It is shown that a compatible family of densities $\rho = (\rho_A)_{A \Subset \mathbb{R}^d}$ can be written as a family of Boltzmann distributions for some interaction potential V, i.e.,

$$\rho_A(\omega) \propto \exp\Big(-\sum_{\eta \Subset \omega:\, \eta \cap A \neq \emptyset} V(\eta, \omega)\Big),$$

if the densities are sufficiently local. However, V often shows poor summability properties. Therefore, also a representation of ρ is given for absolutely summable potential V' using a regrouping as depicted in Figure 2.

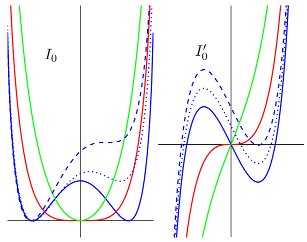

Fig. 3: *Five initial rate functions and their derivatives*

In [4], the evolution of mean-field models under stochastic dynamics is considered. The two main examples are the Curie–Weiss model under Glauber dynamics and Brownian dynamics in a potential. The Gibsianness of the mean-field model at a given time t is characterized in terms of the regularity of the rate function I_t of the large deviation principle in the thermodynamic limit at that time. Indeed, it is proved that the model at time t has the Gibbs property if and only if I_t is differentiable. Since the (generalized) gradient of I_t evolves according to a Hamiltonian flow, one can use this flow to analyze differentiability of I_t. This tool enables to decide the Gibbs property at any time for various models. For the Curie–Weiss model under Glauber dynamics, e.g., one encounters, for various choices of the parameters, interesting scenarios for the initial rate function I_0 (see Figure 3) and for the differentiability of the corresponding I_t's. Indeed, for I_0 represented as the green and the red curves, I_t is differentiable at any time t, while for all the blue curves, there is a loss of differentiability after some time. Furthermore, the time evolution of the shows a later recovery of differentiability, but the one of and do not. The conclusion about the transition of the underlying mean-field model from Gibbs to non-Gibbs and back is rather appealing.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

The Research Group 6 focuses on the research projects *Statistical data analysis* and *Stochastic modeling, optimization, and algorithms*. Applications are mainly in economics, financial engineering, medical imaging, life sciences, and mathematical physics. Special interest is in the modeling of complex systems using methods from nonparametric statistics, statistical learning, risk assessment, and valuation in financial markets using efficient stochastic algorithms and various tools from classical, stochastic, and rough path analysis.

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

Members of RG 6 participated in the DFG Collaborative Research Center (CRC) 649 *Economic Risk*, DFG Research Unit FOR 1735 *Structural Inference in Statistics: Adaptation and Efficiency*, DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*, and in the Research Center MATHEON.

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

Scientific highlights achieved by the research group in 2017 are provided below.

Statistical data analysis

The focus within the project area *Statistical data analysis* is on methods that automatically adapt to unknown structures using some weak qualitative assumptions. The research includes, e. g., methods for dimension reduction, change-point detection, regularization and estimation in inverse problems, model selection, feature identification, inference for random networks, and complex statistical objects using Wasserstein barycenters. Research within this subarea covered both theoretical and applied statistical problems.

Highlights 2017:

- Approval of CRC 1294 *Data Assimilation* at Universität Potsdam, start of project A06.
- Approval of project SE22 of Research Center MATHEON.
- Approval of project OT7 of Research Center MATHEON.
- Prolongation of IRTG 1792 *High Dimensional Non-stationary Time Series* at Humboldt-Universität zu Berlin until September 2022.
- Organization of the Workshop "Mathematics of Deep Learning" at WIAS.
- Development of the statistical package AWC for adaptive nonparametric clustering.

In 2017, the members of the group made some significant contributions to statistical literature.

In [1], a new bootstrap-based approach to the estimation of the spectral projector of a large random matrix is presented. The theoretical study is based on novel results in high-dimensional probability. The approach is very promising for the problem of dimensionality reduction.

Paper [2] offered a complete solution of the so-called *large-ball probability* problem that naturally arises in the study of the bootstrap validity and prior impact in Bayesian inference. The obtained results will be used for data assimilation problems within project A06 of CRC 1294.

Paper [3] provides a rigorous study of the problem of adaptive clustering using the adaptive weights procedure AWC. The result was presented as an invited plenary talk at the 2017 Oberwolfach Workshop “Statistical Recovery of Discrete, Geometric and Invariant Structures”, March 21–24, 2017. The statistical package AWC was developed and added to the software list of WIAS.

Wasserstein spaces of probability measures are widely used for the modeling and analysis of geometric objects, such as images and shapes. A construction procedure for non-asymptotic confidence sets for empirical barycenters in 2-Wasserstein space was proposed in [4]. This procedure is used to construct a non-parametric two-sample test for the detection of structural breaks in data with complex geometry.

Statistical numerical procedures based on the geometry of Wasserstein spaces include the optimal transport optimization problem as a building block. Paper [5] provides a numerically stable alternative to ubiquitous Sinkhorn’s algorithm for solving optimal transport problems. The proposed algorithm outperforms Sinkhorn’s algorithm in the regime of the strong requirements for the accuracy of the obtained solution.

The expertise of the research group with respect to the modeling and analysis of imaging data was further developed in several new directions. In cooperation with the Max Planck Institute for Human Cognitive and Brain Sciences in Leipzig (MPI CBS) and the University Medical Center Hamburg-Eppendorf (UKE), the group worked on new methods for emerging quantitative magnetic resonance imaging modalities. This collaboration includes adaptive algorithms for noise reduction in high-dimensional and multi-modal imaging data and the removal of the estimation bias due to the noise floor in the low signal-to-noise ratio data. RG 6 further established new exact analytic formulas for parameter estimation. The procedures were implemented in software packages. This also contributes to a new comprehensive toolbox that combines major developments from a large European consortium under the lead of MPI CBS.

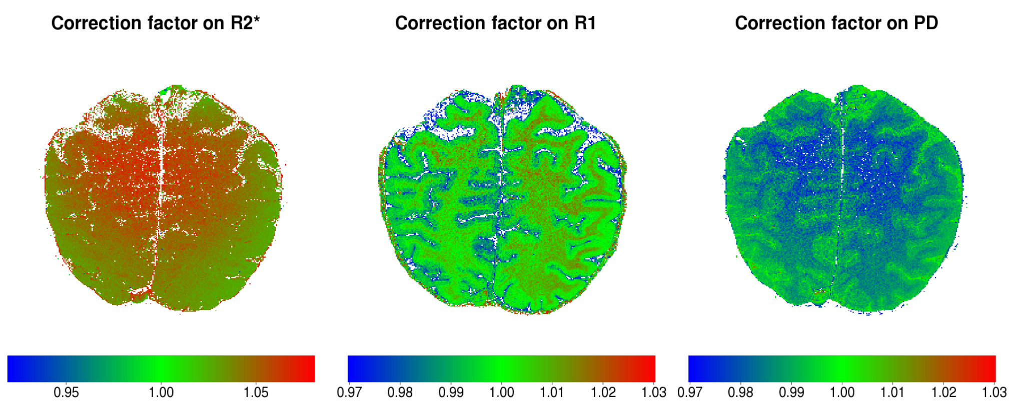

Fig. 1: *Bias correction in quantitative relaxometry parameter maps* $R_2^\star$, R_1, *and proton density* PD

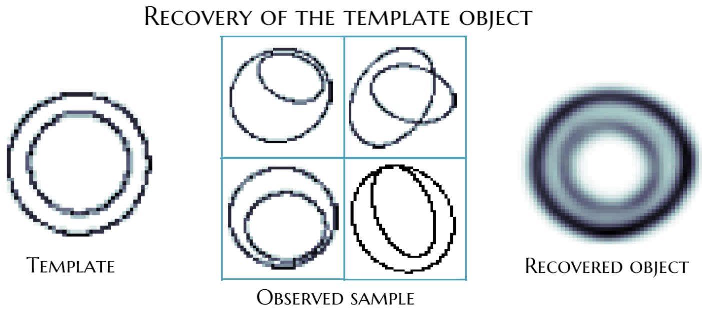

Fig. 2: *An estimator (right) of the unknown template object (left) by an observed sample (middle)*

Together with RG 1 *Partial Differential Equations*, work started on an ECMath project (OT7) on a novel reconstruction method for quantitative properties of quantum dots from images from transmission electron microscopy (TEM). In the project, methods for structuring the image space are applied (deep learning) and are being developed (shape space analysis).

Together with RG 1, see page 68, the group also contributed to the development of representation methods for mathematical models as research data in mathematics. While the project started with PDE-based models in semi-conductor simulation, RG 6 also worked on the inclusion of statistical and stochastic models into the general concept of model representation.

Stochastic modeling, optimization, and algorithms

This project area focuses on the solution of challenging mathematical problems in the field of optimization, stochastic optimal control, and stochastic and rough differential equations. These problems are particularly motivated by applications in the finance and energy industries. One central theme is the rigorous mathematical analysis of innovative methods and algorithms based on fundamental stochastic principles. These methods provide effective solutions to optimal control and decision problems for real-world high-dimensional problems appearing in the energy markets, for instance. Another focus of the project area is on financial (interest rate and equity) modeling, volatility modeling, effective calibration, and the modeling of financial derivatives, such as complex-structured interest rate, energy, and volatility derivatives.

Highlights 2017:

- Start of Focus Platform *Quantitative Analysis of Rough and Stochastic Systems*.
- Outstanding publication jointly with RG 4 *Nonlinear Optimization and Inverse Problems* and RG 3 *Numerical Mathematics and Scientific Computing* in the context of interaction between analysis and stochastics within WIAS:
  F. Anker, Ch. Bayer, M. Eigel, M. Ladkau, J. Neumann, J. Schoenmakers, *SDE based regression for linear random PDEs*, SIAM J. Sci. Comput., **39**:3 (2017), pp. A1168–A1200.

Modern mathematical finance takes into account the illiquidity of markets in a fundamental way, for instance, by fully modeling the limit order book of an asset. Mathematically, limit order books can be most directly described as high-dimensional (but discrete) queuing systems, where orders arrive, are executed, but can also be cancelled according to specific rules, thereby producing market price changes. On the other hand, a different class of models of the limit order book has been proposed that describe the limit order book as an infinite-dimensional random surface, i.e., a stochastic partial differential equation. In [6], these two modeling paradigms were linked: A queuing model was proposed, which exhibits an event-by-event description of the evolution of a limit order book. Then, a corresponding system of stochastic partial differential equations was derived as scaling limit.

In the area of regression-based methods for optimal stopping and control, a new approach that involves the incorporation of "deep learning" ideas was proposed. The main goal is to amend or replace the usually fixed regression basis in a dynamic program by basis functions "learned" from the estimation results of the preceding steps. More specifically, the new basis functions are directly related or related via an application of the underlying propagation operator to the solution estimate of the preceding step. As such this approach has a flavor of dictionary learning, and has the potential advantage of reducing the complexity of several regression-based methods for dynamic programs connected with stopping or control problems.

The research on nonlinear Markov or McKean–Vlasov processes, which are stochastic processes related to nonlinear Fokker–Planck equations whose transition functions may depend on the current distribution of the process, was continued. These processes naturally arise in a wide range of applications, including lithium battery modeling (in RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*), population dynamics, neuroscience, and financial mathematics. In a collaboration with Denis Belomestny (Universität Duisburg-Essen), the focus was on the analysis of novel regression-based estimators for solving McKean–Vlasov-related boundary value problems globally in space. These estimators are based on the realization of an interacting particle system connected with the McKean–Vlasov equation. The very challenge in this study is the fact that the particles are interacting, and hence not independent unlike the case of classical Monte Carlo regression. As a consequence, the regression analysis for independent samples developed in the last decade, based on the theory of empirical processes, needs to be completely reconsidered. The newly developed regression estimators may be naturally effectuated in the context of numerical methods for subsequent problems connected with nonlinear Markov or McKean–Vlasov processes, such as optimal stopping and variance reduction.

Focus Platform *Quantitative Analysis of Rough and Stochastic Systems*

The Focus Platform *Quantitative Analysis of Rough and Stochastic systems* was established in 2017. Its main research efforts are in understanding and computing in the context of systems driven by noise that is rougher than Brownian motion. In particular, numerical algorithms for rough and stochastic partial differential equations are developed. The focus platform also works on the theoretical and numerical analysis of rough models in finance, i.e., models based on fractional Brownian motion with very low Hurst index H.

Work has continued on simulation-based numerical methods for random and rough partial differential equations. In particular, in the context of the research unit FOR 2402, the group develops a new regression algorithm for parabolic rough partial differential equations based on Feynman–Kac-type stochastic representations.

When solving stochastic partial differential equations numerically, usually a high-order spatial discretization is needed. Model order reduction (MOR) techniques are often used to reduce the order of spatially discretized systems and hence reduce computational complexity. In [8], a new MOR approach for linear stochastic systems with Lévy noise was developed. It is based on precise estimates for the controllability and observability energy of the system, which allow to identify the unimportant states within the system. After removing the unimportant states, a low-order reduced system is obtained that well approximates the original stochastic differential equation. The most important results are an accurate a priori error bound for the approximation and the stability preservation in the reduced system. In WIAS Preprint no. 2425, a similar idea was successfully applied to spatially discretized deterministic bilinear equations, an important subclass of nonlinear equations.

The research on the rough volatility model continued successfully in 2017. In particular, asymptotic formulas for option prices and implied volatilities are provided in WIAS Preprint no. 2406, based on moderate deviations. These results are especially important in the context of rough volatility models, since the available numerical approximation schemes are typically much slower than in the diffusion case. With the aim of reproducing the extreme skews and asymmetries, observed on empirical implied volatility surfaces and under rough volatility, threshold models for local volatility were investigated in WIAS Preprints no. 2467 and no. 2468. It was shown that these models are able to reproduce extreme skews and asymmetries similarly to rough volatility models.

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

Research Group 7 conducts research on multiscale modeling, analysis, and numerical simulation of complex materials. The main expertise of the group is in the thermodynamically consistent modeling of phase transitions, the derivation of systematic asymptotic methods, in particular, singularly perturbed problems, and the analysis of hysteresis properties. The application areas of RG 7 focus on electrochemical processes, fundamental processes of micro- and nano-structuring of interfaces, the dynamics of complex liquids, and electro-magneto-mechanical components.

For these application areas the research group developed material models of electrochemistry, such as for lithium-ion batteries and nanopores, phase field models for thin-film solar cells, models for magnetostrictive materials, models of damage, as well as models for liquid polymers and active liquid crystals, and investigates the mathematical theory and numerical algorithms for the corresponding initial boundary value problems of systems of coupled partial differential equations.

Atomistically-informed phase field models for liquid-phase crystallization (LPC)

In order to describe and understand the LPC process, it is essential to investigate the microscale kinetics in a systematic and atomistically consistent way. In the Helmholtz Virtual Institute *Microstructure Control for Thin Film Solar Cells*, RG 7 collaborates as a project partner (headed by Barbara Wagner) with TU Darmstadt to develop an atomistically consistent phase field model to quantitatively capture the solid-liquid interface energy in silicon; see [1], a paper that was selected for inclusion in the "Highlights of 2017" collection of the journal *Modelling and Simulation in Materials Science and Engineering*.

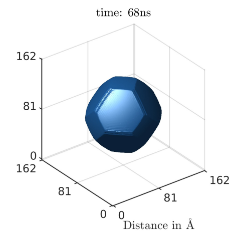

Fig. 1: *Simulation of a 3D Si grain in an undercooled melt. Intialized as a sphere, it developed the typical {100} and {111} facets.*

Numerical simulations, based on pseudo-spectral methods, show that the three-dimensional extension of the new model reproduces the critical nucleation radius, and correctly captures the facets of a silicon grain (see Figure 1) as compared to experimental results and the solid-liquid interface velocities calculated with molecular dynamics. In addition, using asymptotic analysis, a phase field model was developed such that the initially microscopic model parameters depend on the interface thickness. In the numerical algorithm, the value of the variable *interface thickness* dictates the number of necessary gridpoints and, hence, the speed of the simulation. Combining this calculation with the asymptotic analysis resulted in a highly efficient implementation that will allow to simulate grains with higher radii for comparison with experiments. A convergence analysis demonstrates the extent of the increase of the interface thickness, such that the model preserves the kinetic properties of Si. Furthermore, the convergence analysis depicts that the relative error for the comparison between the simulated and the asymptotic velocities decreases rapidly for decreasing undercoolings, which can be seen in Figure 2.

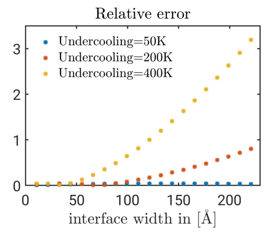

Fig. 2: *The relative error between simulation and asymptotics decreases with decreasing undercooling*

Phase field models for rate-dependent damage and fracture

Starting from models developed in the Young Scientists' Group of WIAS, a continuum model was proposed that incorporates rate-dependent damage and fracture, a material order-parameter field, and temperature within a phase field approach. The model covers partial damage as well as the formation of macro-cracks. For the material order parameter, a Cahn–Larché-type dynamics was assumed, which makes the model, in particular, applicable to binary alloys. With the help of an adaptive finite element code, numerical experiments of different complexity and including anisotropic linear elasticity were conducted to investigate the effect on the crack pattern.

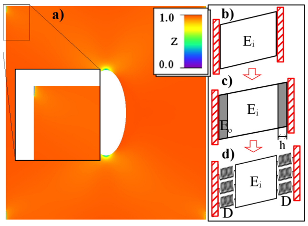

Fig. 3: *Effect of Dirichlet conditions on the displacement*

The particular form of the damage contribution to the free energy and its dissipation functional permits the following interpretation: Micro-cracks, which are not resolved by the model, appear as partial damage. They precede the nucleation and formation of macro-cracks, which are resolved in the model. Although the damage model is rate dependent, the time adaptivity of the algorithm over several orders of magnitude enables us to deal with (almost) brittle dynamics.

If there are flaws or cracks present during the process of phase separation in an alloy, these affect the formation of domains. It is demonstrated that stress concentrators serve as nucleators for the spinodal instability and that soft material is favored to accumulate at these sites. During propagation, cracks are deflected by domain boundaries, [2]. The degree of deflection is determined by the inclination angle and the stiffness ratio of the domains. Samples of failed $SnPb$-solder joints show fracture, in particular, at the interface between the material phases.

Mathematical models and theory of electrochemical processes

Modeling and analysis of many-particle electrodes and a new Nernst–Planck–Poisson model for lithium-ion batteries. Funding was obtained for the ECMath project SE17 "Stochastic methods for the analysis of lithium-ion batteries", headed by Jean-Dominique Deuschel (TU Berlin), Wolfgang Dreyer (RG 3 *Numerical Mathematics and Scientific Computing*), Clemens Guhlke (RG 7), and Peter Friz (RG 6 *Stochastic Algorithms and Nonparametric Statistics*). The previously developed mathematical model for many-particle electrodes of lithium-ion batteries is further extended to include new features such as volume expansion of the particles due to the lithium intercalation process and nonlinear constitutive relations of Butler–Volmer type for the surface reactions.

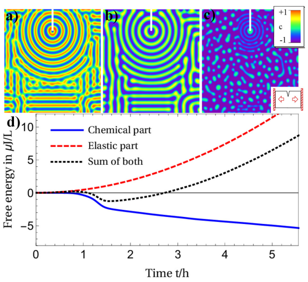

Fig. 4: *Material phase field evolution under linearly increasing mechanical stress*

Another focus concerns the rigorous analysis of models developed for the flow of liquid electrolytes. Here, a breakthrough existence result for global-in-time weak solutions [3] was achieved. Multiple challenges arising from coupling a nondiagonal reaction-diffusion system to the compressible Navier–Stokes equations for the barycentric velocity of the fluid and the Poisson equation for the electrical potential were overcome, allowing, in particular, to treat the chemical reactions without the technique of renormalization. Further results regarding the nondiagonal doubly nonlinear parabolic system with quasilinear flux functions, both for the local- and the global-in-time analysis were obtained in [4]. Funding for a new DFG proposal "Analysis of improved Nernst–Planck–Poisson models for incompressible electrolytic mixtures subject to chemical reactions" was obtained by Pierre-Etienne Druet as the Principal Investigator.

Sensing with nanopores. The focus of the new ECMath project CH11 “Sensing with nanopores”, headed by Jürgen Fuhrmann (RG 3) and Clemens Guhlke (RG 7), concerns the detection and analysis of macromolecules like DNA strands via their electrical response when passing a nanopore in a membrane separating two electrolyte reservoirs with an applied potential difference. In order to achieve a better understanding of the generated current and characteristic properties of the macromolecule, an appropriate nanopore model in the context of non-equilibrium thermodynamics is being developed that accounts for the geometrical properties of pore and analyte, the charged boundary layers, ion diffusion, and fluid flow. Novel numerical discretization schemes, like pressure-robust methods for fluid flow, and novel finite volume discretization approaches for the Poisson–Nernst–Planck system were derived in order to provide physically meaningful numerical models of the double layer structure and its impact on the fluid flow. Asymptotic analysis is used to derive reduced models that include the relevant features of the complete thermodynamic model and to drastically reduce the computation time of the numerical simulation.

Successful proposal within the BMBF Call *Mathematics for Innovation as a Contribution to the “Energiewende”.*

Within the BMBF call, RG 7 submitted a joint proposal with Prof. Mario Ohlberger (WWU Münster), Prof. Volker Schmidt (Universität Ulm), Prof. Sven Simon and Prof. Kai Birke (both Universität Stuttgart), as well as four partners from industry. The proposal “MALLi ^{2} – Modellbasierte Abschätzung der Lebensdauer von gealterten Li-Batterien für die 2nd-Life Anwendung als stationärer Stromspeicher” (Model-based assessment of the life span of aged Li batteries for second-life use for stationary energy storage) was positively evaluated by the end of 2017 with Manuel Landstorfer and Barbara Wagner of RG 7 as project coordinators.

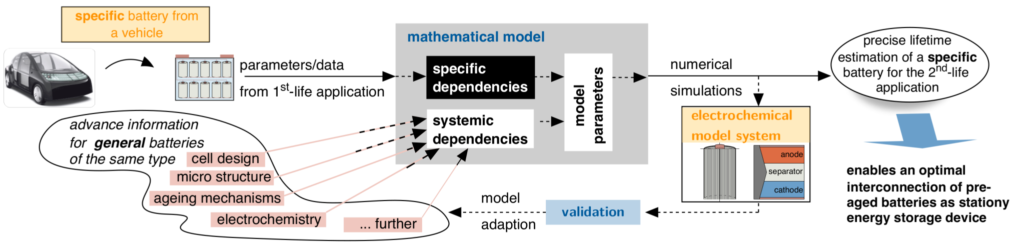

Fig. 5: *Model-based assessment of the life span of aged Li batteries for second-life use for stationary energy storage*

The project aims to improve the lifetime estimation of lithium-ion batteries from electric vehicles for their continued use as stationary energy storage devices. Lithium-ion batteries are used in electric cars up to a capacity of 80% of their initial value, which is reached after about 10 years. Beyond, the capacity/weight ratio is not sufficient anymore for mobile applications, but the batteries can be *recycled* to become stationary devices for at least another 10 years. This so-called *second-life* application provides a substantial electricity storage capacity by the year 2020, which is urgently needed for the German *Energiewende* (exit from nuclear and fossil-fuel energy), and which recently drew a lot of attention in politics and industry.

In order to ensure safety and capacity obligations for the second-life application, detailed knowledge of the battery behavior at a 20-year scale is required. Since this is a very time-consuming task in a laboratory, mathematical modeling and simulation can help to identify the central ageing mechanisms and quantify their impact on the battery capacity degradation. Homogenization and multi-scale techniques will be used within the project MALLi [2] to embed various ageing phenomena in the electrochemical model framework, which was developed at WIAS in the last years.

Free boundary problems of active gels

A new free boundary problem for an active liquid crystal based on the Beris–Edwards theory is formulated that uses a tensorial order parameter to allow for a description of the rich defect structure observed in applications, such as the adenosine triphosphate (ATP)-driven motion of a thin film of an actin filament network. In addition, the small aspect ratio of the film geometry allows for a reduction of the free boundary problem under the assumption of weak elasticity of the network and strong activity terms. For these simplified models it is found for various boundary and anchoring conditions that the active terms can completely change the dynamics and flow structure of the active film [6].

Hysteresis, electromagnetic-mechanical components, and uncertainty quantification

The application of the methods of uncertainty quantification to models involving hysteresis operators were presented in a series of talks by Olaf Klein at the Summer School on Multi-Rate Processes, Slow-Fast Systems and Hysteresis MURPHYS-HSFS-2017, June 19–20, 2017, in Turin, Italy.

Moreover, using experimental data for Terfenol-D provided by Daniele Davino (Benevento), appropriate values for the parameters for a generalized Prandtl–Ishlinskiĭ operator as in Sec. 5.1 of Davino–Krejčí–Visone (2013) and the information on the uncertainty of these parameters were determined by applying Bayes' theorem.

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4.8 Research Group 8 "Nonsmooth Variational Problems and Operator Equations"

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

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

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

RG 8 commenced its research activities in 2016 and continued to expand in 2017. Within WIAS, it broadened its agenda and scope, and added personnel over the year. In particular, Kostas Papafitsoros and Carlos N. Rautenberg became members of the group in the period of report. Several new members started via funding from the Einstein Center for Mathematics Berlin and the DFG Priority Program SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization*, in some cases also in joint activities with Humboldt-Universität zu Berlin. Specifically, this concerns Guozhi Dong, Steven-Marian Stengl, Andrea Ceretani, and Rafael Arndt.

General relevance of the scientific topics considered by the RG

Many challenging problems in applied sciences involve non-differentiable structures together with partial differential operators. In general, the nonsmoothness arises via problem formulation, is determined by competition/hierarchy, or appears by constraints, complementarity, or switching systems. For example, in the manufacturing process of thermoforming, a heated plastic sheet in a pliable stage is forced towards a mold to acquire a desired shape. The associated mathematical formulation rests on a non-penetration condition determining a natural nonsmoothness and, in addition, heat transfer and the heat expansion of the mold add a new nonsmooth structure leading to a quasi-variational inequality. Additionally, when optimization problems are considered, like in the optimal control of conservation laws or, again, quasi-variational inequalities, novel differentiability concepts and results (for the control-to-state map) are required to provide further structural insight.

Nonsmooth energies have been considered in recent years in the context of medical image processing. In particular, RG 8 was involved in this line of research by optimally choosing specific nonsmooth regularization functionals in weighted total variation models leading to better image reconstructions than state-of-the-art methods.

In optimal control of technical processes or pertinent game-theoretic approaches in case of multi-objective/multi-control situations, one typically needs to account for constraints on the common state of the underlying system. Generalized Nash equilibria provide the proper concept in such a context, thus leading to a nonsmooth and typically set-valued generalized PDE system characterizing such equilibria.

The research development within RG 8 is aimed at properly capturing the nonsmooth nature of underlying mathematical models, and control problems thereof. In this vein, compromising smoothing techniques are avoided, suitable generalized differentiability concepts are established, and discretization schemes are tailored to each specific application. In light of such approaches, large problem classes like scalar nonlinear conservation laws and quasi-variational inequalities together with their control are addressed. Besides theoretical developments, also mesh-independent/adaptive solvers are analyzed, designed, and further advanced.

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

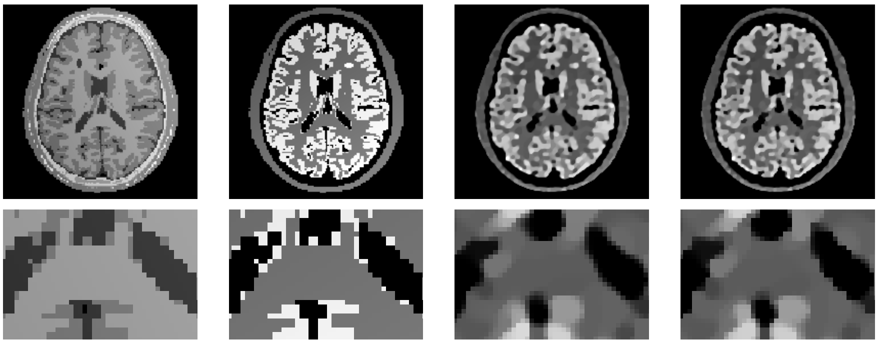
Selected research results

Nonsmooth models for energy functionals and/or state systems. Nonsmooth regularization functionals play a central role in variational approaches for inverse problems due to their excellent ability to preserve edges. During the recent years, total variation-type functionals, which exploit structural similarity of the reconstruction u to some a priori known information v, have become increasingly popular. They typically incorporate gradient information in a pointwise fashion:

$$J(u) = \int_\Omega j_v(x, \nabla u(x))\, dx.$$

These techniques are particularly relevant in multimodal medical imaging, where, for instance, information from one modality, e.g., a magnetic resonance (MR) image can be exploited in the reconstruction process of another modality, e.g., positron emission tomography (PET). In a recently completed project [1], we introduced and analyzed a function space framework for a large class of such structural total variation (TV) functionals that are typically used in the above context. This is particularly important, since in function space there is a thorough mathematical description of prominent image features, e.g., edges, which are modeled as discontinuities of functions that typically belong to the space of functions of bounded variation. We defined the structural TV functionals in function space, as appropriate L^p lower semicontinuous envelopes (relaxations) of functionals of the type J as above — note that J is well-defined only when ∇u is an integrable function. We showed that these relaxations J^{**} can have a precise integral representation only in certain restrictive cases. However, we showed through a general duality result that formulation of the Tikhonov regularization problem in function space can still be understood via its equivalence to a corresponding saddle-point formulation, where no knowledge of the precise formulation of

J^{**} is needed. Thus, our work allows the function space formulation of a wide class of multimodal medical imaging problems.



MRI prior Ground truth PET Standard TV Structural TV

Fig. 1: *Better reconstruction of the edges of a PET image using an MRI image as structural prior*

Figure 1 depicts such an example where the structural TV functional is appropriately tuned to promote edge alignment of a PET reconstruction to an already reconstructed MRI image. As a result, the edges in the PET reconstruction are more enhanced.

Additionally, in [3] an extension to TV-type models was addressed, a solution algorithm developed, and numerical tests were provided.

ECMath Einstein Center for Mathematics Berlin

The ECMath CH12 project "Advanced magnetic resonance imaging: Fingerprinting and geometric quantification", which was initiated in June 2017, is also focused on the precise mathematization and incorporation of analytical techniques that target to improve modern medical imaging modalities. In particular, in a recent work associated with the project, we applied uncertainty quantification techniques in image segmentation. Here, we developed a better understanding on the behavior of edges with respect to certain error types and we gave a mathematical meaning to the informal term of random edges, based on the Ambrosio–Tortorelli approximation of the Mumford–Shah segmentation model. We developed methods that can detect areas where it is likely to encounter an edge under the presence of uncertainty; see Figure 2.

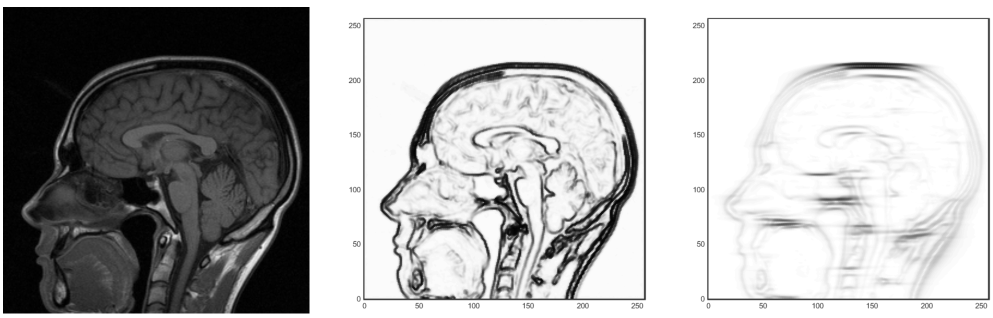
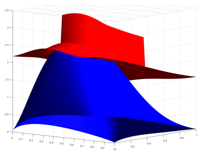


Fig. 2: *Left: original image; middle: result for the noise model; right: result for a motion blur model*

Quasi-variational inequalities and their optimal control. Project P11 "Optimal control of elliptic and parabolic quasi-variational inequalities" in the DFG Priority Program SPP 1962 considered optimization problems and differentiability issues involving quasi-variational inequalities. In the reported period, directional differentiability of the control-to-state map for a class of elliptic quasi-variational inequalities was studied, and a positive answer to this research question was obtained. The result was proven involving selection procedures for the solution set and represents the directional derivative as the limit of a monotonic sequence of directional derivatives associated with specific variational inequalities; see Figure 3 for a numerical realization.


State (blue), obstacle (red)

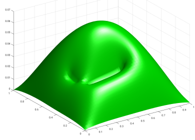

Directional derivative

Fig. 3: *Solution to the thermoforming model. Left: state/membrane/plastic sheet (blue) and compliant obstacle (red). Right: directional derivative of the state in direction* $h = 1$

Additionally, RG 8 made contributions to the study of quasi-variational problems of dissipative and non-dissipative type with gradient constraints in [7]. A semi-discretization in time was employed for the study of the problems and the derivation of a numerical solution scheme, respectively. Convergence of the discretization procedure was proven and properties of the original infinite-dimensional problem, such as existence, extra regularity and non-decrease in time, were derived. The proposed numerical solver reduces to a finite number of gradient-constrained convex optimization problems, which can be solved rather efficiently. Particular applications of the latter involve superconductivity, where the evolution of the magnetic field in a type-II superconductor can be modeled via Bean's critical state model, which admits an equivalent quasi-variational formulation. In Figure 4, we depict the behavior of the magnetic field for large times obtained with the proposed algorithm.

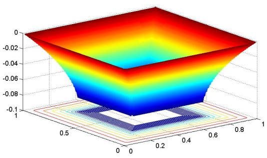
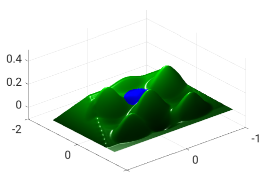
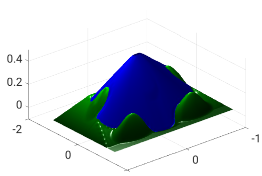


Fig. 4: *Magnetic field in a type-II superconductor*

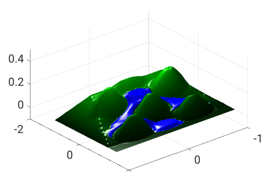
In a similar vein, in [8] the development of solvers for quasi-variational inequality models determined by fixed points of discontinuous maps was carried out. Particular applications are the evolution of the free growth surface for accumulation of granular cohensionless materials and the determination of river and lake networks over complex topographies depending on the respective angle of repose[1]. In Figure 5, we show the accumulation of material for high and low angle of repose, resembling a sandpile and accumulation of water and watercourses, respectively.



$t = 0$, Source location (blue)



$t = 0.3$, high angle of repose



$t = 0.3$, low angle of repose

Fig. 5: *Accumulation of material for high and low angles of repose at time* $= 0.3$

Optimal control and inverse problems of balance laws with applications in gas networks The current shift in energy policy from nuclear energy to renewable ones and other energy carriers such as hydrogen has triggered a surge in need for optimal use of such energy resources. It is

[1] The steepest angle at which a sloping surface formed of loose material is stable.

widely believed that gas plays a paramount role as an intermediate energy resource during this transition. In this regard, RG 8 participates in the DFG Collaborative Research Center SFB/TRR 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks*.

In the report period, discretization methods for scalar hyperbolic conservation laws in the optimal control context were investigated. In [4], stability properties of the *Total Variation Diminishing Runge–Kutta* (TVD-RK) methods, which are crucial for the convergence of the discretizations of the hyperbolic problems, were shown. Moreover, properties of the TVD-RK methods were studied in the context of optimal control; see [4, 5].

Moreover, within the SFB/TRR 154 project, for semilinear systems of balance laws, modeling gas flow in pipes, identification problems for the friction coefficient were addressed. Generally speaking, the friction coefficient describes the roughness of the interior walls of the pipes and influences the transport in a decisive way. In [6], the existence of broad solutions of the underlying PDE is proven and sensitivity results for the corresponding solution operator are obtained. In this way, the identification problem was addressed in a deterministic setting.

Important questions in the optimization of gas networks are related to the study of probabilistic constraints, involving the friction coefficient, which is uncertain in general. The associated mathematical formulations indeed depend on statistical properties of the associated uncertain quantities, such as the mean value, standard deviation, or even the entire distribution. For this purpose, a Bayesian framework for the inversion process in infinite dimensions was employed. Some numerical results in this direction are shown in Figure 6, where the identified friction coefficients with highest probability (blue lines) are plotted against the true friction coefficient (orange line). This project also led to the release of a public software package for Bayesian inverse problems of gas pipes which is available at https://github.com/fg8/UQ.

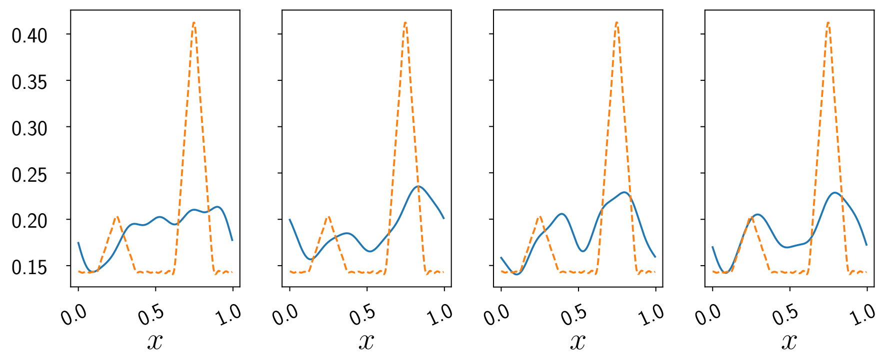


Fig. 6: *Application of the Bayesian inversion in the identification of the friction coefficient of the gas pipes*

Further highlights in 2017

The DFG Priority Program SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* coordinated by Michael Hintermüller with WIAS as the coordinating institution is successfully running, and the annual meeting was held in October 9–11 scheduling additional keynote lectures. In connection to this event, the Autumn

School on Nonsmooth Structures in Mathematical Models 2017 was organized from October 11–14.

From August 29 to December 20, Michael Hintermüller co-organized the program "Variational Methods and Effective Algorithms for Imaging and Vision" at the Isaac Newton Institute for Mathematical Sciences, University of Cambridge, UK.

The CIM-WIAS Workshop was coorganized with the International Center for Mathematics in Lisbon on "Topics in Applied Analysis and Optimisation" and took place in Lisbon from December 6–8. Additionally, Michael Hintermüller was part of the conference organizers for the 4th Conference on Optimization Methods and Software that took place from December 16–20 in Havana, Cuba.

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4.9 Weierstrass Group 1 "Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes"

This group was installed at WIAS in April 2017 as a new element of the Flexible Research Platforms. It is partly funded from WIAS budget for three years with an evaluation at the end of this period.

The research goals of the group are the development of mathematical methods for systems with bulk-interface processes for the thermodynamically consistent modeling of bulk-interface interaction with dissipative, Hamiltonian, and coupled dynamics, the theory for the existence and qualitative properties of solutions, and the derivation and justification of interfacial processes and coupling conditions.

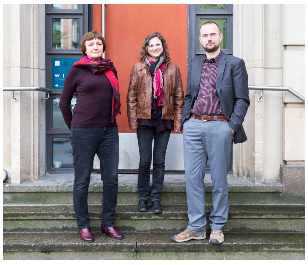

Fig. 1: *Start of the Weierstrass Group in April 2017*

The analytical results form the basis for the development of numerical algorithms supporting simulations for applications with bulk-interface interaction. The applications treated in the group belong to three main application areas of WIAS, namely *Materials Modeling*, *Nano- and Optoelectronics*, and *Flow and Transport*. In particular, the following applications are currently on the agenda of the group: (1) dissipative processes in elastic solids with bulk-interface interaction, such as, e.g., damage, fracture, plastification; (2) optoelectronic processes in mechanically strained semiconductor devices; (3) viscous flows with free boundaries and contact lines. The group also contributes to the organization of the Materials Modeling Seminar and the Semiconductor Seminar of the institute.

The following is a summary of the results from 2017 for these three topics:

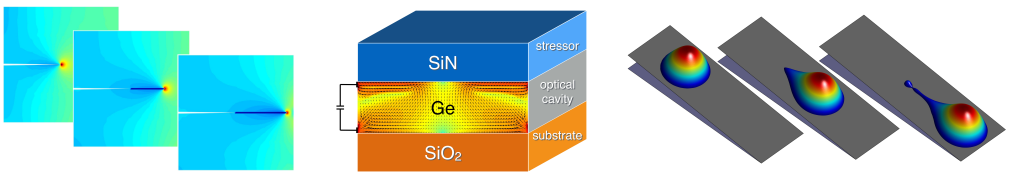

Fig. 2: *Left: mechanical stresses and progression of damage for a tension test with a notched bar. Middle: electrical current in an optimized germanium laser. Right: P1 FEM solution of free boundary problem showing droplets sliding down an inclined plane.*

Dissipative processes in elastic solids. The fourth quarter of 2017 saw the start of the second phase of the DFG Priority Programme SPP 1748 *Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretisation Methods, Mechanical and Mathematical Analysis*. Based on their previous project "Finite element approximation of functions of bounded variation and application to models of damage, fracture, and plasticity", Marita Thomas and Sören Bartels (U Freiburg) participate in the second funding phase with the joint project "Reliability of efficient approximation schemes for material discontinuities described by functions of bounded variation".

Figure 2 (left) shows the progression of fracture and the mechanical stresses in a mode-I tension test. It is based on a variable alternating-direction method-of-multipliers algorithm for a damage model with a spatial bounded variation (BV) regularization for a rate-independent damage evolution and a quasistatic evolution of the displacements. The new project will also deal with approximation techniques for dynamic fracture.

In 2017, also the proceedings volume of "PDE 2015: Theory & Applications of Partial Differential Equations" was published as the special volume of DCDS-S Discrete Contin. Dyn. Syst. Ser. S, 10:4

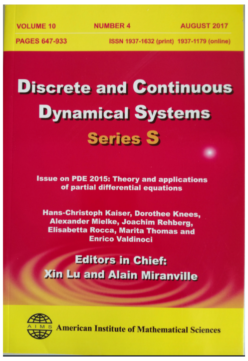

Fig. 3: *DCDS-S Special Volume 10:4 (2017)*

(2017), guest-edited by Hans-Christoph Kaiser, Joachim Rehberg, Alexander Mielke (RG 1 *Partial Differential Equations*) and Marita Thomas (WG 1) together with Dorothee Knees (U Kassel), Elisabetta Rocca (U Pavia), and Enrico Valdinoci (Politecnico di Milano). Organized by this group of researchers, the international workshop was held at WIAS, Nov. 30 – Dec. 04, 2015, and brought together analysts furthering the theory of PDEs and analysts working on applications involving nonsmooth PDEs. It was attended by more than 100 mathematicians from these fields of research from 16 different countries. The proceedings volume with its 16 contributed research papers gives good insights into recent questions and results in the theory and applications of PDEs with contributions on harmonic and geometric analysis & inequalities, evolution equations, and elliptic systems as well as on results in applications with free or moving boundaries, and dissipative solids.

Optoelectronic processes in mechanically strained semiconductor devices. In June 2017, the ECMath-funded MATHEON Subproject OT8 “Modeling, analysis, and optimization of optoelectronic semiconductor devices driven by experimental data” started as a successor of Subproject OT1 “Mathematical modeling, analysis, and optimization of strained germanium microbridges”, which bases on the collaboration with experimentalists from the Leibniz institute IHP – Innovations for High-Performance Microelectronics in Frankfurt (Oder). The goal of the project is the development of a reliable second-order doping optimization framework for the system of optoelectronics as shown in Figure 2 (middle), combined with a topology optimization as an input; the latter was designed in collaboration with RG 8 *Nonsmooth Variational Problems and Operator Equation*. Based on this, methods for the parameter indentification of material data for strained germanium are to be developed. The current state of research was presented at the NUSOD 2017 Conference in Copenhagen and will appear in the journal Optical and Quantum Electronics. Since the numerical approach is based on finite element methods (FEM), a study in the WIAS `ddfermi` initiative, jointly with RG 3 *Numerical Mathematics and Scientific Computing*, examines the convergence of the corresponding method compared to improved Scharfetter–Gummel methods for general distribution functions; see `https://www.wias-berlin.de/software/ddfermi/`.

ECMath Einstein Center for Mathematics Berlin

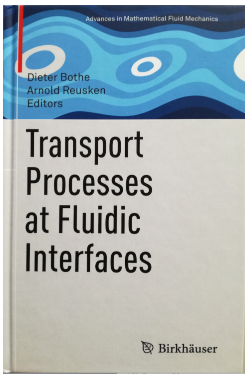

Fig. 4: D. PESCHKA, B. WAGNER, S. JACHALSKI, S. BOMMER, R. SEEMANN, *Chapter 18: Structure Formation in Thin Liquid–Liquid Films, Springer, 2017, pp. 531–574.*

Viscous flows with free boundaries and contact lines. The group works on the modeling and simulation of viscous fluid flows with a particular focus on multiphysics descriptions including mixtures and suspensions, multiphase flows, interface and contact line models, and also aims at their coupling to elasticity models for solids. A common topic in these problems is the presence of a free interface with extra contributions to energy and dissipation. Their implementation requires careful and systematic modeling and simulation approaches. Results from this research were presented in 2017, among others, in invited lectures at an ICERM workshop at the Brown University in Providence (USA), at the Universität der Bundeswehr (Munich), and at the SISSA International School for Advanced Studies (Trieste). Moreover, to advance the available tools for the FE simulation of free boundary problems, a cooperation with Prof. Luca Heltai (SISSA) was established with regard to the *deal.II FEM-library* (`www.dealii.org`). From the past joint project “Structure formation in thin liquid–liquid films” in the DFG SPP 1506 *Transport Processes at Fluidic Interfaces* with Barbara Wagner (RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*) and Ralf Seemann (U Saarland), a review article was published in the book “Advances in Mathematical Fluid Mechanics” in 2017. The simulation results in Figure 2 (right) are generated by a novel free boundary problem formulation for thin films and are based on an energetic formulation that combines FEM and *arbitrary Lagrangian–Eulerian* methods for moving meshes.

A Facts and Figures

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

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

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

A.1.1 Offers of Professorships

1. Ch. Mukherjee, Junior Professorship, April 1, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik.

A.1.2 Awards and Distinctions

1. Ch. D'Alonzo, *Leibniz-Auszubildendenpreis, 2. Platz (Leibniz Award for Apprentices, second place)*, November 29, 2017.
2. M. Hintermüller, *Chair of the Einstein Center for Mathematics Berlin*.
3. ———, *Member of* Matheon*'s Executive Board*.
4. D. Hömberg, *Member of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization*.
5. ———, *Vice Chair of Cost Action TD1409 (Mi-NET)*.
6. ———, *President of the European Consortium for Mathematics in Industry (ECMI)*, 2016/17.
7. H.-Chr. Kaiser, *Deputy Spokesperson of the Representative Bodies for Disabled Employees of the Leibniz Association*, 2017.
8. W. König, *Member of* Matheon*'s Executive Board*.
9. M. Liero, *Member of the Executive Board of the Einstein Center for Mathematics Berlin (Scientific Employee Representative)*.
10. A. Mielke, *Chair of the Prize Committee for the ICIAM Prizes 2019*.
11. ———, *Head of the Secretariat of the International Mathematical Union (IMU)*.
12. ———, *Member of* Matheon*'s Executive Board*.
13. ———, *Member of the Executive Board of the Einstein Center for Mathematics Berlin*.
14. ———, *Member of the IMU Berlin Einstein Foundation Program Committee*.
15. ———, *Treasurer of IMU*.
16. D. Peschka, *Member of* Matheon*'s Executive Board (Scientific Employee Representative)*.

A.1.3 Habilitations

1. M.H. Farshbaf Shaker, *Optimization problems governed by Allen–Cahn and Cahn–Hilliard type systems with control and state constraints*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, February 14.
2. K. Disser, *Optimal elliptic and maximal parabolic regularity in non-smooth settings and applications to bulk-interface processes*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, October 18.

A.1.4 Defenses of Ph.D. Theses

1. N.L. Naumann, *Quantum control of light and matter fields in the nonlinear regime*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Priv.-Doz. Dr. U. Bandelow, Prof. Dr. A. Knorr, November 29.
2. S. Rösel, *Approximation of nonsmooth optimization problems and elliptic variational inequalities with applications to elasto-plasticity*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, February 7.
3. L. Andreis, *McKean–Vlasov limits, propagation of chaos and long-time behavior of some mean field interacting particle systems*, Università degli Studi di Padova, Dipartimento di Matematica Pura ed Applicata, supervisor: Prof. Dr. P. Dai Pra, November 16.
4. A. Suvorikova, *Detection of structural breaks in complex data*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, June 15.

A.1.5 Supervision of Undergraduate Theses

1. R. Arndt, *A time-dependent quasi-variational inequality with a gradient constraint arising from a model of sandpile growth* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, August 23.
2. M. Bahn, *From diffusion to reactions via EDP convergence* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, October 4.
3. F.L. Bierbüsse, *Ultrakurze dunkle optische Solitonen – Herleitung der "Short Pulse Equation" für eine defokussierende Nichtlinearität und Untersuchung von solitären Lösungen* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Priv.-Doz. Dr. U. Bandelow, June 27.
4. Y. Freytag, *Optimal experimental design to estimate the time of death in a Bayesian context* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, March 2.
5. Ch. Gramstat, *Irrfahrten auf Netzwerken* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 20.
6. B. Gross, *Robust higher order decomposition via optimization on manifolds* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, January 9.
7. C. Hinsen, *Das parabolische Anderson-Modell mit korreliertem Potential* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 1.
8. T. Kalinowski, *Ein Gibbs-Ansatz für Nachrichtentrajektorien in einem hochdichten Kommunikationsnetzwerk mit mehreren Basisstationen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 6.
9. M. Labib, *Optimalität in dynamischen Zuweisungsproblemen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 4.
10. R. Marquardt, *Zeit- und energiebezogene Optimierung in Dioiden* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, January 25.

11. T. MASSEL, *Informationskapazität in großen zufälligen Kommunikationsnetzwerken* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 26.
12. S. MASSHAFI, *Voraussagen im Poisson-Cluster-Modell* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 28.
13. K. METZGER, *Optimale Steuerung eines nichtlinearen Produktionsmodells* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, March 2.
14. K. MUNDINGER, *Perkolation mit Interferenz bei beschränkter Sprungzahl* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 16.
15. L. NEUMS, *Das Kreisgesetz für das Spektrum großer zufälliger Matrizen* (bachelor's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 25.
16. K. NOWORYTA, *Modellierung und Analyse eines hochdichten zufälligen Telekommunikationssystems* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 4.
17. A. PAN, *Regularität des Coulomb-Funktionals bezüglich des Brownschen Aufenthaltsmaßes* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 17.
18. S. PETER, *Higher-order robust principal component pursuit by inexact alternating minimisation on tensor manifolds* (master's thesis), Humboldt-Unversität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, April 20.
19. F. PETERS, *Punktprozesskonvergenz der lokalen Maxima eines Gauß'schen Feldes* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 17.
20. P.M. REIF, *Lösung eines inversen Problems in einem diffusiven Phasenübergangsmodell* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, September 11.
21. J. RUTZ, *Optimierung der Zeitdifferenz bis zum Auftreten eines besseren zufälligen Wertes* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 30.
22. L. SCHMELLER, *Innere-Punkte-Verfahren mit Filter und Liniensuche* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, October 3.
23. J. SCHMIDT, *Die Gesamtmasse der Lösung des parabolischen Anderson-Modells* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 7.
24. S. SIVAGNANASUNDARAM, *Fluktuation prozesswertiger Ordnungsstatistiken* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 4.
25. A. WAPENHANS, *Das parabolische Anderson-Modell mit zeitabhängigem Katalysator* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 16.

26. ST.-M. STENGL, *Bildsegmentierung im Mumford-Shah-Modell: Analysis und Numerik mit anschließender Quantifizierung von Unsicherheiten für fehlerhafte Bilder* (master's thesis), Humboldt-Unversität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, June 12.

A.2 Grants[1]

European Union, Brussels

- **Seventh Framework Programme**

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

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

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

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

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

The EID project MIMESIS started in October 2015. Driven by the five partners EFD Induction (Norway), SSAB Europe Oy and Outokumpu Stainless OY (Finland), the University of Oulu (Finland), and WIAS, eight doctoral thesis projects are jointly carried out, providing a unique interdisciplinary and inter-sectorial training opportunity. The research is focused on three major topics: induction heating, phase transformations in steel alloys, and gas stirring in steelmaking ladles. MIMESIS has a budget of 2.1 million euros and is coordinated by the head of RG 4, Prof. D. Hömberg.

EU Framework Eurostars (in RG 2)

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

European Cooperation in Science & Technology (COST) Actions (in RG 4)

The "Mathematics for Industry Network (MI-NET)" is a COST-funded action, which aims to facilitate more effective widespread application of mathematics to all industrial sectors, by encouraging greater interaction between mathematicians and industrialists.

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

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

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

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

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

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

- **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) ran 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 were German experimental and theoretical groups in the field of electrochemistry.

ENERGIESPEICHER
Forschungsinitiative der Bundesregierung

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

- **Support Programme EXIST: EXIST Business Start-up Grants**

  "MSim – Microelectronic Simulations" is the preparation for a spin-off of WIAS (RG 3). Dr. Lennard Kamenski, Dr. Klaus Gärtner, and Dr. André Fiebach are preparing a business start-up in connection with an innovative industrial software for microelectronic simulations during the design phase of the semiconductor device development for the estimation of the design potential. Particularly, sophisticated power electronics and semiconductor detectors are in the focus of interest.

  The project is based on the research results achieved at WIAS in the field of numerical semiconductor simulations and the innovative semiconductor simulator Oskar3, which will be extended from a scientific tool to a commercial software.

- **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)

Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Bonn

TRR 154 | Mathematische Modellierung, Simulation und Optimierung am Beispiel von Gasnetzwerken

- **Collaborative Research Center/Transregio (TRR) 154**, Friedrich-Alexander-Universität Erlangen-Nürnberg
  "Mathematische Modellierung, Simulation und Optimierung am Beispiel von Gasnetzwerken" (Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks)

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

Halbleiter-Nanophotonik SFB 787

- **Collaborative Research Center (SFB) 787**, Technische Universität Berlin
  "Halbleiter-Nanophotonik: Materialien, Modelle, Bauelemente" (Semiconductor Nanophotonics: Materials, Models, Devices)

  This collaborative research center began its work on January 1, 2008. In the third funding period (2016–2019), WIAS participates in the subprojects B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters" (in RG 1 and RG 2) and B5 "Effective models, simulation and analysis of the dynamics in quantum dot devices" (in RG 2).

SFB 910

- **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 "Pattern formation in systems with multiple scales" (in RG 1) focuses on the interaction between nonlinear effects relevant in pattern formation and the microstructures including the periodic settings as well as localized structures. Starting from 2015, also the Subproject A3 "Activity patterns in delay-coupled systems" (in RG 2) has been treated by WIAS staff members, jointly with TU Berlin.

SFB 1114

- **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).

SFB 1294 Data Assimilation

- **Collaborative Research Center (SFB) 1294**, Universität Potsdam
  "Datenassimilation: Die nahtlose Verschmelzung von Daten und Modellen" (Data Assimilation – The Seamless Integration of Data and Models)

  This center started in July 2017 for four years. It is coordinated by Universität Potsdam together with HU Berlin, TU Berlin, WIAS, Geoforschungszentrum Potsdam, and Universität Magdeburg. The research is focused on the seamless integration of large data sets into sophisticated computational models. When the computational model is based on evolutionary equations and the data set is time ordered, the process of combining models and data is called data assimilation.

The Subproject A06 "Approximative Bayesian inference and model selection for stochastic differential equations (SDEs)" is carried out jointly between the TU Berlin, with the focus on variational Bayesian methods on combined state and drift estimation for SDEs, WIAS, on prior selection for semi- and non-parametric statistics applied to SDEs, and the Universität Potsdam, on sequential Monte Carlo methods for high-dimensional inference problems arising from SDEs.

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

  This interdisciplinary priority program aims at a mathematically rigorous understanding of the behavior of complex multiphase flow problems with a focus on the local processes at interfaces. WIAS participated 2017 in the subprojects "Mathematical analysis, numerical simulation of thin liquid bilayers and validation experiments" (in RG 7) and "Fully adaptive and integrated numerical methods for the simulation and control of variable density multiphase flows governed by diffuse interface models" (in RG 8).

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

  This interdisciplinary nationwide priority program aims at the development of new mathematical methods for the study and understanding of an innovative evolution biology. In the prolongation of the Subproject "Branching processes in random environment and their application to population genetics" for 2016–2018 (in RG 5), the interest was concentrated in 2017 on the description of genetics-driven biologic evolution in complex population models with additional effects and features like seed banks.

- **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 (three funding periods Oct. 2013 – Sept. 2019) with the Subproject "Numerische Lösungsverfahren für gekoppelte Populationsbilanzsysteme zur dynamischen Simulation multivariater Feststoffprozesse am Beispiel der formselektiven Kristallisation" (Numerical methods for coupled population balance systems for the dynamic simulation of multivariate particulate processes using the example of shape-selective crystallization; in RG 3). The project aims at assessing and improving numerical methods for population balance systems. The assessment of the methods is based on data from experiments that are conducted by one of the project's partners.

- **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

  WG 1 participated 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) and participates now, again jointly with Universität Freiburg, from December 2017 to November 2020 in the Subproject "Reliability of efficient approximation schemes for material discontinuities described by functions of bounded variation".

- **Priority Program SPP 1886: "Polymorphe Unschärfemodellierungen für den numerischen Entwurf von Strukturen" (Polymorphic Uncertainty Modelling for the Numerical Design of Structures)**, Technische Universität Dresden

  RG 4 participates in this priority program with the subproject "Mehrskalige Versagensanalyse unter polymorphen Unsicherheiten für den optimalen Entwurf von Rotorblättern" (Multi-scale failure analysis with polymorphic uncertainties for optimal design of rotor blades), which is a collaboration with Prof. Yuriy Petryna at the TU Berlin. Main goals of the project are a possibilistic-probabilistic modeling of an adhesion layer described by a non-periodic random microstructure, and the numerical upscaling to a macroscopic random representation.

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

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

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

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

  Complex data is often modeled using some structural assumptions. Structure adaptive methods attempt to recover this structure from the data and to use it for estimation. RG 6 is studying the convergence and efficiency of such algorithms (second funding period until March 2018) in the Subproject "Semiparametric structural analysis in regression estimation".

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

  This research unit has been funded since December 2015. One of the two spokesmen is Prof. P. Friz (RG 6). The unit works on innovative methods for applying rough path theory to the analysis of stochastic partial differential equations (SPDEs), like rough flow transformations, paracontrolled distributions, and regularity structures, to push forward the understanding of the solution theory of various types of SPDEs and the analysis of the most important physical properties of the solution processes.

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

  In the Subproject TP5 "Singular SPDEs – Approximation and statistical properties" (in RG 5), two important and prominent types of equations are studied – the Kardar–Parisi–Zhang (KPZ) equation and the (time-dependent) parabolic Anderson equation. The main goal is the investigation of their most important long-time properties like ageing for the KPZ equation and intermittency of the Anderson equation.

- **Normalverfahren (Individual Grants)**

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

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

  "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)**

"Negative Frequenzen bei der Streuung von Pumpenwellen an Solitonen" (Contribution of negative frequencies to scattering of dispersive waves at solitons; Dr. S. Amiranashvili)

Leibniz-Gemeinschaft (Leibniz Association), Berlin

- **Leibniz-Strategiefonds (Leibniz Strategic Fund)**

"Leibniz-MMS: Mathematische Modellierung und Simulation" (Leibniz MMS: Mathematical Modeling and Simulation; July 2017 – June 2019, in Director's office)

- **Leibniz-Wettbewerb (Leibniz Competition)**

"Probabilistische Methoden für Kommunikationsnetzwerke mit mobilen Relais" (Probabilistic methods for communication networks with mobile relays; July 2014 – June 2018, in LG 4)

Einstein Stiftung Berlin (Einstein Foundation Berlin)

- **Einstein-Zentrum für Mathematik Berlin (Einstein Center for Mathematics Berlin)**

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

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

Research Center MATHEON

The highlight of the collaboration with the mathematical institutions in Berlin was again the joint operation of the Research Center MATHEON "Mathematics for key technologies". Since June 2014, the funding of MATHEON is about 2 million euros per year through the Einstein Center for Mathematics (ECMath), which is funded by the Einstein Foundation Berlin. In September 2016, the reviewing for the second phase was successful, and the funding was extended until December 2018.

In 2017, WIAS again dedicated considerable financial and personal resources to the Center: Its director, Prof. M. Hintermüller (RG 8), and deputy directors, Prof. A. Mielke (RG 1) and Prof. W. König (RG 5), were members of MATHEON's Executive Board; Prof. B. Wagner (RG 7), Deputy Chairperson of its Council; Prof. D. Hömberg (RG 4), Scientist in Charge of the Application Area C "Energy and Materials", Priv.-Doz. Dr. U. Bandelow (RG 2), Scientist in Charge of the Application Area D "Electronic and Photonic Devices", Priv.-Doz. Dr. R. Henrion (RG 4), Scientist in Charge of the Application Area "Networks", Dr. D. Peschka Scientific Employee Representative of the Executive Board; and WIAS members participated in the successful running of the following subprojects:

until May 31, 2017:

OT1: "Mathematical modeling, analysis, and optimization of strained germanium microbridges" (in RG 1, RG 8, and WG 1)

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

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

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

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

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

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

since June 1, 2017:

CH11: “Sensing with nanopores” (in RG 3 and RG 7)

MI11: “Data mobility in ad-hoc networks: Vulnerability and security” (in RG 5)

OT7: “Model-based geometry reconstruction of quantum dots from TEM” (in RG 1 and RG 6)

OT8: “Modeling, analysis, and optimization of optoelectronic semiconductor devices driven by experimental data” (in WG 1)

SE17: “Stochastic methods for the analysis of lithium-ion batteries” (in RG 3, RG 6, and RG 7)

SE18: “Models for heat and charge-carrier flow in organic electronics” (in RG 1)

SE22: “Decisions in energy markets via deep learning and optimal control” (in RG 6)

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

- Programm Projektbezogener Personenaustausch (PPP) “Emergent Dynamics in Systems of Coupled Excitable Units” (Cooperation wit Institute of Physics Belgrade; in RG 2)
- A DAAD-IAESTE Fellowship holder (International Association for the Exchange of Students for Technical Experience; in RG 1; see 173)

Helmholtz-Gemeinschaft (Helmholtz Association), Berlin/Bonn

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

  In this virtual institute, which is coordinated by the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), the formation of structural defects and related strain during the growth of thin-film solar cells is investigated by combining experimental as well as simulation approaches. The aim is to understand and control the formation of structural defects and strain during the growth of polycrystalline silicon and Cu(In,Ga)Se2 (CIGSe) thin films by optimized growth parameters. RG 7 participates in the project “Phase field modeling for multi-phase systems applied to the growth of Si and Cu(In,Ga)Se2 thin films”.

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

- Two Humboldt Research Fellowship holders (in RG 8); see page 173

International projects

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

Mission-oriented research (examples)

- General Electric (Switzerland) GmbH, Baden: “Prozesssimulation bei industriellen Gasturbinen” (Process simulation for industrial gas turbines; in RG 3 and RG 6)
- Mathshop Limited, Salisbury, Wiltshire, UK: Consulting contract (in RG 5)

- Orange Labs Research, Paris, France: “Continuum percolation theory applied to device-to-device” (in LG 4). This one-year research project aims at a deeper understanding of device-to-device networks based on the idea of network “überisation” using continuum percolation theory.
- TRUMPF Laser GmbH, Schramberg: Consulting contract “Introduction to the simulation of the nonlinear dynamics of edge-emitting broad-area semiconductor lasers using the software BALaser” (in RG 2)

A.3 Membership in Editorial Boards[2]

1. J. Sprekels, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
2. ———, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
3. ———, Editorial Board, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
4. ———, Editorial Board, Applied Mathematics and Optimization, Springer-Verlag, New York, USA.
5. P. Friz, Editorial Board, Monatshefte der Mathematik, Springer-Verlag, Berlin.
6. ———, Editorial Board, Stochastic Processes and Applications, Elsevier, Oxford, UK.
7. R. Henrion, 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, Mathematical Programming, Series A, Springer-Verlag, Heidelberg.
11. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
12. M. Hintermüller, Editorial Board, Interfaces and Free Boundaries, European Mathematical Society Publishing House, Zurich, Switzerland.
13. ———, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
14. ———, Editorial Board, ESAIM: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
15. ———, Editorial Board, Optimization Methods and Software, Taylor & Francis, Oxford, UK.
16. ———, Editorial Board, SIAM Journal on Scientific Computing, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
17. ———, Editorial Board, SIAM Journal on Numerical Analysis, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
18. ———, Series Editor, International Series of Numerical Mathematics, Springer-Verlag, Basel, Switzerland.
19. ———, Series Editor, Handbook of Numerical Analysis, Elsevier, Amsterdam, Netherlands.
20. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
21. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
22. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
23. ———, Area Editor, Bernoulli Journal, International Statistical Institute/Bernoulli Society for Mathematical Statistics and Probability, The Hague, Netherlands.
24. ———, Series Editor, Pathways in Mathematics, Birkhäuser, Basel, Switzerland.

[2] Memberships in editorial boards by nonresident members have been listed in front of those by the WIAS staff members.

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

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

2nd Leibniz MMS Days
Hanover, February 22–24
Organized by: WIAS, TIB Hannover
Supported by: Leibniz Association

The second Leibniz MMS Days were again an activity of the Leibniz Network "Mathematical Modeling and Simulation" (MMS) coordinated by WIAS. The President of the Leibniz Association, Prof. Kleiner, opened the workshop, highlighting the particular importance of state-of-the-art methods in MMS for a multiplicity of Leibniz institutions.

The event brought together participants from varied fields from natural to social sciences. Fifty-five scientists from 18 Leibniz institutes took part in the workshop. The goal was to further exploit the potential of modern methods of MMS and create synergistic effects. On account of the thematic diversity, the workshop comprised both general, plenary discussions and smaller groups that focused on specific themes.

Three keynote talks were delivered: Klaus-Robert Müller (TU Berlin) talked on "Machine learning and applications", Stefan Turek (TU Dortmund) on "Extreme fluids – Some examples, challenges and simulation techniques for flow problems with complex rheology", and Peter Maaß (Universität Bremen) gave "An introduction to inverse problems with applications in machine learning".

A particular focus was also on legislation concerning research software and open access-related issues.

Nonlinear Waves and Turbulences in Optics and Hydrodynamics (NOWATOH2017)
Berlin, March 22–24
Organized by: WIAS (RG 2)
Supported by: Einstein Center for Mathematics (ECMath), WIAS

The workshop "Nonlinear Waves and Turbulences in Optics and Hydrodynamics (NOWATOH17)", organized with the support of the Einstein Center for Mathematics (ECMath), brought together renowned experts in the field of nonlinear optics and hydrodynamics. The objective of this workshop was to strengthen the interdisciplinary approach to our understanding of physical systems that exhibit heavy-tailed statistics and extreme events. In the theoretical description of these phenomena, remarkable parallels emerged between nonlinear optics and hydrodynamics in the recent years. While optical rogue waves induce damage to semiconductor laser diodes, oceanic rogue waves pose a considerable risk to seafarers.

The subjects of our workshop included the theoretical modeling of rogue events with nonlinear and integrable wave models, stochastic aspects related to rogue wave predictability, optical rogue waves in fibers and laser resonators, and dissipative solitons and localized structures. The workshop featured 21 invited and contributed talks presented by international speakers from eight countries and was attended by 28 participants.

7th Annual ERC Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis
Berlin, May 18–20
Organized by: WIAS (RG 6), TU Berlin, Oxford University
Supported by: European Research Council, WIAS

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

– Nonlinear stochastic partial differential equations

- Regularity structures
- Expected signatures
- Stochastic Loewner Evolution
- Statistics and machine learning
- Gaussian rough path analysis
- Numerical analysis for stochastic and rough differential equations

The three-day workshop attracted around 70 participants and featured 28 invited speakers, mostly early career researchers from Berlin, Oxford, and Warwick, on topics related to the afore-mentioned fields. The following, eighths, Berlin-Oxford meeting took place in Oxford in the week of December 14–16, 2017.

The workshop was jointly organized by RG *Stochastic Algorithms and Nonparametric Statistics* (P. Friz, ERC-funded, M. Maurelli), Technische Universität (TU) Berlin (T. Kastberg Nilssen), and Oxford University (T. Lyons, ERC-funded; H. Boedihardjo, H. Oberhauser).

CRC 1114 Spring School 2017: Methods for Particle Systems with Multiple Scales
Berlin, May 29 – June 2
Organized by: CRC 1114 and WIAS (RG 1 and RG 5)
Supported by: DFG through CRC 1114, with the support of BMS

The workshop aimed at acquainting young researchers of the interdisciplinary DFG Collaborative Research Center (CRC) 1114 *Scaling Cascades in Complex Systems*, who did not necessarily have a mathematical background, with mathematical methods. It centered around three minicourses on molecular dynamics and social and stochastic interacting particle systems, including exercise sessions. Furthermore, the minicourses were augmented with contributed talks from CRC members and additional Ph.D. talks. In order to spark interaction and active involvement, the number of participants was kept deliberately low. In total, there were 11 participants from within the CRC, 5 from the Berlin Mathematical School (BMS), and 6 with other affiliations. A questionnaire at the end of the workshop showed that the participants were in average very satisfied with the minicourses, talks, and the overall format.

Workshop on Mathematics of Deep Learning
Berlin, September 13 –15
Organized by: WIAS (RG 4 and RG 6), TU Berlin
Supported by: ECMath/Matheon, FOR 1735, FOR 2402, WIAS

Deep Learning has evolved into one of the hot topics in industry and science with a wide range of applications related to the processing and interpretation of large amounts of data. The workshop with more than 60 participants was jointly organized by WIAS and the Technische Universität (TU) Berlin and supported by the Einstein Center for Mathematics (ECMath) / Research Center Matheon as well as the Research Units FOR 1735 *Structural Inference in Statistics: Adaptation and Efficiency* and FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*. The event gathered experts from different disciplines to present and discuss approaches towards a mathematically rigorous understanding of deep learning architectures and their applications.

Homogenization Theory and Applications (HomTAp)
Berlin, October 4–6
Organized by: WIAS (RG 1 and RG 3) and TU Dortmund
Supported by: DFG CRC 910 and 1114, WIAS

The first HomTAp workshop was supported by the Collaborative Research Centers (CRC) 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*, and 1114 *Scaling Cascades in Complex Systems* and WIAS. The workshop focused on periodic, stochastic, and numerical methods for homogenization of multiscale problems. The aim of the workshop was to bring together researchers from analysis, numerics, and scientific computing and to give them the opportunity to exchange experience in the field of homogenization.

The program featured 9 invited talks, 23 contributed talks, and 12 posters. In total, 64 scientists participated in the workshop. There has been a very high demand among national and international scientists to participate in this workshop such that the organizers were forced to close the online registration early. Therefore, due to limited capacities of the Erhard Schmidt lecture room, several interested researchers had, unfortunately, to be rejected. For the second time, a live stream was established such that WIAS colleagues had the opportunity to follow the talks on their computers.

Fig. 1: *The participants of the Workshop on Homogenization Theory and Applications*

SPP 1962 Annual Meeting
Kremmen, October 9–11
Organized by: WIAS (RG 8), HU Berlin
Supported by: DFG SPP 1962

The Annual Meeting of the DFG Priority Programme (SPP) 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* coordinated by the WIAS Director, Prof. Dr. Michael Hintermüller, took place from October 9 to 11 in Kremmen near Berlin. A total of 69 participants attended the annual meeting of whom 64 were from outside WIAS. Each of the 23 scientific projects in the SPP was represented by a talk of 25 minutes where a presentation of results obtained or a concrete plan for future work was given. Four of the attendees — Radu Bot (Universität Wien), Martin Brokate (Technische Universität München), Jiří Outrata (Czech Academy of Sciences), and Sven Leyffer (Argonne National Laboratory) — were plenary speakers specially chosen for the annual meeting, and each plenary speaker gave a talk of 45 minutes.

In addition, a meeting for principal investigators also took place on October 10 where important matters related to the upkeep and continual improvement of SPP issues were discussed. Concurrently, also a Young Researchers' Meeting took place, which helped to identify an organizational team (outside WIAS) who will be responsible for running a Young Researchers' event for the younger SPP members in 2018.

In summary, the meeting was well attended and opinions of the venue and format were generally quite favorable.

Autumn School on Nonsmooth Structures in Mathematical Models 2017
Berlin, October 11–14
Organized by: WIAS (RG 8)
Supported by: DFG SPP 1962

A number of complex problems in the applied and physical sciences involve non-differentiable structures that lead to non-smooth systems and models. Some examples of these include models describing frictional contact problems, magnetization of superconductors, and optimal system design in biomechanics and robotics; these are all highly nonlinear and nonsmooth, and represent novel mathematical structures. Analytical, algorithmical and numerical obstacles need to be overcome to fully study these problems.

The aim of this autumn school was to present formulations of models, their rigorous analysis and resulting numerical analysis in a series of lectures held by Radu Bot (Universität Wien), Martin Brokate (Technische Universität München), and Jiří Outrata (Czech Academy of Sciences).

The autumn school took place directly after the SPP 1962 Annual Meeting in order to facilitate ease of attendance for the doctoral and postdoctoral students of the SPP, however the school was also open for other interested persons.

Twenty-six participants from outside WIAS took part in the school. A social dinner on Thursday evening was organized at a local restaurant in Berlin.

Colloquium in Mathematical Statistics
Berlin, November 22
Organized by: WIAS (RG 6)
Supported by: DFG CRC 1294, FOR 1735, IRTG 1792, WIAS

The aim of this international workshop was to discuss recent results on modern mathematical statistics on the occasion of 50 years of the Seminar of Mathematical Statistics in Berlin. The lectures focused particularly on statistical problems arising in quantum tomography, econometrics, adaptive density estimation, and others. The program featured six invited lectures of high-calibre scientists from renowned universities.

The conference was supported by the DFG Collaborative Research Center(CRC) 1294 *Data Assimilation*, the DFG Research Unit FOR 1735 *Structural Inference in Statistics: Adaptation and Efficiency*, the International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, and WIAS. It was attended by 58 participants, mainly from Germany and France as well as from Sweden, Singapore, Denmark, and the United States.

CIM-WIAS Workshop "Topics in Applied Analysis and Optimisation (Stochastic, Partial Differential Equations and Numerical Analysis)"
Lisbon, December 6–8
Organized by: CIM, University of Lisbon, CMAF-CIO, CMUC, WIAS
Supported by: Portuguese Foundation for Science and Technology FCT, WIAS

This workshop was organized with the aim of inciting scientific activities among member institutions of the European Research Centres on Mathematics (ERCOM). In Lisbon, current scientific interests of the research groups of the Weierstrass Institute and mathematics centres in Portugal were presented and discussed. This joint workshop of the Portugese Centro Internacional de Matemática (CIM) and WIAS brought together a selection of experts in Europe in order to launch and strengthen further collaborations. Topics of interest included partial differential equations with applications to material sciences, thermodynamics, and laser dynamics, scientific computing, nonlinear optimization, and stochastic analysis. The workshop was organized and supported by the Department of Mathematics of the University of Lisbon, the Centre for Mathematics of the University of Coimbra (CMUC), and WIAS. Twenty-four talks were presented to thirty-eight participants.

Dynamics of novel mode-locked and frequency-swept lasers (DNMFL2017)
Berlin, December 18–19
Organized by: WIAS (RG 2)

This international minisymposium was focused on the discussion of novel technological trends and modeling approaches in optoelectronics. The aim of the two-day minisymposium was to bring together applied mathematicians and physicists in order to provide them an opportunity to exchange knowledge and latest developments with their colleagues and young scientists by presenting their recent theoretical and experimental results in the field of nonlinear dynamics of frequency-swept and mode-locked lasers. The subjects of the workshop included the experimental and theoretical investigation of the dynamics of frequency-swept lasers used in optical coherence tomography, the transition to optical turbulence in long-cavity laser systems, the modeling of Fourier domain mode-locked lasers, the application of delay-differential equation models in laser dynamics, the reduction of laser models using dynamical systems theory, bifurcation theory and singular perturbation theory, numerical methods for the simulation of mode-locked and frequency-swept lasers, the investigation of temporal cavity solitons and light bullets in broad-area mode-locked lasers.

The program featured nine invited and contributed talks presented by speakers from four countries, and was attended by 17 registered participants.

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

BMS Summer School "Probabilistic and statistical methods for networks"
Berlin, August 21 – September 1
Organized by: BMS, EPSRC at the University of Bath, WIAS (RG 5)

The annual BMS Summer School 2017 (more precisely, one of the two in this year) was devoted to a very timely topic that plays an increasingly important role in the research of RG 5: networks in various applications having important connections with randomness in any sense. Eight speakers talked about more or less theoretical or applied aspects of networks for various kinds of applications, like neuroscience, traffic, and telecommunication, statistical inference, or information science. Two WIAS members were among the speakers (from RG 5 and RG 6) and introduced the audience to probabilistic spatial models for wireless communication and to statistic network modeling for the analysis of learning processes in brains, respectively.

The school was jointly organized by the *Engineering and Physical Sciences Research Council (EPSRC) Centre for Doctoral Training in Statistical Applied Mathematics (SAMBa)* at the University of Bath and the Berlin Mathematical School (BMS). The speakers were jointly appointed. About 60 young scientists, ten of which from Bath and the rest mainly from Germany, but also from all over the world, were selected for participation after the application process. In the ten morning sessions of the school, 20 challenging lectures were delivered, and in the afternoons, several exercise sessions were offered by young instructors. Additional research talks by scientists from Berlin and Bath, as well as contributed talks by the young participants were given as well.

A.4.3 Oberwolfach Workshops co-organized by WIAS

Workshop "Mathematics of Quantitative Finance"
Mathematisches Forschungsinstitut Oberwolfach, February 26 – March 4
Organized by: Antoine Jacquier (Imperial College, London), Josef Teichmann (ETH Zurich), Peter Friz (TU Berlin and RG 6)

The workshop focused on cutting-edge areas of mathematical finance, with an emphasis on the applicability of the new techniques and models presented by the participants.

Over 50 invited participants attended the workshop. These scientists came from a diverse set of countries, and young mathematicians were especially well-represented among them. Fundamental topics of modern mathematical finance, such as rough volatility, nonlinear partial differential equation methods, and model-free finance were investigated in detail in the 42 talks. Citing the concluding report: "[...] 20 years after settling the fundamental theorems [of mathematical finance, due to Delbaen–Schachermayer], the field is sparkling with new ideas from all directions of applied mathematics and beyond."

Workshop "Variational Methods for Evolution"
Mathematisches Forschungsinstitut Oberwolfach, November 12–18
Organized by: Alexander Mielke (RG 1), Mark Peletier (TU Eindhoven), Dejan Slepcev (Carnegie Mellon University Pittsburgh)

About 50 mathematicians from calculus of variations, partial differential equations, metric geometry, and stochastics, as well as applied and computational scientists discussed a variety of topics and exchanged ideas, thereby continuing two earlier meetings (in 2011 and 2014) at the Mathematical Research Institute in Oberwolfach.

The workshop focused on variational tools such as incremental minimization approximations, Gamma convergence, optimal transport, gradient flows, and large-deviation principles for time-continuous Markov processes. Relevant applications that arise in mechanics of fluids and solids, in reaction-diffusion systems, and in many-particle models were discussed, too.

From WIAS, eight participants took part in the workshop. The photo by Petra Lein (Copyright MFO) shows the organizers.

Fig. 2: *The organizers of the Oberwolfach Workshop "Variational Methods for Evolution"*

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

1. N. Ahmed, member of the Organizing Committee, *CASM International Conference on Applied Mathematics*, Lahore University of Management Sciences, Centre for Advanced Studies in Mathematics, Pakistan, May 22–24.
2. M. Eigel, co-organizer of the Section S15 “Uncertainty Quantification”, *88th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2017)*, Bauhaus Universität Weimar/Technische Universität Ilmenau, Weimar, March 6–10.
3. ———, co-organizer of the Minisymposium “Uncertainty Computations with Reduced Order Models and Low-Rank Representations”, *2nd International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2017)*, Rhodos, Greece, June 15–17.
4. P. Friz, organizer, *Workshop “Mathematics of Quantitative Finance”*, Mathematisches Forschungsinstitut Oberwolfach, February 26 – March 4.
5. ———, co-organizer of the Section S13 “Probability Theory”, *19th International Congress of the ÖMG and Annual DMV Meeting*, Austrian Mathematical Society (ÖMG) and Deutsche Mathematiker-Vereinigung (DMV), Paris-Lodron University of Salzburg, Austria, September 11–15.
6. ———, member of the Scientific Committee, *Quantitative Finance Conference in honour of Jim Gatheral’s 60th Birthday*, New York University, Courant Institute, USA, October 13–15.
7. ———, scientific organizer, *Berlin-Leipzig Workshop in Analysis and Stochastics*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29 – December 1.
8. ———, member of the Scientific Board, *8th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis*, University of Oxford, Mathematical Institute, UK, December 14–16.
9. J. Fuhrmann, A. Linke, members of the Organizing Committee, *8th International Symposium on Finite Volumes for Complex Applications (FVCA 8)*, Université Lille 1, Villeneuve d’Ascq, France, June 12–16.
10. M. Hintermüller, co-organizer of the Minisymposium MS 111 “Optimization with Balance Laws on Graphs”, *SIAM Conference on Optimization*, Vancouver, British Columbia, Canada, May 22–25.
11. ———, co-organizer of the Minisymposium MS 122 “Recent Trends in PDE-Constrained Optimization”, *SIAM Conference on Optimization*, Vancouver, British Columbia, Canada, May 22–25.
12. ———, co-organizer of the Theme Session 8 “Optimization and Control of Interfaces”, *14th International Conference on Free Boundary Problems: Theory and Applications*, Shanghai Jiao Tong University, China, July 9–14.
13. ———, co-organizer, *Programme “Variational Methods and Effective Algorithms for Imaging and Vision” including the Workshop “Generative Models, Parameter Learning and Sparsity” (Oct. 30 – Nov. 3, 2017) and the Satellite Workshop “MiR@W Day: Image Analysis and Processing in the Life Sciences” (Oct. 2–3, 2017)*, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, August 29 – December 20.
14. ———, co-organizer of the Section S10 “Numerical Analysis”, *19th ÖMG Congress and Annual DMV Meeting*, Austrian Mathematical Society (ÖMG) and Deutsche Mathematiker-Vereinigung (DMV), Paris-Lodron University of Salzburg, Austria, September 11–15.
15. ———, co-chair of the Organizing Committee, *4th Conference on Optimization Methods and Software*, Havana, Cuba, December 16–20.
16. M. Hintermüller, V. John, members of the Scientific Board, *2nd Leibniz MMS Days 2017*, German National Library of Science (TIB), Hannover, February 22–24.

17. M. Hintermüller, W. König, A. Mielke, members of the Scientific Organizing Committee, *CIM-WIAS Workshop "Topics in Applied Analysis and Optimisation"*, International Center for Mathematics, University of Lisbon, Portugal, December 6–8.
18. V. John, member of the Scientific Committee, *12th International Workshop on Variational Multiscale and Stabilization Methods (VMS-2017)*, Campus Reina Mercedes, Sevilla, Spain, April 26–28.
19. W. König, organizer, *Summer School 2017: Probabilistic and Statistical Methods for Networks*, Technische Universität Berlin, Berlin Mathematical School, August 21 – September 1.
20. Th. Koprucki, member of the Program Committee, *10th Conference on Intelligent Computer Mathematics (CICM 2017)*, University of Edinburgh, UK, July 17–21.
21. ———, member of the Steering Committee, *17th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD17)*, Technical University of Denmark, Copenhagen, July 23–28.
22. A. Mielke, member of the Scientific Committee and co-organizer of the Minisymposium "Deformation Accumulation in Seismic Faults and Networks", *CRC 1114 Conference "Scaling Cascades in Complex Systems 2017"*, Freie Universität Berlin, March 27–29.
23. A. Mielke, S. Reichelt, organizers, *SFB 910 Symposium "Stability versus Oscillations in Complex Systems"*, Technische Universität Berlin, Institut für Theoretische Physik, February 10.
24. O. Omel'chenko, co-organizer of the Minisymposium 14a "Synchronization Patterns In Networks: Theory And Applications", *XXXVII Dynamics Days Europe*, University of Szeged, Faculty of Science and Informatics, Hungary, June 5–9.
25. M. Radziunas, member of the International Scientific Committee, *22nd International Conference „Mathematical Modelling and Analysis"*, European Consortium for Mathematics in Industry (ECMI) and Vilnius Gediminas Technical University, Druskininkai, Lithuania, May 30 – June 2.
26. V. Spokoiny, organizer, *Spring School "Structural Inference" 2017*, DFG Research Unit FOR 1735 "Structural Inference in Statistics: Adaptation and Efficiency", Bad Malente, March 5–10.
27. ———, chair of the Local Organizing Commitee, *The 39th Conference on Stochastic Processes and their Applications (SPA2017)*, Russian Academy of Sciences, Kharkevich Institute of Information Transmissions Problems, Moscow, July 24–28.
28. M. Thomas, co-organizer of the Section S14 "Applied Analysis", *88th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2017)*, Bauhaus Universität Weimar/Technische Universität Ilmenau, Weimar, March 6–10.

A.6 Publications[3]

A.6.1 Monographs (to appear)

[1] B. Błaszczyszyn, M. Haenggi, P. Keeler, S. Mukherjee, *Stochastic Geometry Analysis of Cellular Networks*, Cambridge University Press, Cambridge.

A.6.2 Editorship of Proceedings and Collected Editions

[1] P. Colli, A. Favini, E. Rocca, G. Schimperna, J. Sprekels, eds., *Solvability, Regularity, and Optimal Control of Boundary Value Problems for PDEs: In Honour of Prof. Gianni Gilardi*, vol. 22 of Springer INdAM Series, Springer International Publishing AG, Cham, 2017, xii+571 pages.

[2] F.J. Aragón Artacho, R. Henrion, M.A. López-Cerdá, C. Sagastizábal, J.M. Borwein, eds., *Special Issue: Advances in Monotone Operators Theory and Optimization*, vol. 25, issues 3 and 4, of Set-Valued and Variational Analysis, Springer International Publishing AG, Cham, 2017, 396 pages.

[3] L. Ghezzi, D. Hömberg, Ch. Landry, eds., *Math for the Digital Factory*, vol. 27 of Mathematics in Industry / The European Consortium for Mathematics in Industry, Springer International Publishing AG, Cham, 2017, x+348 pages.

[4] H.-Chr. Kaiser, D. Knees, A. Mielke, J. Rehberg, E. Rocca, M. Thomas, E. Valdinoci, eds., *PDE 2015: Theory and Applications of Partial Differential Equations*, vol. 10 of Discrete and Continuous Dynamical Systems – Series S, no. 4, American Institute of Mathematical Science, Springfield, 2017, iv+933 pages.

A.6.3 Outstanding Contributions to Monographs

[1] P. Farrell, N. Rotundo, D.H. Doan, M. Kantner, J. Fuhrmann, Th. Koprucki, *Chapter 50: Drift-Diffusion Models, in: Vol. 2 of Handbook of Optoelectronic Device Modeling and Simulation: Lasers, Modulators, Photodetectors, Solar Cells, and Numerical Methods*, J. Piprek, ed., Series in Optics and Optoelectronics, CRC Press, Taylor & Francis Group, Boca Raton, 2017, pp. 733–771.

[2] M. Hintermüller, D. Wegner, *Distributed and Boundary Control Problems for the Semidiscrete Cahn–Hilliard/Navier–Stokes System with Nonsmooth Ginzburg–Landau Energies, in: Topological Optimization and Optimal Transport in the Applied Sciences*, M. Bergounioux, E. Oudet, M. Rumpf, G. Carlier, Th. Champion, F. Santambrogio, eds., vol. 17 of Radon Series on Computational and Applied Mathematics, De Gruyter, Berlin, 2017, pp. 40–63.

[3] M. Hintermüller, M. Hinze, Ch. Kahle, T. Keil, *Chapter 13: Fully Adaptive and Integrated Numerical Methods for the Simulation and Control of Variable Density Multiphase Flows Governed by Diffuse Interface Models, in: Transport Processes at Fluidic Interfaces*, D. Bothe, A. Reusken, eds., Advances in Mathematical Fluid Mechanics, Birkhäuser, Springer International Publishing AG, Cham, 2017, pp. 305–353.

[4] O. Marquardt, V.M. Kaganer, P. Corfdir, *Chapter 12: Nanowires, in: Vol. 1 of Handbook of Optoelectronic Device Modeling and Simulations: Fundamentals, Materials, Nanostructures, LEDs, and Amplifiers*, J. Piprek, ed., Series in Optics and Optoelectronics, CRC Press, Taylor & Francis Group, Boca Raton, 2017, pp. 395–415.

[5] H.-G. Bartel, H.-J. Mucha, *Chapter 2: Incomparability/Inequality Measures and Clustering, in: Partial Order Concepts in Applied Sciences*, M. Fattore, R. Brüggemann, eds., Springer International Publishing, New York, 2017, pp. 21–34.

[3] Publications that have been written by nonresident members and scholarship holders during their stay at WIAS have been listed in front of those written by the WIAS staff members.

[6] S. Jachalski, D. Peschka, St. Bommer, R. Seemann, B. Wagner, *Chapter 18: Structure Formation in Thin Liquid–Liquid Films, in: Transport Processes at Fluidic Interfaces*, D. Bothe, A. Reusken, eds., Advances in Mathematical Fluid Mechanics, Birkhäuser, Springer International Publishing AG, Cham, 2017, pp. 531–574.

[7] M. Radziunas, *Chapter 31: Traveling Wave Modeling of Nonlinear Dynamics in Multisection Semiconductor Laser Diodes, in: Vol. 2 of Handbook of Optoelectronic Device Modeling and Simulation: Lasers, Modulators, Photodetectors, Solar Cells, and Numerical Methods*, J. Piprek, ed., Series in Optics and Optoelectronics, CRC Press, Taylor & Francis Group, Boca Raton, 2017, pp. 153–182.

Outstanding Contributions to Monographs (to appear)

[1] L. Andreis, P. Dai Pra, M. Fischer, *Chapter 6: Simultaneous Jumps in Interacting Particle Systems: From Neuronal Networks to a General Framework, in: Mathematical and Computational Neuroscience: Cell, Network and Data Analysis*, G. Naldi, Th. Nieus, eds., Springer INdAM Series, Springer.

A.6.4 Articles in Refereed Journals

[1] K. Bredies, H. Sun, *A proximal point analysis of the preconditioned alternating direction method of multipliers*, J. Optim. Theory Appl., 173 (2017), pp. 878–907.

[2] P. Colli, G. Gilardi, E. Rocca, J. Sprekels, *Asymptotic analyses and error estimates for a Cahn–Hilliard type phase field system modelling tumor growth*, Discrete Contin. Dyn. Syst., 10 (2017), pp. 37–54.

[3] ———, *Optimal distributed control of a diffuse interface model of tumor growth*, Nonlinearity, 30 (2017), pp. 2518–2546.

[4] P. Colli, G. Gilardi, J. Sprekels, *Distributed optimal control of a nonstandard nonlocal phase field system with double obstacle potential*, Evol. Equ. Control Theory, 6 (2017), pp. 35–58.

[5] ———, *Global existence for a nonstandard viscous Cahn–Hilliard system with dynamic boundary condition*, SIAM J. Math. Anal., 49 (2017), pp. 1732–1760.

[6] ———, *Recent results on the Cahn–Hilliard equation with dynamic boundary condition*, Bull. South Ural State Univ. Ser. Math. Model. Program. Comput. Softw., 10 (2017), pp. 5–21.

[7] P. Krejčí, E. Rocca, J. Sprekels, *Unsaturated deformable porous media flow with thermal phase transition*, Math. Models Methods Appl. Sci., 27 (2017), pp. 2675–2710.

[8] J. Sprekels, E. Valdinoci, *A new type of identification problems: Optimizing the fractional order in a nonlocal evolution equation*, SIAM J. Control Optim., 55 (2017), pp. 70–93.

[9] N. Ahmed, *On the grad-div stabilization for the steady Oseen and Navier–Stokes equations*, Calcolo, 54 (2017), pp. 471–501.

[10] N. Ahmed, S. Becher, G. Matthies, *Higher-order discontinuous Galerkin time stepping and local projection stabilization techniques for the transient Stokes problem*, Comput. Methods Appl. Mech. Engrg., 313 (2017), pp. 28–52.

[11] A. Wahab, T. Abbas, N. Ahmed, Q.M. Zaigham Zia, *Detection of electromagnetic inclusions using topological sensitivity*, 35 (2017), pp. 642–671.

[12] N. Ahmed, T.C. Rebollo, V. John, S. Rubino, *Analysis of a full space-time discretization of the Navier–Stokes equations by a local projection stabilization method*, IMA J. Numer. Anal., 37 (2017), pp. 1437–1467.

[13] ———, *A review of variational multiscale methods for the simulation of turbulent incompressible flows*, Arch. Comput. Methods Eng., 24 (2017), pp. 115–164.

[14] N. Ahmed, A. Linke, Ch. Merdon, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Comput. Methods Appl. Math., published online on 18.11.2017, https://doi.org/10.1515/cmam-2017-0047.

[15] V. Wiedmeyer, F. Anker, C. Bartsch, A. Voigt, V. John, K. Sundmacher, *Continuous crystallization in a helically-coiled flow tube: Analysis of flow field, residence time behavior and crystal growth*, Ind. Eng. Chem. Res., 56 (2017), pp. 3699–3712.

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[17] F. Anker, Ch. Bayer, M. Eigel, M. Ladkau, J. Neumann, J.G.M. Schoenmakers, *SDE based regression for random PDEs*, SIAM J. Sci. Comput., 39 (2017), pp. A1168–A1200.

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[33] M. Eigel, M. Pfeffer, R. Schneider, *Adaptive stochastic Galerkin FEM with hierarchical tensor representations*, Numer. Math., 136 (2017), pp. 765–803.

[34] M. Eigel, K. Sturm, *Reproducing kernel Hilbert spaces and variable metric algorithms in PDE constrained shape optimisation*, Optim. Methods Softw., 33 (2018), pp. 268–296 (published online on 03.05.2017).

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[2] H. Abels, J. Daube, Ch. Kraus, D. Kröner, *The sharp-interface limit for the Navier–Stokes–Korteweg equations*, in: Hyp2016, XVI International Conference on Hyperbolic Problems Theory, Numerics, Applications, Aachen, August 1–5, Springer Proceedings in Mathematics and Statistics.

[3] P. Mathé, S. Agapiou, *Posterior contraction in Bayesian inverse problems under Gaussian priors*, in: New Trends in Parameter Identification for Mathematical Models, Trends in Mathematics, Springer.

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A.7 Preprints, Reports

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[2] ———, *On a Cahn–Hilliard system with convection and dynamic boundary conditions*, Preprint no. 2391, WIAS, Berlin, 2017.

[3] ———, *Optimal velocity control of a convective Cahn–Hilliard system with double obstacles and dynamic boundary conditions: A 'deep quench' approach*, Preprint no. 2428, WIAS, Berlin, 2017.

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[6] A. Grin, K.R. Schneider, *Global bifurcation analysis of a class of planar systems*, Preprint no. 2426, WIAS, Berlin, 2017.

[7] P. Krejčí, E. Rocca, J. Sprekels, *Unsaturated deformable porous media flow with phase transition*, Preprint no. 2384, WIAS, Berlin, 2017.

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[11] N. Ahmed, A. Linke, Ch. Merdon, *On really locking-free mixed finite element methods for the transient incompressible Stokes equations*, Preprint no. 2368, WIAS, Berlin, 2017.

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[14] Ch. Bayer, P. Friz, A. Gulisashvili, B. Horvath, B. Stemper, *Short-time near-the-money skew in rough fractional volatility models*, Preprint no. 2406, WIAS, Berlin, 2017.

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[23] P.-É. Druet, *Global–in–time solvability of thermodynamically motivated parabolic systems*, Preprint no. 2455, WIAS, Berlin, 2017.

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[29] P. Dondl, Th. Frenzel, A. Mielke, *A gradient system with a wiggly energy and relaxed EDP-convergence*, Preprint no. 2459, WIAS, Berlin, 2017.

[30] M. Becker, Th. Frenzel, Th. Niedermeyer, S. Reichelt, A. Mielke, M. Bär, *Local control of globally competing patterns in coupled Swift–Hohenberg equations*, Preprint no. 2457, WIAS, Berlin, 2017.

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[32] A. González Casanova Soberón, D. Spanò, *Duality and fixation in Ξ-Wright–Fisher processes with frequency-dependent selection*, Preprint no. 2390, WIAS, Berlin, 2017.

[33] M. Heida, *On convergences of the squareroot approximation scheme to the Fokker–Planck operator*, Preprint no. 2399, WIAS, Berlin, 2017.

[34] L. Donati, M. Heida, M. Weber, B. Keller, *Estimation of the infinitesimal generator by square-root approximation*, Preprint no. 2416, WIAS, Berlin, 2017.

[35] M. Heida, R. Kornhuber, J. Podlesny, *Fractal homogenization of a multiscale interface problem*, Preprint no. 2453, WIAS, Berlin, 2017.

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[37] M. Heida, St. Neukamm, M. Varga, *Stochastic unfolding and homogenization*, Preprint no. 2460, WIAS, Berlin, 2017.

[38] T. González Grandón, H. Heitsch, R. Henrion, *A joint model of probabilistic/robust constraints for gas transport management in stationary networks*, Preprint no. 2401, WIAS, Berlin, 2017.

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[45] M. Hintermüller, C.N. Rautenberg, N. Strogies, *Dissipative and non-dissipative evolutionary quasi-variational inequalities with gradient constraints*, Preprint no. 2446, WIAS, Berlin, 2017.

[46] Ch. Hirsch, B. Jahnel, E. Cali, *Continuum percolation for Cox point processes*, Preprint no. 2445, WIAS, Berlin, 2017.

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[48] Ch. Hirsch, B. Jahnel, *Large deviations for the capacity in dynamic spatial relay networks*, Preprint no. 2463, WIAS, Berlin, 2017.

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[52] M. Kantner, M. Mittnenzweig, Th. Koprucki, *Hybrid quantum-classical modeling of quantum dot devices*, Preprint no. 2412, WIAS, Berlin, 2017.

[53] W. König, A. Tóbiás, *A Gibbsian model for message routing in highly dense multi-hop network*, Preprint no. 2392, WIAS, Berlin, 2017.

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[55] M. Biskup, R. Fukushima, W. König, *Eigenvalue fluctuations for lattice Anderson Hamiltonians: Unbounded potentials*, Preprint no. 2439, WIAS, Berlin, 2017.

[56] B. Drees, A. Kraft, Th. Koprucki, *Reproducible research through persistently linked and visualized data*, Preprint no. 2430, WIAS, Berlin, 2017.

[57] Th. Koprucki, M. Kohlhase, K. Tabelow, D. Müller, F. Rabe, *Model pathway diagrams for the representation of mathematical models*, Preprint no. 2431, WIAS, Berlin, 2017.

[58] M. Kohlhase, Th. Koprucki, D. Müller, K. Tabelow, *Mathematical models as research data via flexiformal theory graphs*, Preprint no. 2385, WIAS, Berlin, 2017.

[59] M. Landstorfer, *On the dissociation degree of ionic solutions considering solvation effects*, Preprint no. 2443, WIAS, Berlin, 2017.

[60] P. Dupuis, V. Laschos, K. Ramanan, *Exit time risk-sensitive stochastic control problems related to systems of cooperative agents*, Preprint no. 2407, WIAS, Berlin, 2017.

[61] V. Laschos, A. Mielke, *Geometric properties of cones with applications on the Hellinger–Kantorovich space, and a new distance on the space of probability measures*, Preprint no. 2458, WIAS, Berlin, 2017.

[62] M. Liero, St. Melchionna, *The weighted energy-dissipation principle and evolutionary Gamma-convergence for doubly nonlinear problems*, Preprint no. 2411, WIAS, Berlin, 2017.

[63] M. Liero, J. Fuhrmann, A. Glitzky, Th. Koprucki, A. Fischer, S. Reineke, *3D electrothermal simulations of organic LEDs showing negative differential resistance*, Preprint no. 2420, WIAS, Berlin, 2017.

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[65] P.W. Schroeder, Ch. Lehrenfeld, A. Linke, G. Lube, *Towards computable flows and robust estimates for inf-sup stable FEM applied to the time-dependent incompressible Navier–Stokes equations*, Preprint no. 2436, WIAS, Berlin, 2017.

[66] A. Linke, Ch. Merdon, M. Neilan, F. Neumann, *Quasi-optimality of a pressure-robust nonconforming finite element method for the Stokes problem*, Preprint no. 2374, WIAS, Berlin, 2017.

[67] E. Meca Álvarez, A. Münch, B. Wagner, *Localized instabilities and spinodal decomposition in driven systems in the presence of elasticity*, Preprint no. 2387, WIAS, Berlin, 2017.

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[72] I. Omelchenko, O.E. Omel'chenko, A. Zakharova, E. Schöll, *Optimal design of the tweezer control for chimera states*, Preprint no. 2449, WIAS, Berlin, 2017.

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[74] I. Franović, O.E. Omel'chenko, M. Wolfrum, *Phase sensitive excitability of a limit cycle*, Preprint no. 2465, WIAS, Berlin, 2017.

[75] A.P. Willis, Y. Duguet, O.E. Omel'chenko, M. Wolfrum, *Surfing the edge: Finding nonlinear solutions using feedback control*, Preprint no. 2389, WIAS, Berlin, 2017.

[76] R.I.A. Patterson, S. Simonella, W. Wagner, *A kinetic equation for the distribution of interaction clusters in rarefied gases*, Preprint no. 2365, WIAS, Berlin, 2017.

[77] St. Bommer, S. Jachalski, D. Peschka, R. Seemann, B. Wagner, *Structure formation in thin liquid-liquid films*, Preprint no. 2380, WIAS, Berlin, 2017.

[78] S. Pickartz, C. Brée, U. Bandelow, S. Amiranashvili, *Cancellation of Raman self-frequency shift for compression of optical pulses*, Preprint no. 2419, WIAS, Berlin, 2017.

[79] P. Pigato, *Extreme at-the-money skew in a local volatility model*, Preprint no. 2468, WIAS, Berlin, 2017.

[80] A. Lejay, P. Pigato, *A threshold model for local volatility: Evidence of leverage and mean reversion effects on historical data*, Preprint no. 2467, WIAS, Berlin, 2017.

[81] G. Slavcheva, M.V. Koleva, A. Pimenov, *The impact of microcavity wire width on polariton soliton existence and multistability*, Preprint no. 2381, WIAS, Berlin, 2017.

[82] T. Schemmelmann, F. Tabbert, A. Pimenov, A.G. Vladimirov, S.V. Gurevich, *Delayed feedback control of self-mobile cavity solitons in a wide-aperture laser with a saturable absorber*, Preprint no. 2400, WIAS, Berlin, 2017.

[83] M. Radziunas, M. Khoder, V. Tronciu, J. Danckaert, G. Verschaffelt, *Tunable semiconductor ring laser with filtered optical feedback: Traveling wave description and experimental validation*, Preprint no. 2438, WIAS, Berlin, 2017.

[84] M. Radziunas, A. Zeghuzi, J. Fuhrmann, Th. Koprucki, H.-J. Wünsche, H. Wenzel, U. Bandelow, *Efficient coupling of inhomogeneous current spreading and dynamic electro-optical models for broad-area edge-emitting semiconductor devices*, Preprint no. 2421, WIAS, Berlin, 2017.

[85] M. Redmann, *Type II balanced truncation for deterministic bilinear control systems*, Preprint no. 2425, WIAS, Berlin, 2017.

[86] ———, *Type II singular perturbation approximation for linear systems with Lévy noise*, Preprint no. 2398, WIAS, Berlin, 2017.

[87] M. Redmann, P. Kürschner, *An H_2 -type error bound for time-limited balanced truncation*, Preprint no. 2440, WIAS, Berlin, 2017.

[88] P. Goyal, M. Redmann, *Towards time-limited H_2 -optimal model order reduction*, Preprint no. 2441, WIAS, Berlin, 2017.

[89] A.F.M. ter Elst, J. Rehberg, *Consistent operator semigroups and their interpolation*, Preprint no. 2382, WIAS, Berlin, 2017.

[90] P. Gurevich, S. Reichelt, *Pulses in FitzHugh–Nagumo systems with rapidly oscillating coefficients*, Preprint no. 2413, WIAS, Berlin, 2017.

[91] D.R.M. Renger, *Flux large deviations of independent and reacting particle systems, with implications for macroscopic fluctuation theory*, Preprint no. 2375, WIAS, Berlin, 2017.

[92] R. Schlundt, *A multilevel Schur complement preconditioner for complex symmetric matrices*, Preprint no. 2452, WIAS, Berlin, 2017.

[93] D. Belomestny, J.G.M. Schoenmakers, *Regression on particle systems connected to mean-field SDEs with applications*, Preprint no. 2464, WIAS, Berlin, 2017.

[94] O. Blondel, M.R. Hilário, R. Soares dos Santos, V. Sidoravicius, A. Teixeira, *Random walk on random walks: Higher dimensions*, Preprint no. 2435, WIAS, Berlin, 2017.

[95] ———, *Random walk on random walks: Low densities*, Preprint no. 2434, WIAS, Berlin, 2017.

[96] St. Muirhead, R. Pymar, R. Soares dos Santos, *The Bouchaud–Anderson model with double-exponential potential*, Preprint no. 2433, WIAS, Berlin, 2017.

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[98] M. Thomas, C. Bilgen, K. Weinberg, *Analysis and simulations for a phase-field fracture model at finite strains based on modified invariants*, Preprint no. 2456, WIAS, Berlin, 2017.

[99] S. Bartels, M. Milicevic, M. Thomas, *Numerical approach to a model for quasistatic damage with spatial BV -regularization*, Preprint no. 2388, WIAS, Berlin, 2017.

[100] R. Rossi, M. Thomas, *From nonlinear to linear elasticity in a coupled rate-dependent/independent system for brittle delamination*, Preprint no. 2409, WIAS, Berlin, 2017.

[101] R. Kraaij, F. Redig, W. van Zuijlen, *A Hamilton–Jacobi point of view on mean-field Gibbs-non-Gibbs transitions*, Preprint no. 2461, WIAS, Berlin, 2017.

[102] G. Kitavtsev, A. Münch, B. Wagner, *Thin film models for an active gel*, Preprint no. 2451, WIAS, Berlin, 2017.

[103] O. Muscato, W. Wagner, *A stochastic algorithm without time discretization error for the Wigner equation*, Preprint no. 2415, WIAS, Berlin, 2017.

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A.7.2 WIAS Reports Series

[1] H.-J. Mucha, *Big data clustering: Data preprocessing, variable selection, and dimension reduction*, WIAS Report no. 29, WIAS, Berlin, 2017.

A.7.3 Preprints/Reports in other Institutions

[1] L. Andreis, A. Asselah, P. Dai Pra, *Ergodicity of a system of interacting random walks with asymmetric interaction*, arXiv:1702.02754, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

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[15] M. Hintermüller, N. Strogies, *On the identification of the friction coefficient in a semilinear system for gas transport through a network*, Preprint, DFG SFB Transregio 154 "Mathematical Modelling, Simulation and Optimization using the Example of Gas Networks", Friedrich-Alexander-Universität Erlangen-Nürnberg, 2017.

[16] P. Mathé, B. Hofmann, *Tikhonov regularization with oversmoothing penalty for non-linear ill-posed problems in Hilbert scales*, arXiv:1705.03289, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

[17] L.T. Ding, P. Mathé, *Minimax rates for statistical inverse problems under general source conditions*, arXiv:1707.01706, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

[18] B. Gess, M. Maurelli, *Well-posedness by noise for scalar conservation laws*, arXiv:1701.05393, Cornell University Library, arXiv.org, Ithaca, 2017.

[19] D.R.M. Renger, P. Koltai, *From large deviations to transport semidistances: Coherence analysis for finite Lagrangian data*, arXiv:1709.02352, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

[20] F. Götze, A. Naumov, V. Spokoiny, V. Ulyanov, *Gaussian comparison and anti-concentration inequalities for norms of Gaussian random elements*, arXiv:1708.08663, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

[21] A. Naumov, V. Spokoiny, V. Ulyanov, *Bootstrap confidence sets for spectral projectors of sample covariance*, arXiv:1703.00871, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

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[23] J. Ebert, V. Spokoiny, A. Suvorikova, *Construction of non-asymptotic confidence sets in 2-Wasserstein space*, arXiv:1703.03658, Cornell University Library, arXiv.org, Ithaca, USA, 2017.

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A.8 Talks and Posters

A.8.1 Main and Plenary Talks

1. P. Friz, *Aspects of rough volatility*, The 5th Imperial – ETH Workshop on Mathematical Finance, March 27–29, Imperial College London, UK, March 27.
2. R. Henrion, *Probabilistic constraints: Convexity issues and beyond*, XII International Symposium on Generalized Convexity and Monotonicity, August 27 – September 2, Hajdúszoboszló, Hungary, August 29.
3. ———, *A friendly tour through the world of calmness*, 11th International Conference on Parametric Optimization and Related Topics (ParaoptXI), September 19–22, Prague, Czech Republic, September 19.
4. ———, *Comparing and verifying calmness conditions for MPECs*, Second Workshop on Metric Bounds and Transversality (WoMBaT 2017), November 30 – December 2, RMIT University, Melbourne, Australia, November 30.
5. M. Hintermüller, *Recent trends in PDE-constrained optimization with non-smooth structures*, Fourth Conference on Numerical Analysis and Optimization (NAOIV-2017), January 2–5, Sultan Qaboos University, Muscat, Oman, January 4.
6. D. Hömberg, *European collaboration in industrial and applied mathematics*, 25th Conference on Applied and Industrial Mathematics (CAIM), September 14–17, University of Iaşi, Romania, September 14.
7. ———, *MSO for steel production and manufacturing*, Workshop “Future and Emerging Mathematical Technologies in Europe”, December 11–15, Lorentz Center, Leiden, Netherlands, December 11.
8. A. Mielke, *Optimal transport versus growth and decay*, International Conference “Calculus of Variations and Optimal Transportation” in the Honor of Yann Brenier for his 60th Birthday, January 9–11, Institut Henri Poincaré, Paris, France, January 11.
9. V. Spokoiny, *Adaptive clustering and network clustering*, 60th MIPT Scientific Conference, Moscow State University, Moscow Institute of Physics and Technology, Russian Federation, November 25.
10. B. Wagner, *Mathematical opportunities and challenges in sustainable energies*, SIAM Annual Meeting, July 10–14, Pittsburgh, USA, July 14.

A.8.2 Scientific Talks (Invited)

1. J. Sprekels, *A nonstandard viscous Cahn–Hilliard system with dynamic boundary condition and the DCH*, Analysis of Boundary Value Problems for PDEs – Workshop on the Occasion of the 70th Birthday of Gianni Gilardi, Pavia, Italy, February 20.
2. ———, *Well-posedness and optimal control of a nonstandard Cahn–Hilliard system with dynamic boundary condition*, Fudan University, School of Mathematical Sciences, China, April 10.
3. ———, *Optimal control of PDEs: From basic principles to hard applications*, 3 talks, International School “Frontiers in Partial Differential Equations and Solvers”, May 22–25, University of Pavia, Department of Mathematics, Italy, May 25.
4. H. Sun, *Locating and determining shapes of multiple scatterers with finite electromagnetic point sources*, Applied Inverse Problems 2017, Minisymposium M47-2 “Visibility and Invisibility for Wave Scattering”, May 29 – June 2, Hangzhou, China, May 30.
5. N. Ahmed, *Higher-order discontinuous Galerkin time discretizations for the evolutionary Navier–Stokes equations*, Technische Universität Dresden, Institut für Numerische Mathematik, March 9.

6. ———, *On really locking-free mixed finite element methods for the transient incompressible Stokes equations*, CASM International Conference on Applied Mathematics, May 22–24, Lahore University of Management Sciences, Centre for Advanced Studies in Mathematics, Pakistan, May 22.

7. ———, *A numerical study of residual based variational multiscale methods for turbulent incompressible flow problems*, American University of the Middle East, Dasman, Kuwait, November 2.

8. A. Alphonse, *A coupled bulk-surface reaction-diffusion system on a moving domain*, Workshop “Emerging Developments in Interfaces and Free Boundaries”, January 23–28, Mathematisches Forschungszentrum Oberwolfach, January 25.

9. C. Bartsch, *ParMooN – A parallel finite element solver, Part I*, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, India, March 16.

10. Ch. Bayer, *Smoothing the payoff for efficient computation of basket option prices*, Workshop “Mathematics of Quantitative Finance”, February 26 – March 4, Mathematisches Forschungsinstitut Oberwolfach, February 27.

11. ———, *Smoothing the payoff for efficient computation of basket options*, Workshop on Recent Developments in Numerical Methods with Applications in Statistics and Finance, June 8–9, University of Mannheim, Graduate School of Economics and Social Sciences, June 9.

12. ———, *Numerics for rough volatility models*, Ninth Workshop on Random Dynamical Systems, June 14–17, University of Bielefeld, Department of Mathematics, June 14.

13. ———, *Smoothing the payoff for efficient computation of basket options*, Conference on Mathematical Modelling in Finance 2017, August 30 – September 2, Imperial College London, UK, September 2.

14. ———, *Rough volatility models in finance*, 19th International Congress of the ÖMG and Annual DMV Meeting, 6th Austrian Stochastics Days, September 11–15, Austrian Mathematical Society (ÖMG) and Deutsche Mathematiker-Vereinigung (DMV), Paris-Lodron University of Salzburg, Austria, September 13.

15. ———, *Smoothing the payoff for efficient computation of basket option*, Financial Math Seminar, Princeton University, Operations Research & Financial Engineering, USA, October 11.

16. ———, *A regularity structure for rough volatility*, Quantitative Finance Conference in honour of Jim Gatheral’s 60th Birthday, October 13–15, New York University, Courant Institute, USA, October 14.

17. ———, *Rough volatility models in finance*, AMCS Seminar, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering Division, Thuwal, Saudi Arabia, October 25.

18. C. Brée, *Detection of dynamic resonances in femtosecond filaments via the transient plasma grating effect*, Workshop „Nonlinear Phenomena in Strong Fields”, Leibniz Universität Hannover, January 25.

19. A. Caiazzo, *Homogenization methods for weakly compressible elastic materials forward and inverse problem*, Workshop on Numerical Inverse and Stochastic Homogenization, February 13–17, Universität Bonn, Hausdorff Research Institute for Mathematics, February 17.

20. R. dos Santos, *Mass concentration in the parabolic Anderson model*, Université Claude Bernard Lyon 1, Institut Camille Jordan, France, February 2.

21. W. Dreyer, *Space-time transformations and the principle of material objectivity*, 2 talks, Technische Universität Darmstadt, Fachbereich Mathematik, May 3–5.

22. P.-É. Druet, *Existence of weak solutions for improved Nernst–Planck–Poisson models of compressible electrolytes*, Seminar EDE, Czech Academy of Sciences, Institute of Mathematics, Department of Evolution Differential Equations (EDE), Prague, Czech Republic, January 10.

23. M. Eigel, *Adaptive stochastic FE for explicit Bayesian inversion with hierarchical tensor representations*, Institut National de Recherche en Informatique et en Automatique (INRIA), SERENA (Simulation for the Environment: Reliable and Efficient Numerical Algorithms) research team, Paris, France, June 1.

24. ———, *Explicit Bayesian inversion in hierarchical tensor representations*, 4th GAMM Junior's and 1st GRK2075 Summer School 2017 "Bayesian Inference: Probabilistic Way of Learning from Data", July 10–14, Braunschweig, July 14.

25. ———, *Aspects of stochastic Galerkin FEM*, Universität Basel, Mathematisches Institut, Switzerland, November 10.

26. S. Eydam, *Phase oscillator mode-locking*, Forschungsseminar "Applied Dynamical Systems", TU Berlin, June 14.

27. P. Farrell, *Numerical solution of PDEs via RBFs and FVM with focus on semiconductor problems*, Technische Universität Hamburg, Institut für Mathematik, Harburg, January 6.

28. F. Flegel, *Spectral localization vs. homogenization in the random conductance model*, 19th ÖMG Congress and Annual DMV Meeting, Minisymposium M6 "Spectral and Scattering Problems in Mathematical Physics", September 11–15, Austrian Mathematical Society (ÖMG) and Deutsche Mathematiker-Vereinigung (DMV), Paris-Lodron University of Salzburg, Austria, September 12.

29. ———, *Spectral localization vs. homogenization in the random conductance model*, Berlin-Leipzig Workshop in Analysis and Stochastics, November 29 – December 1, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29.

30. P. Friz, *A regularity structure for rough volatility*, Global Derivates Trading & Risk Management Conference 2017, May 8–12, Barcelona, Spain, May 10.

31. ———, *An application of regularity structures to the analysis of rough volatility*, Fractional Brownian Motion and Rough Models, June 8–9, Barcelona Graduate School of Economics, Spain, June 9.

32. ———, *General semimartingales and rough paths*, Durham Symposium on Stochastic Analysis, July 10–20, Durham University, Department of Mathematical Sciences, UK, July 13.

33. ———, *Geometric aspects in pathwise stochastic analysis*, High Risk High Gain – Groundbreaking Research in Berlin, August 31 – September 3, Technische Universität Berlin, Stabsstelle Presse, September 2.

34. ———, *Rough differential equations with jumps and their applications*, Japanese-German Open Conference on Stochastic Analysis 2017, September 4–8, Technische Universität Kaiserslautern, Fachbereich Mathematik, September 5.

35. ———, *Multiscale systems, homogenization and rough paths*, Berlin-Leipzig Workshop in Analysis and Stochastics, November 29 – December 1, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29.

36. A. González Casanova Soberón, *Modelling selection via multiple parents*, Probability Seminar, University of Oxford, Mathematical Institute, UK, January 24.

37. ———, *Modelling selection via multiple parents*, Seminar Probability, National Autonomous University of Mexico, Mexico City, February 23.

38. ———, *Branching processes with interactions and their relation to population genetics*, The 3rd Workshop on Branching Processes and Related Topics, May 8–12, Beijing Normal University, School of Mathematical Sciences, China, May 8.

39. ———, *The ancestral efficiency graph*, Spatial Models in Population Genetics, September 6–8, University of Bath, Department of Mathematical Sciences, UK, September 6.

40. ———, *Modelling the Lenski experiment*, 19th ÖMG Congress and Annual DMV Meeting, Section S16 "Mathematics in the Science and Technology", September 11–15, Austrian Mathematical Society (ÖMG) and Deutsche Mathematiker-Vereinigung (DMV), Paris-Lodron University of Salzburg, Austria, September 14.

41. ———, *The discrete ancestral selection graph*, Seminar, Center for Interdisciplinary Research in Biology, Stochastic Models for the Inference of Life Evolution SMILE, Paris, France, October 23.

42. R. Gruhlke, *Multi-scale failure analysis with polymorphic uncertainties for optimal design of rotor blades*, Frontiers of Uncertainty Quantification in Engineering (FrontUQ 2017), September 6–8, München, September 6.

43. H. Heitsch, *A probabilistic approach to optimization problems in gas transport networks*, SESO 2017 International Thematic Week "Smart Energy and Stochastic Optimization", May 30 – June 1, ENSTA ParisTech and École des Ponts ParisTech, Paris, France, June 1.

44. ———, *On probabilistic capacity maximization in stationary gas networks*, 21st Conference of the International Federation of Operational Research Societies (IFORS 2017), Invited Session TB20 "Optimization of Gas Networks 2", July 17–21, Quebec, Canada, July 18.

45. R. Henrion, *Contraintes en probabilité: Formules du gradient et applications*, Workshop "MAS-MODE 2017", Institut Henri Poincaré, Paris, France, January 9.

46. ———, *On a joint model for probabilistic/robust constraints with an application to gas networks under uncertainties*, Workshop "Models and Methods of Robust Optimization", March 9–10, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Kaiserslautern, March 10.

47. ———, *On M-stationary condition for a simple electricity spot market model*, Workshop "Variational Analysis and Applications for Modelling of Energy Exchange", May 4–5, Université Perpignan, France, May 4.

48. ———, *Subdifferential estimates for Gaussian probability functions*, HCM Workshop: Nonsmooth Optimization and its Applications, May 15–19, Hausdorff Center for Mathematics, Bonn, May 17.

49. ———, *Subdifferential characterization of Gaussian probability functions*, SESO 2017 International Thematic Week "Smart Energy and Stochastic Optimization", May 30 – June 1, ENSTA ParisTech and École des Ponts ParisTech, Paris, France, June 1.

50. ———, *Problèmes d'optimisation sous contraintes en probabilité*, Université de Bourgogne, Département de Mathématiques, Dijon, France, October 25.

51. ———, *Probabilistic constraints in infinite dimensions*, Universität Wien, Institut für Statistik und Operations Research, Austria, November 6.

52. ———, *Probabilistic programming: Structural properties and applications*, Control and Optimization Conference on the occasion of Frédéric Bonnans 60th birthday, November 15–17, Electricité de France, Palaiseau, France, November 17.

53. ———, *Optimization problems under robust constraints with applications to gas networks under uncertainty*, The Eighth Australia-China Workshop on Optimization (ACWO 2017), December 4, Curtin University, Perth, Australia, December 4.

54. ———, *Subdifferential of probability functions under Gaussian distribution*, The Second Pacific Optimization Conference (POC2017), December 4–7, Curtin University, Perth, Australia, December 6.

55. ———, *Probabilistic programming in infinite dimensions*, The South Pacific Optimization Meeting in Western Australia 2017 (SPOM in WA 2017), December 8–10, Curtin University, Perth, Australia, December 9.

56. M. Hintermüller, *Non-smooth structures in PDE-constrained optimization*, Mathematisches Kolloquium, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, January 11.

57. ———, *Bilevel optimization and applications in imaging*, Mathematisches Kolloquium, Universität Wien, Austria, January 18.

58. ———, *Presentation of the GAMM-related DFG Priority Programme 1962 "Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization"*,

88th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2017), March 6–10, Bauhaus Universität Weimar/Technische Universität Ilmenau, Weimar, March 9.

59. ———, *Optimal control of nonsmooth phase-field models*, DFG-AIMS Workshop on "Shape Optimization, Homogenization and Control", March 13–16, Mbour, Senegal, March 14.

60. ———, *Optimal control of multiphase fluids and droplets*, Kolloquium, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, Erlangen, May 2.

61. ———, *(Pre)Dualization, dense embeddings of convex sets, and applications in image processing*, HCM Workshop: Nonsmooth Optimization and its Applications, May 15–19, Hausdorff Center for Mathematics, Bonn, May 15.

62. ———, *Adaptive finite element solvers for MPECs in function space*, SIAM Conference on Optimization, Minisymposium MS122 "Recent Trends in PDE-Constrained Optimization", May 22–25, Vancouver, British Columbia, Canada, May 25.

63. ———, *Total variation diminishing Runge–Kutta methods for the optimal control of conservation laws: Stability and order-conditions*, SIAM Conference on Optimization, Minisymposium MS111 "Optimization with Balance Laws on Graphs", May 22–25, Vancouver, British Columbia, Canada, May 25.

64. ———, *Generalized Nash equilibrium problems in Banach spaces: Theory, Nikaido–Isoda-based path-following methods, and applications*, The Third International Conference on Engineering and Computational Mathematics (ECM2017), Stream 3 "Computational Optimization", May 31 – June 2, The Hong Kong Polytechnic University, China, June 2.

65. ———, *Nonsmooth structures in PDE constrained optimization*, Optimization Seminar, Chinese Academy of Sciences, State Key Laboratory of Scientific and Engineering Computing, Beijing, China, June 6.

66. ———, *Generalized Nash games with partial differential equations*, Kolloquium Arbeitsgruppe Modellierung, Numerik, Differentialgleichungen, Technische Universität Berlin, June 20.

67. ———, *Optimal control of multiphase fluids based on non smooth models*, 14th International Conference on Free Boundary Problems: Theory and Applications, Theme Session 8 "Optimization and Control of Interfaces", July 9–14, Shanghai Jiao Tong University, China, July 10.

68. ———, *On (pre)dualization, dense embeddings of convex sets, and applications in image processing*, Seminar, Isaac Newton Institute, Programme "Variational Methods and Effective Algorithms for Imaging and Vision", Cambridge, UK, August 30.

69. ———, *Bilevel optimization and some "parameter learning" applications in image processing*, LMS Workshop "Variational Methods Meet Machine Learning", September 18, University of Cambridge, Centre for Mathematical Sciences, UK, September 18.

70. ———, *On (pre)dualization, dense embeddings of convex sets, and applications in image processing*, University College London, Centre for Inverse Problems, UK, October 27.

71. D. Hömberg, *Mathematical aspects of multi-frequency induction heating*, Universidade Técnica de Lisboa, Instituto Superior Técnico, Portugal, February 2.

72. ———, *On a robust phase field approach to topology optimization*, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, April 28.

73. ———, *Joule heating models – Modelling, analysis and industrial application*, Beijing Computational Science Research Center, China, October 10.

74. ———, *Optimal coefficient control for semilinear parabolic equations*, The 15th Annual Meeting of the China Society for Industrial and Applied Mathematics, Embedded Meeting EM02 "A3 Workshop on Modeling and Computation of Applied Inverse Problems", October 12–15, Qingdao, China, October 14.

75. ———, *The Digital Factory – A perspective for a closer cooperation between Math and Industry*, Meeting "M414 Mathematics for Industry 4.0", November 7, Vicenza Convention Centre, Italy, November 7.

76. B. Jahnel, *The Widom–Rowlinson model under spin flip: Immediate loss and sharp recovery of quasilocality*, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, January 18.

77. ———, *The Widom–Rowlinson model under spin flip: Immediate loss and sharp recovery of quasilocality*, Oberseminar Wahrscheinlichkeitstheorie, Ludwig-Maximilians-Universität München, Fakultät für Mathematik, Informatik und Statistik, February 13.

78. ———, *The Widom–Rowlinson model under spin flip: Immediate loss and sharp recovery of quasilocality*, Oberseminar Stochastik, Johannes Gutenberg Universität Mainz, Institut für Mathematik, April 25.

79. B. Jahnel, *Stochastic geometry in telecommunications*, 3 talks, Summer School 2017: Probabilistic and Statistical Methods for Networks, August 21 – September 1, Technische Universität Berlin, Berlin Mathematical School, August 23–25.

80. ———, *Large deviations in relay-augmented wireless networks*, Sharif University of Technology Tehran, Mathematical Sciences Department, Teheran, Iran, September 17.

81. ———, *Continuum percolation for Cox processes*, Seminar, Ruhr Universität Bochum, Fakultät für Mathematik, October 27.

82. ———, *Continuum percolation theory applied to Device to Device*, Telecom Orange Paris, France, November 17.

83. ———, *Gibbsian representation for point processes via hyperedge potentials*, Workshop on Stochastic Analysis and Random Fields, Second Haifa Probability School, December 18–22, Technion Israel Institute of Technology, Haifa, Israel, December 18.

84. V. John, *Variational multiscale (VMS) methods for the simulation of turbulent incompressible flows*, Mahindra École Centrale, School of Natural Sciences, Hyderabad, India, March 9.

85. ———, *Variational multiscale (VMS) methods for the simulation of turbulent incompressible flows*, CDS: Computational Science Symposium, March 16–18, Indian Institute of Science, Department of Computer and Data Sciences, Bangalore, India, March 16.

86. ———, *Variational multiscale (VMS) methods for the simulation of turbulent incompressible flows*, Chinese Academy of Sciences, Academy of Mathematics and Systems Science, Beijing, May 10.

87. ———, *Variational multiscale (VMS) methods for the simulation of turbulent incompressible flows*, Peking University, School of Mathematical Sciences, Beijing, China, May 11.

88. ———, *Finite element methods for incompressible flow problems*, 10 talks, Beijing Computational Science Research Center, Applied and Computational Mathematics, China, May 14–18.

89. ———, *Finite elements for scalar convection-dominated equations and incompressible flow problems — A never ending story?*, 30th Chemnitz FEM Symposium, September 25–27, Bundesinstitut für Erwachsenenbildung, St. Wolfgang / Strobl, Austria, September 27.

90. P. Keeler, *Optimizing spatial throughput in device-to-device networks*, Applied Probability @ The Rock – An International Workshop celebrating Phil Pollett's 60th Birthday, April 17–21, University of Adelaide, School of Mathematical Sciences, Uluru, Australia, April 20.

91. T. Keil, *Strong stationarity conditions for the optimal control of a Cahn–Hilliard–Navier–Stokes system*, 14th International Conference on Free Boundary Problems: Theory and Applications, Theme Session 8 "Optimization and Control of Interfaces", July 9–14, Shanghai Jiao Tong University, China, July 10.

92. O. Klein, *Uncertainty quantification for models involving hysteresis operators*, 3 talks, Summer School on Multi-Rate Processes, Slow-Fast Systems and Hysteresis MURPHYS-HSFS-2017, June 19–23, DISMA Politecnico di Torino, Dipartimento di Scienze Matematiche "Giuseppe Luigi Lagrange", Italy, June 19–20.

93. W. König, *A variational formula for an interacting many-body system*, Probability Seminar, University of California, Los Angeles, Department of Mathematics, USA, January 19.

94. ———, *The principal part of the spectrum of a random Schrödinger operator in a large box*, Mathematisches Kolloquium, Oberseminar Stochastik und Analysis, Technische Universität Dormund, May 15.

95. ———, *Connectivity in large mobile ad-hoc networks*, Summer School 2017: Probabilistic and Statistical Methods for Networks, August 21 – September 1, Technische Universität Berlin, Berlin Mathematical School, August 29.

96. ———, *Moment asymptotics of branching random walks in random environment*, Modern Perspective of Branching in Probability, September 26–29, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, September 28.

97. ———, *Intersections of Brownian motions*, Workshop "Peter's Network", October 31 – November 1, University of Bath, Department of Mathematical Sciences, UK, November 1.

98. ———, *Cluster-size distributions in a classical many-body system*, Berlin-Leipzig Workshop in Analysis and Stochastics, November 29 – December 1, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29.

99. TH. KOPRUCKI, *How to tidy up the jungle of mathematical models? A prerequisite for sustainable research software*, 2nd Conference on Non-Textual Information "Software and Services for Science (S3)", May 10–11, Technische Informationsbibliothek, Hannover, May 11.

100. ———, *Über das L-Konzept einer physikalischen Theorie*, Seminar Wissensrepräsentation und -verarbeitung, Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Informatik, Erlangen, May 17.

101. ———, *On the Scharfetter–Gummel scheme for the discretization of drift-diffusion equations and its generalization beyond Boltzmann*, Kolloquium Modellierung, Numerik, Differentialgleichungen, Technische Universität Berlin, Institut für Mathematik, May 30.

102. M. LANDSTORFER, *Theory, structure and experimental justification of the metal/electrolyte interface*, Universität Münster, Institut für Analysis und Numerik, July 11.

103. M. LIERO, *On entropy-transport problems and the Hellinger–Kantorovich distance*, Seminar of Team EDP-AIRSEA-CVGI, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, Grenoble, France, January 26.

104. M. LIERO, *The Hellinger–Kantorovich distance as natural generalization of optimal transport distance to (scalar) reaction-diffusion equations*, Workshop "Variational Methods for Evolution", November 12–17, Mathematisches Forschungsinstitut Oberwolfach, November 14.

105. ———, *The Hellinger–Kantorovich distance as natural generalization of optimal transport distance to (scalar) reaction-diffusion equations*, Oberseminar "Angewandte Analysis", Universität Dortmund, Institut für Mathematik, November 29.

106. A. LINKE, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, Neubiberg, January 18.

107. ———, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Technische Universität Dortmund, Institut für Angewandte Mathematik, March 23.

108. ———, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Freie Universität Berlin, Institut für Mathematik, May 3.

109. ———, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, CASM International Conference on Applied Mathematics, May 22–24, Lahore University of Management Sciences, Centre for Advanced Studies in Mathematics, Pakistan, May 23.

110. ———, *Towards pressure-robust mixed methods for the incompressible Navier–Stokes equations*, Technische Universität Darmstadt, Fachbereich Mathematik, July 20.

111. C. Löbhard, *A function space based solution method with space-time adaptivity for parabolic optimal control problems with state constraints*, PGMO Days 2017, November 13–14, EDF Lab Paris Saclay, France, November 14.

112. M. Marschall, *Sampling-free Bayesian inversion with adaptive hierarchical tensor representation*, Frontiers of Uncertainty Quantification in Engineering (FrontUQ 2017), September 6–8, München, September 7.

113. ———, *Sampling-free Bayesian inversion with adaptive hierarchical tensor representation*, International Conference on Scientific Computation and Differential Equations (SciCADE2017), MS21 “Tensor Approximations of Multi-Dimensional PDEs”, September 11–15, University of Bath, UK, September 14.

114. P. Mathé, *Complexity of supervised learning*, ibc-paris2017 : Information Based Complexity, High-Dimensional Problems, March 14–15, Institut Henri Poincaré, Paris, France, March 15.

115. ———, *Bayesian inverse problems with non-commuting operators*, Statistical Foundations of Uncertainty Quantification for Inverse Problems Workshop, June 19–22, University of Cambridge, Center for Mathematical Sciences, UK, June 21.

116. ———, *Tikhonov regularization with oversmoothing penalty*, 7th German-Polish Conference on Optimization (GPCO 2017), August 27 – September 1, Mathematical Research and Conference Center of IMPAN, Będlewo, Poland, August 28.

117. ———, *Numerical integration (mini course)*, 3 talks, Fudan University, School of Mathematical Sciences, China, November 20 – December 4.

118. M. Maurelli, *Regularization by noise for scalar conservation laws*, Stochastic Analysis Day, February 27, Università di Pisa, Dipartimento di Matematica, Italy, February 27.

119. ———, *Regularization by noise for scalar conservation laws*, Séminaire de Probabilité et Statistique, Université de Nice Sophia-Antipolis, Laboratoire Jean Alexandre Dieudonné, France, September 26.

120. ———, *Stochastic 2D Euler equations with transport noise*, Chalmers University of Technology, Department of Mathematical Sciences, Gothenburg, Sweden, November 28.

121. ———, *A McKean–Vlasov SDE with reflecting boundaries*, 8th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 14–16, University of Oxford, Mathematical Institute, UK, December 15.

122. ———, *A McKean–Vlasov SDE with reflecting boundaries*, Seminar of SPASS – Probability, Stochastic Analysis and Statistics in Pisa, Università di Pisa, Dipartimento di Matematica, Italy, December 18.

123. Ch. Merdon, *Druckrobuste Finite-Elemente-Methoden für die Navier-Stokes-Gleichungen*, Universität Paderborn, Institut für Mathematik, April 25.

124. ———, *Pressure-robustness in mixed finite element discretisations for the Navier–Stokes equations*, Universität des Saarlandes, Fakultät für Mathematik und Informatik, July 12.

125. A. Mielke, *A geometric approach to reaction-diffusion equations*, Institutskolloquium, Universität Potsdam, Institut für Mathematik, January 25.

126. ———, *Uniform exponential decay for energy-reaction-diffusion systems*, Analysis Seminar, University of Pavia, Department of Mathematics, Italy, March 21.

127. ———, *On self-induced oscillations for friction reduction with applications to walking*, Conference “Dynamical Systems and Geometric Mechanics”, June 12–14, Technische Universität München, Zentrum für Mathematik, June 13.

128. ———, *Entropy-induced geometry for classical and quantum Markov semigroups*, SMS Colloquium, University College Cork, School of Mathematical Science, Ireland, September 11.

129. ———, *Perspectives for gradient flows*, GAMM-Workshop on Analysis of Partial Differential Equations, September 27–29, Eindhoven University of Technology, Mathematics and Computer Science Department, Netherlands, September 28.

130. M. MITTNENZWEIG, *An entropic gradient structure for quantum Markov semigroups*, Workshop "Applications of Optimal Transportation in the Natural Sciences", January 30 – February 3, Mathematisches Forschungsinstitut Oberwolfach, January 31.

131. M. MITTNENZWEIG, *A variational approach to the Lindblad equations*, Scientific Computing Seminar, École des Ponts ParisTech, CERMICS, Paris, France, April 24.

132. ———, *Gradient flow structures for quantum master equations*, Analysis-Seminar Augsburg-München, Universität Augsburg, Institut für Mathematik, June 8.

133. ———, *Variational methods for quantum master equations*, BMS – BGSMath Junior Meeting, October 9–10, Berlin Mathematical School and Barcelona Graduate School of Mathematics, Barcelona, Spain, October 10.

134. ———, *A variational approach to quantum master equations coupled to a semiconductor PDE*, Workshop "Variational Methods for Evolution", November 12–17, Mathematisches Forschungsinstitut Oberwolfach, November 14.

135. H.-J. MUCHA, *Big data clustering: Comparison of the performance of a new fast pre-clustering and subsampling*, German Polish Seminar on Data Analysis and Applications 2017, September 25–26, Wrocław University of Economics, Poland, September 26.

136. CH. MUKHERJEE, *Asymptotic behavior of the mean-field polaron*, Probability and Mathematical Physics Seminar, Courant Institute of Mathematical Sciences, Department of Mathematics, New York, USA, March 20.

137. R. MÜLLER, *A posteriori analysis for coupled bulk-surface problems*, Oberseminar "Angewandte Analysis und Numerische Simulation", Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, June 1.

138. ———, *Consistent coupling of charge transport and fluid flow with application to nanopores*, ACOMEN 2017 – 7th International Conference on Advanced Computational Methods in Engineering, Minisymposium MS7 "Electrokinetic and Electrochemical Flows for Batteries and Fuel Cells: Analysis, Simulation, Upscaling", September 18–22, Ghent University, Belgium, September 21.

139. O. OMEL'CHENKO, *Introduction to chimera states*, Seminar of the Scientific Computing Laboratory, University of Belgrade, Institue of Physics, Serbia, May 4.

140. ———, *Bifurcations mediating the appearance of chimera states*, SIAM Conference on Applications of Dynamical Systems (DS 17), Minisymposium "Large Scale Dynamics In Coupled Systems On Networks", May 21–25, Society for Industrial and Applied Mathematics (SIAM), Snowbird, USA, May 24.

141. ———, *Bifurcations mediating appearance of chimera states*, XXXVII Dynamics Days Europe, Minisymposium 3 "Complex Networks: Delays And Collective Dynamics", June 5–9, University of Szeged, Faculty of Science and Informatics, Hungary, June 8.

142. ———, *Controlling unstable complex dynamics: From coupled oscillators to fluid mechanics*, XV Latin American Workshop on NonLinear Phenomena, November 6–10, Facultad de Ciencias y Astronomía, Universidad de La Serena, Chile, November 7.

143. R.I.A. PATTERSON, *Confidence intervals for coagulation–advection simulations*, Clausthal-Göttingen International Workshop on Simulation Science, April 27–28, Georg-August-Universität Göttingen, Institut für Informatik, April 28.

144. R.I.A. PATTERSON, *Simulation of particle coagulation and advection*, Numerical Methods and Applications of Population Balance Equations, October 13, GRK 1932, Technische Universität Kaiserslautern, Fachbereich Mathematik, October 13.

145. D. Peschka, *Modelling and simulation of suspension flow*, Graduate Seminar PDE in the Sciences, Universität Bonn, Institut für Angewandte Mathematik, January 20.

146. ———, *Motion of thin droplets over surfaces*, Making a Splash – Driplets, Jets and Other Singularities, March 20–24, Brown University, Institute for Computational and Experimental Research in Mathematics (ICERM), Providence, USA, March 22.

147. ———, *Variational structure of fluid motion with contact lines in thin-film models*, Kolloquium Angewandte Mathematik, Universität der Bundeswehr, München, May 31.

148. ———, *Mathematical and numerical approaches to moving contact lines*, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, December 6.

149. P. Pigato, *The oscillating Brownian motion: Estimation and application to volatility modeling*, Probability Seminar, Università degli Studi di Padova, Dipartimento di Matematica Pura ed Applicata, Italy, September 26.

150. ———, *The oscillating Brownian motion: Estimation and application to volatility modelling*, Finance and Stochastics Seminar, Imperial College London, Department of Mathematics, UK, November 15.

151. A. Pimenov, *Time-delay models of multi-mode laser dynamics*, SIAM Conference on Applications of Dynamical Systems (DS17), May 21–25, Society for Industrial and Applied Mathematics (SIAM), Snowbird, USA, May 24.

152. J. Polzehl, *Toward in-vivo histology of the brain*, Neuro-Statistics: The Interface between Statistics and Neuroscience, University of Minnesota, School of Statistics (IRSA), Minneapolis, USA, May 5.

153. ———, *Connectivity networks in neuroscience – Construction and analysis*, 2 talks, Summer School 2017: Probabilistic and Statistical Methods for Networks, August 21 – September 1, Technische Universität Berlin, Berlin Mathematical School, August 21–22.

154. ———, *Neue statistische Methoden zur Biomarkerselektion*, Symposium “Biomarker: Objektive Parameter als Grundlage für die erfolgreiche individuelle Therapie”, November 21, Leibniz Gesundheitstechnologien, Berlin, November 21.

155. ———, *Structural adaptation – A statistical concept for image denoising*, Seminar, Isaac Newton Institute, Programme “Variational Methods and Effective Algorithms for Imaging and Vision”, Cambridge, UK, December 5.

156. ———, *Towards in-vivo histology of the brain*, Berlin Symposium 2017: Modern Statistical Methods From Data to Knowledge, December 14–15, organized by Indiana Laboratory of Biostatistical Analysis of Large Data with Structure (IL-BALDS), Berlin, December 14.

157. M. Redmann, *A regression method to solve parabolic rough PDEs*, Ninth Workshop on Random Dynamical Systems, June 14–17, Universität Bielefeld, Fakultät für Mathematik, June 15.

158. ———, *Type II singular perturbation approximation for linear systems with Levy noise*, London Mathematical Society – EPSRC Durham Symposium: Model Order Reduction, Durham University, Department of Mathematical Sciences, UK, August 14.

159. J. Rehberg, *On optimal elliptic Sobolev regularity*, Oberseminar Prof. Ira Neitzel, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Numerische Simulation, February 2.

160. ———, *Explicit and uniform resolvent estimates for second order divergence operators on L^p spaces*, Oberseminar Analysis, Technische Universität Darmstadt, Fachbereich Mathematik, November 9.

161. S. Reichelt, *Pulses in FitzHugh–Nagumo systems with periodic coefficients*, Seminar “Dynamical Systems and Applications”, Technische Universität Berlin, Institut für Mathematik, May 3.

162. ———, *Corrector estimates for elliptic and parabolic equations with periodic coefficients*, Analysis Seminar, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, Erlangen, May 18.

163. ———, *Corrector estimates for elliptic and parabolic equations with periodic coefficients*, Analysis Seminar, Universität Augsburg, Institut für Mathematik, May 23.

164. D.R.M. Renger, *Large deviations and gradient flows*, Spring School 2017: From Particle Dynamics to Gradient Flows, February 27 – March 3, Technische Universität Kaiserslautern, Fachbereich Mathematik, March 1.

165. ———, *Banach-valued functions of bounded variation*, Oberseminar Analysis, Universität Regensburg, Fakultät für Mathematik, July 28.

166. ———, *Was sind und was sollen die Zahlen*, Tag der Mathematik, Universität Regensburg, Fakultät für Mathematik, July 28.

167. ———, *Gradient flows and GENERIC in flux space*, Workshop "Variational Methods for Evolution", November 12–18, Mathematisches Forschungsinstitut Oberwolfach, November 16.

168. J.G.M. Schoenmakers, *Projected particle methods for solving McKean–Vlasov SDEs*, Dynstoch 2017, April 5–7, Universität Siegen, Department Mathematik, April 6.

169. ———, *Projective simulation and regression methods for Mckean–Vlasov SDE systems*, Mathematisches Kolloquium, Universität Duisburg-Essen, Fakultät für Mathematik, November 29.

170. H. Si, *On tetrahedralisations containing knotted and linked line segments*, Dalian University, School of Software and Technology, China, August 10.

171. ———, *An introduction to Delaunay-based mesh generation and adaptation*, 10th National Symposium on Geometric Design and Computing (GDC 2017), August 12–14, Shandong Business School, Yantai, China, August 12.

172. ———, *On tetrahedralisations containing knotted and linked line segments*, 26th International Meshing Roundtable and User Forum "Mesh Modeling for Simulations and Visualization", Session 4A "Tet Meshing", September 18–22, Barcelona, Spain, September 19.

173. ———, *Challenges in tetrahedral mesh generation*, PaMPA: Parallel Mesh Partitioning and Adaptation, 1st PaMPA Day Workshop, October 18, INRIA Bordeaux – Sud-Ouest, France, October 18.

174. ———, *Tetrahedral mesh improvement using moving mesh smoothing and lazy searching flips*, University Beijing, School of Mathematics and Systems Science, China, December 1.

175. R. Soares dos Santos, *Random walk on random walks*, Mathematical Probability Seminar, New York University Shanghai, China, March 21.

176. ———, *Concentration de masse dans le modèle parabolique d'Anderson*, Séminaire de Probabilités, Université de Grenoble, Institut Fourier, Laboratoire des Mathematiques, France, April 11.

177. ———, *Complete localisation in the Bouchaud–Anderson model*, Leiden University, Institute of Mathematics, Netherlands, May 9.

178. ———, *Eigenvalue order statistics of random Schrödinger operators and applications to the parabolic Anderson model*, 19th ÖMG Congress and Annual DMV Meeting, Minisymposium M6 "Spectral and Scattering Problems in Mathematical Physics", September 11–15, Austrian Mathematical Society (ÖMG) and Deutsche Mathematiker-Vereinigung (DMV), Paris-Lodron University of Salzburg, Austria, September 12.

179. V. Spokoiny, *Nonparametric estimation: Parametric view*, 6 talks, Advanced Statistical Methods, Independent University of Moscow, Russian Federation, February 7–22.

180. ———, *Adaptive nonparametric clustering*, Workshop "Statistical Recovery of Discrete, Geometric and Invariant Structures", March 19–25, Mathematisches Forschungsinstitut Oberwolfach, March 24.

181. ———, *Subset selection using the smallest accepted rule*, Structure Learning Seminar, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, April 6.

182. ———, *Gaussian approximation of the squared norm of a high dimensional vector*, Structural Learning Seminar, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, May 18.

183. ———, *Gaussian approximation for a probability of a ball*, Structural Learning Seminar, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, June 5.

184. ———, *Structural learning*, Structural Learning Seminar, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, October 25.

185. ———, *Bootstrap confidence sets for spectral projectors of sample covariance (joint with A. Naumov and V. Ulyanov)*, Séminaire de Statistique, Université de Toulouse, Institut de Mathématiques, France, November 7.

186. ———, *Adaptive nonparametric clustering*, Rencontres de Statistique Mathématique, December 18–22, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, December 18.

187. A. SUVORIKOVA, *Construction of confidence sets in 2-Wasserstein space*, Haindorf Seminar 2017, January 24–28, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, Hejnice, Czech Republic, January 26.

188. ———, *Construction of confidence sets in 2-Wasserstein space*, Machine Learning Seminar, Université Paul-Sabatier, Institut de Mathématiques de Toulouse, France, December 1.

189. K. TABELOW, *To smooth or not to smooth in fMRI*, Cognitive Neuroscience Seminar, Universitätsklinikum Hamburg-Eppendorf, Institut für Computational Neuroscience, April 4.

190. ———, *High resolution MRI by variance and bias reduction*, Channel Network Conference 2017 of the International Biometric Society (IBS), April 24–26, Hasselt University, Diepenbeek, Belgium, April 25.

191. ———, *Adaptive smoothing of multi-parameter maps*, Berlin Symposium 2017: Modern Statistical Methods From Data to Knowledge, December 14–15, organized by Indiana Laboratory of Biostatistical Analysis of Large Data with Structure (IL-BALDS), Berlin, December 14.

192. M. THOMAS, *Rate-independent delamination processes in visco-elasticity*, Miniworkshop on Dislocations, Plasticity, and Fracture, February 13–16, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, February 15.

193. ———, *Why scientist in Academia?*, I, SCIENTIST: The Conference on Gender, Career Paths and Networking, May 12–14, Freie Universität Berlin, May 14.

194. ———, *Mathematical modeling and analysis of evolution processes in solids and the influence of bulk-interface-interaction*, Humboldt-Universität zu Berlin, Institut für Mathematik, October 20.

195. W. VAN ZUIJLEN, *Mean-field Gibbs-non-Gibbs transitions*, Mark Kac Seminar, Utrecht University, Mathematical Institute, Netherlands, February 3.

196. ———, *The principal eigenvalue of the Anderson Hamiltonian in continuous space*, Berlin-Leipzig Workshop in Analysis and Stochastics, November 29 – December 1, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29.

197. A.G. VLADIMIROV, *Mathematical modeling of dispersive and diffractive multimode lasers*, 1st Sino-German Symposium on Fiber Photonics for Light Matter Interaction, September 17–21, Shanghai University, China, September 19.

198. ———, *Mathematical modelling of multimode laser dynamics*, Seminar of the Ultrafast Laser Laboratory, Institute for Quantum Optics, Leibniz University of Hannover, November 17.

199. A. WAPENHANS, *Data mobility in ad-hoc networks: Vulnerability & security*, Telecom Orange Paris, France, November 17.

200. U. Wilbrandt, *ParMooN – A parallel finite element solver, Part II*, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, India, March 16.

201. M. Wolfrum, *Synchronization transitions in systems of coupled phase oscillators*, IPB Colloquium, Institute of Physics Belgrade, Serbia, May 9.

202. ———, *Chimera states in systems of coupled phase oscillators*, Emerging Topics in Network Dynamical Systems, June 6–9, Lorentz Center, Leiden, Netherlands, June 6.

A.8.3 Talks for a More General Public

1. M. Eigel, *Revolution im dritten Anlauf: Der bemerkenswerte Siegeszug des Deep Learnings*, MathInside – Mathematik ist überall, Urania, Berlin, March 21.
2. C. Guhlke, *Lithium-Ionen-Batterien und Luftballons – Ein Fall für die Mathematik!*, MathInside – Mathematik ist überall, Urania, Berlin, March 21.
3. B. Jahnel, *Stochastische Geometrie und das Internet der Dinge*, Tag der Mathematik 2017, Humboldt-Universität zu Berlin, Institut für Mathematik, April 22.
4. W. König, *Universalität der Fluktuationen: Warum ist alles Gauß-verteilt?*, MathInside – Mathematik ist überall, Urania, Berlin, January 5.
5. C. Löbhard, *Simpson sucht die Null: Wie eine uralte Idee heute genutzt wird*, Girls' Day, WIAS Berlin, April 27.
6. S. Reichelt, *Achilles und die Schildkröte*, Girls' Day, WIAS Berlin, April 27.
7. D.R.M. Renger, *Wie man nicht-differenzierbare Funktionen differenzieren kann*, Tag der Mathematik 2017, Humboldt-Universität zu Berlin, Institut für Mathematik, April 22.
8. H. Stephan, *Denkblockaden und mathematische Paradoxa (I) und (II)*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2017, WIAS at Leibniz Association Headquarters, Berlin, June 24.

A.8.4 Posters

1. W. Dreyer, J. Fuhrmann, P. Gajewski, C. Guhlke, M. Landstorfer, M. Maurelli, R. Müller, *Stochastic model for LiFePO4-electrodes*, ModVal14 – 14th Symposium on Fuel Cell and Battery Modeling and Experimental Validation, Karlsruhe, March 2–3.
2. P. Dvurechensky, *Gradient method with inexact oracle for non convex optimization*, 3rd Applied Mathematics Symposium Münster: Shape, Imaging and Optimization, February 28 – March 3.
3. ———, *Gradient method with inexact oracle for composite non-convex optimization*, Optimization and Statistical Learning, Les Houches, France, April 10–14.
4. ———, *Gradient method with inexact oracle for composite non-convex optimization*, Foundations of Computational Mathematics (FoCM 2017), Barcelona, Spain, July 17–19.
5. ———, *A unified view on accelerated randomized optimization methods: Coordinate descent, directional search, derivative-free method*, Foundations of Computational Mathematics (FoCM 2017), Barcelona, Spain, July 17–19.
6. ———, *Faster algorithms for optimal transport*, 3. International Matheon Conference on Compressed Sensing and its Applications 2017, Berlin, December 4–8.
7. J. Fuhrmann, A. Glitzky, M. Liero, *Hybrid finite-volume/finite-element schemes for p(x)-Laplace thermistor models*, 8th International Symposium on Finite Volumes for Complex Applications (FVCA 8), Université Lille 1, Villeneuve d'Ascq, France, June 15.

8. J. FUHRMANN, A. LINKE, CH. MERDON, *Models and numerical methods for ionic mixtures with volume constraints*, 12th International Symposium on Electrokinetics, Dresden, September 10–12.

9. C. GUHLKE, *Vom Luftballon zur Lithium-Ionen-Batterie*, Lange Nacht der Wissenschaften, Technische Universität Berlin, Haus der Mathematik, June 24.

10. ———, *Modelling of ion transport in electrolytes – A thermodynamic approach*, 2nd Dresden Battery Days, Dresden, September 18–20.

11. M. HEIDA, A. MIELKE, *Effective models for interfaces with many scales*, CRC 1114 Conference "Scaling Cascades in Complex Systems 2017", Berlin, March 27–29.

12. A. FISCHER, M. LIERO, A. GLITZKY, TH. KOPRUCKI, K. VANDEWAL, S. LENK, S. REINICKE, *Predicting electrothermal behavior from lab-size OLEDs to large area lighting panels*, MRS Spring Meeting & Exhibit, Materials Research Society, Phoenix, Arizona, USA, April 17–21.

13. M. LIERO, A. GLITZKY, TH. KOPRUCKI, J. FUHRMANN, *3D electrothermal simulations of organic LEDs showing negative differential resistance*, Multiscale Modelling of Organic Semiconductors: From Elementary Processes to Devices, Grenoble, France, September 12–15.

14. N. KUMAR, J. TEN THIJE BOONKKAMP, B. KOREN, A. LINKE, *A nonlinear flux approximation scheme for the viscous Burgers equation*, 8th International Symposium on Finite Volumes for Complex Applications (FVCA 8), Université Lille 1, Villeneuve d'Ascq, France, June 12–16.

15. V. SPOKOINY, *Adaptive nonparametric clustering*, Optimization and Statistical Learning, Les Houches, France, April 10–14.

16. A. SUVORIKOVA, *Construction of non-asymptotic confidence sets in 2-Wasserstein space*, Spring School "Structural Inference" 2017, Bad Malente, March 5–10.

17. K. TABELOW, CH. D'ALONZO, J. POLZEHL, *Toward in-vivo histology of the brain*, 2nd Leibniz MMs Days 2017, Technische Informationsbibliothek, Hannover, February 22–24.

18. K. TABELOW, CH. D'ALONZO, L. RUTHOTTO, M.F. CALLAGHAN, N. WEISKOPF, J. POLZEHL, S. MOHAMMADI, *Removing the estimation bias due to the noise floor in multi-parameter maps*, The International Society for Magnetic Resonance in Medicine (ISMRM) 25th Annual Meeting & Exhibition, Honolulu, USA, April 22–27.

19. B. WAGNER, *Rheologies of dense suspensions*, Workshop "Form and Deformation in Solid and Fluid Mechanics", Isaac Newton Institute, Cambridge, UK, September 18–22.

A.9 Visits to other Institutions[5]

1. J. Sprekels, University of Pavia, Department of Mathematics, Italy, February 19–24.
2. ———, Fudan University, School of Mathematical Sciences, China, April 4–12.
3. ———, University of Pavia, Department of Mathematics, Italy, November 12–16.
4. N. Ahmed, Technische Universität Dresden, Institut für Numerische Mathematik, March 6–9.
5. N. Alia, University of Oulu Graduate School, Finland, January 1–31.
6. ———, SSAB, Raahe, Finland, February 1 – December 31.
7. L. Andreis, Università degli Studi di Padova, Dipartimento di Matematica Pura ed Applicata, Padua, Italy, November 15–20.
8. M.J. Arenas Jaén, University of Oulu, Faculty of Technology, Finland, November 4, 2016 – January 31, 2017.
9. ———, EFD Induction AS, Skien, Norway, August 15 – September 12.
10. C. Bartsch, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, India, March 7–16.
11. Ch. Bayer, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering Division, Thuwal, Saudi Arabia, May 21 – June 1.
12. ———, Rheinisch-Westfälische Technische Hochschule Aachen, Aachen Institute for Advanced Study in Computational Engineering Science (AICES), July 31 – August 5.
13. ———, King Abdullah University of Science and Technology (KAUST), Computer, Electrical and Mathematical Sciences & Engineering Division, Thuwal, Saudi Arabia, October 24–30.
14. ———, December 11–17.
15. L. Blank, Université de Franche-Comté, Laboratoire de Mathématiques de Besançon, France, January 23–27.
16. C. Brée, Universitat Politecnica de Catalunya, Terrassa, Spain, July 10–14.
17. N. Buzun, Moscow Institute of Physics and Technology, Department of Applied Mathematics and Control, Dolgoprudny, Moscow Region, Russian Federation, May 12–31.
18. L. Capone, University of Oulu, Faculty of Technology, Finland, November 7, 2016 – January 31, 2017.
19. ———, EFD Induction AS, Skien, Norway, July 10–13.
20. P.-É. Druet, Czech Academy of Sciences, Institute of Mathematics, Department of Evolution Differential Equations (EDE), Prague, January 9–13.
21. P. Dvurechensky, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, July 28 – August 15.
22. ———, October 30 – November 10.
23. M. Eigel, Institut National de Recherche en Informatique et en Automatique (INRIA), Team SERENA, Paris, France, May 29 – June 2.
24. S. Eydam, University of Belgrade, Institute of Physics Belgrade, Serbia, September 4 – October 2.
25. A. González Casanova Soberón, University of Oxford, Mathematical Institute, UK, January 16–26.
26. ———, Johann Wolfgang Goethe-Universität Frankfurt, Institut für Mathematik, March 19–24.

[5] Only stays of more than three days are listed.

27. R. Henrion, Université de Bourgogne, Département de Mathématiques, Dijon, France, October 17–27.
28. M. Hintermüller, Hong Kong Polytechnic University, Department of Applied Mathematics, China, May 27 – June 2.
29. ———, Chinese Academy of Sciences, State Key Laboratory of Scientific and Engineering Computing, Beijing, China, June 3–9.
30. ———, Isaac Newton Institute, organization of Trimester Program "Variational Methods and Effective Algorithms for Imaging and Vision", Cambridge, UK, August 28–31.
31. ———, September 4–8.
32. ———, September 13–18.
33. ———, September 26 – October 1.
34. ———, October 14–17.
35. ———, October 25–28.
36. ———, October 30 – November 5.
37. ———, November 6–9.
38. ———, December 3–11.
39. D. Hömberg, Fudan University, School of Mathematical Sciences, Shanghai, China, March 6–10.
40. ———, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, March 20–29.
41. ———, October 20 – November 10.
42. B. Jahnel, Ludwig-Maximilians-Universität München, Fakultät für Mathematik, Informatik und Statistik, May 31 – June 6.
43. ———, August 4–16.
44. V. John, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, India, March 7–16.
45. ———, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, April 2–7.
46. ———, Beijing Computational Science Research Center, Applied and Computational Mathematics, China, May 9–19.
47. W. König, University of California, Los Angeles, Department of Mathematics, USA, January 14–27.
48. Th. Koprucki, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, Erlangen, January 16–19.
49. ———, May 15–18.
50. M. Landstorfer, Tel Aviv University, School of Physics and Astronomy, Israel, June 20–26.
51. M. Liero, Universität Dortmund, Institut für Mathematik, November 28 – December 1.
52. P. Mathé, Technische Universität Chemnitz, Fakultät für Mathematik, September 25–29.
53. ———, Fudan University, School of Mathematical Sciences, China, November 14 – December 6.
54. M. Maurelli, Université de Nice Sophia-Antipolis, Laboratoire Jean Alexandre Dieudonné, France, September 25 – October 6.
55. ———, Università di Pisa, Dipartimento di Matematica, Italy, December 17–20.
56. A. Mielke, University of Pavia, Department of Mathematics, Italy, March 20–24.

57. ———, University College Cork, School of Mathematical Science, Ireland, September 6–15.
58. Ch. Mukherjee, Courant Institute of Mathematical Sciences, Department of Mathematics, New York, USA, March 14–23.
59. O. Omel'chenko, University of Belgrade, Institute of Physics, Serbia, May 2–6.
60. ———, University of California at Berkeley, Department of Physics, USA, May 15–19.
61. K. Papafitsoros, Isaac Newton Institute, Trimester Program "Variational Methods and Effective Algorithms for Imaging and Vision", Cambridge, UK, October 7 – November 14.
62. D. Peschka, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, December 4–8.
63. P. Pigato, École Polytechnique, Centre de Mathématiques Appliquées, Palaiseau, France, July 10–14.
64. ———, Università degli Studi di Padova, Dipartimento di Matematica Pura ed Applicata, Italy, September 24–30.
65. J. Polzehl, University of Minnesota, School of Statistics (IRSA), Minneapolis, USA, April 24 – May 17.
66. ———, University of Cambridge, Isaac Newton Institute, UK, October 23 – November 10.
67. ———, November 27 – December 13.
68. M. Radziunas, Monocrom S.L., Barcelona, Spain, November 5–8.
69. M. Redmann, University of Bath, Department of Mathematical Sciences, UK, November 6–10.
70. J. Rehberg, Technische Universität Darmstadt, Fachbereich Mathematik, November 7–11.
71. D.R.M. Renger, University of Bath, Department of Mathematical Sciences, UK, April 24 – May 1.
72. ———, Universität Regensburg, Fakultät für Mathematik, July 27 – August 7.
73. H. Si, Beihang University, School of Mathematics and Systems Science, Beijing, China, January 2–13.
74. ———, Beijing Computational Science Research Center, China, July 24 – August 6.
75. ———, Dalian University, School of Software and Technology, China, August 7–18.
76. ———, Beijing Computational Science Research Center, China, November 27 – December 8.
77. R. Soares dos Santos, University College London, Department of Mathematics, UK, June 12–18.
78. ———, Université Claude Bernard Lyon 1, Institut Camille Jordan, France, February 1–6.
79. ———, New York University Shanghai, Institute of Mathematical Sciences, China, March 12 – April 2.
80. ———, Leiden University, Institute of Mathematics, Netherlands, October 8–11.
81. V. Spokoiny, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, February 1–9.
82. ———, February 12–25.
83. ———, April 3–7.
84. ———, May 16–20.
85. ———, June 5–10.
86. ———, October 23–27.
87. ———, November 25 – December 2.
88. A. Suvorikova, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, Moscow, April 3 – June 14.

89. ———, Université Paul-Sabatier, Institut de Mathématiques de Toulouse, France, November 13 – December 8.
90. ———, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, Moscow, December 18, 2017 – January 5, 2018.
91. K. Tabelow, University of Cambridge, Isaac Newton Institute, UK, October 30 – November 3.
92. M. Thomas, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, February 16–23.
93. ———, Università di Brescia, Dipartimento di Matematica, Italy, February 28 – March 3.
94. ———, University of Pavia, Department of Mathematics, Italy, May 21–24.
95. ———, Erwin Schrödinger Center, Vienna, Austria, June 10–13.
96. W. van Zuijlen, Delft University of Technology, Faculty Electrical Engineering, Mathematics and Computer Science, Netherlands, May 3–8.
97. ———, Leiden University, Institute of Mathematics, Netherlands, October 18–23.
98. U. Wilbrandt, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, March 7–16.

A.10 Academic Teaching[6]

Winter Semester 2016/2017

1. L. Recke, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. M. Eigel, *Tensor Product Approximation in Uncertainty Quantification* (lecture), Technische Universität Berlin, 2 SWS.
3. P. Friz, *Rough Paths and Regularity Structures* (lecture), Technische Universität Berlin, 2 SWS.
4. D. Becherer, J. Blath, P. Friz, W. König, et al., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin/Technische Universität Berlin/WIAS Berlin, 2 SWS.
5. J. Fuhrmann, *Wissenschaftliches Rechnen (Scientific Computing)* (lecture), Technische Universität Berlin, 4 SWS.
6. A. Glitzky, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
7. M. Hintermüller, *Nichtlineare Optimierung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
8. M. Hintermüller, C. Schillings, *Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
9. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
10. V. John, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
11. J. Blath, W. König, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
12. M. Maurelli, *Numerische Mathematik II für Ingenieure* (practice), Technische Universität Berlin, 2 SWS.
13. A. Mielke, *Analysis I** (lecture), Humboldt-Universität zu Berlin, 5 SWS.
14. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
15. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
16. H. Stephan, *Funktionalanalytische Methoden in der klassischen Physik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. ———, *Funktionalanalytische Methoden in der klassischen Physik* (practice), Humboldt-Universität zu Berlin, 1 SWS.
18. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
19. M. Thomas, *Evolutionary Gamma-Convergence in Continuum Mechanics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. M. Wolfrum, B. Fiedler, P. Gurevich, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

[6] SWS = semester periods per week

Summer Semester 2017

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. A. Caiazzo, *Analysis 1* (lecture), Freie Universität Berlin, 4 SWS.
3. ———, *Analysis 1* (practice), Freie Universität Berlin, 2 SWS.
4. P. Farrell, *Numerical Mathematics II* (lecture), Technische Universität Hamburg-Harburg, 4 SWS.
5. ———, *Numerical Solution of ODEs* (lecture), Technische Universität Hamburg-Harburg, 4 SWS.
6. P. Friz, *Rough Analysis and Quantitative Finance* (seminar), Technische Universität Berlin, 2 SWS.
7. D. Becherer, J. Blath, P. Friz, W. König, et al., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin/Technische Universität Berlin/WIAS Berlin, 2 SWS.
8. A. Glitzky, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
9. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. ———, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
11. M. Hintermüller, *Theorie und Verfahren der nichtglatten Optimierung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
12. ———, *Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
13. D. Hömberg, *Variationsrechnung und optimale Steuerung gewöhnlicher Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS.
14. V. John, *Numerik III* (lecture), Freie Universität Berlin, 4 SWS.
15. J. Blath, W. König, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
16. M. Maurelli, *Maß- und Integrationstheorie* (practice), Technische Universität Berlin, 2 SWS.
17. A. Mielke, *Analysis II** (lecture), Humboldt-Universität zu Berlin, 4 SWS.
18. V. Spokoiny, *Mathematische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
19. ———, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
20. ———, *Mathematische Statistik* (practice), Humboldt-Universität zu Berlin, 2 SWS.
21. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
22. H. Stephan, *Funktionalanalytische Methoden in der klassischen Physik II* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
23. ———, *Funktionalanalytische Methoden in der klassischen Physik II* (practice), Humboldt-Universität zu Berlin, 1 SWS.
24. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
25. M. Thomas, *Partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

26. M. Wolfrum, B. Fiedler, P. Gurevich, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

Winter Semester 2017/2018

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. P. Farrell, *Numerical Mathematics I* (lecture), Technische Universität Hamburg-Harburg, 4 SWS.
3. ———, *Numerical Solution of PDEs* (lecture), Technische Universität Hamburg-Harburg, 4 SWS.
4. P. Friz, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
5. ———, *Rough Analysis and Quantitative Finance* (seminar), Technische Universität Berlin, 2 SWS.
6. D. Becherer, J. Blath, P. Friz, W. König, et al., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin/Technische Universität Berlin/WIAS Berlin, 2 SWS.
7. J. Fuhrmann, *Wissenschaftliches Rechnen* (lecture), Technische Universität Berlin, 4 SWS.
8. A. Glitzky, *Einführung in die Kontrolltheorie und optimale Steuerung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
9. ———, *Einführung in die Kontrolltheorie und optimale Steuerung* (practice), Humboldt-Universität zu Berlin, 1 SWS.
10. A. Glitzky, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
11. M. Hintermüller, A. Kröner, *Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
12. D. Hömberg, *Optimization II – PDE-Constrained Optimal Control (13 two-hour lectures from Oct. 23 to Nov. 10, 2017)* (lecture), Norwegian University of Science and Technology, Trondheim, – SWS.
13. B. Jahnel, *Analysis I und Lineare Algebra für Ingenieurwissenschaften* (lecture), Technische Universität Berlin, 4 SWS.
14. V. John, *Numerik IV: Finite-Elemente-Methoden II (Strömungsmechanik)* (lecture), Freie Universität Berlin, 2 SWS.
15. ———, *Numerik IV: Finite-Elemente-Methoden II (Strömungsmechanik)* (practice), Freie Universität Berlin, 2 SWS.
16. O. Klein, *Mathematische Modellierung von Hystereseeffekten* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. ———, *Mathematische Modellierung von Hystereseeffekten* (practice), Humboldt-Universität zu Berlin, 1 SWS.
18. W. König, *Analysis I für Mathematiker* (lecture), Technische Universität Berlin, 4 SWS.
19. J. Blath, W. König, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
20. M. Liero, *Optimaler Transport und Wasserstein-Gradientenflüsse* (lecture), Humboldt-Universität zu Berlin, 2 SWS.

21. ———, *Optimaler Transport und Wasserstein-Gradientenflüsse* (practice), Humboldt-Universität zu Berlin, 1 SWS.

22. O. Marquardt, *Mathematisch-physikalische Grundlagen, Screen Based Media (BA)* (lecture), Beuth Hochschule für Technik Berlin, 2 SWS.

23. ———, *Brückenkurs Physik für Elektrotechnik und Mechatronik (10 two-hour lectures from Sept. 25 to 29, 2017)* (seminar), Beuth Hochschule für Technik Berlin, – SWS.

24. M. Maurelli, *Fortgeschrittene Themen der Stochastik – Regularization by Noise* (lecture), Technische Universität Berlin, 2 SWS.

25. Ch. Merdon, *Numerik partieller Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

26. A. Mielke, *Analysis III* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

27. J.G.M. Schoenmakers, *Stochastische Finanzmathematik I* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

28. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.

29. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.

30. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.

31. M. Thomas, *Nichtlineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

32. ———, *Nichtlineare partielle Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.

33. B. Wagner, *Asymptotische Analysis* (lecture), Technische Universität Berlin, 4 SWS.

34. M. Wolfrum, B. Fiedler, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

A.11 Visiting Scientists[7]

A.11.1 Guests

1. L. Adam, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – May 31.
2. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, June 5–9.
3. L. Adamyan, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, Berlin, January 1 – December 31.
4. R. Adar, Tel Aviv University, School of Physics and Astronomy, Israel, January 24–28.
5. I. Bačić, University of Belgrade, Institute of Physics Belgrade, Scientific Computing Laboratory, Serbia, November 3–30.
6. Ch. Ben Hammouda, King Abdullah University of Science and Technology (KAUST), Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, July 10–14.
7. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, October 27 – November 2.
8. Ch. Bick, University of Exeter, Department of Mathematics, UK, January 8–11.
9. A. Boitsev, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, St. Petersburg, Russian Federation, November 13–17.
10. E. Bolthausen, Universität Zürich, Institut für Mathematik, Switzerland, March 5–9.
11. R.I. Bot, Universität Wien, Fakultät für Mathematik, Austria, October 11–14.
12. M. Brokate, Technische Universität München, Zentrum Mathematik, Garching, October 11–14.
13. E.A. Carlen, Rutgers University, Department of Mathematics, Piscataway, USA, November 21–26.
14. A. Carpentier, Universität Potsdam, Institut für Mathematik, January 1 – December 31.
15. D. Chapelle, Inria Saclay – Ile de France, Mathematical and Mechanical Modeling with Data Interaction in Simulations for Medicine, Palaiseau, France, September 15–18.
16. J. Chen, Zheijian University, Center for Engineering & Scientific Computation, Hangzhou, China, April 8–13.
17. D. Chetverikov, University of California at Los Angeles (UCLA), Department of Economics, USA, June 20–24.
18. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, September 17–29.
19. ———, December 4–8.
20. P. Colli, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, February 26 – March 3.
21. P. Das, EFD Induction AS, Skien, Norway, March 5–21.
22. ———, May 2 – July 31.
23. ———, November 6, 2017 – January 31, 2018.
24. F. Dassi, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, January 21–31.

[7] Only stays of more than three days are listed.

25. E. Davoli, University of Vienna, Faculty of Mathematics, Austria, May 9–12.
26. P.-O. Dehaye, Universität Zürich, Institut für Mathematik, Switzerland, March 17–25.
27. F. den Hollander, Leiden University, Mathematical Institute, Netherlands, April 19–22.
28. G. Dong, Humboldt-Universität zu Berlin, Institut für Mathematik, September 1, 2017 – December 31, 2018.
29. A. Drewitz, Universität zu Köln, Mathematisches Institut, July 31 – August 3.
30. K. Efimov, Humboldt-Universität zu Berlin, Institut für Mathematik, October 1 – December 31.
31. I. Franovic, University of Belgrade, Institute of Physics Belgrade, Serbia, June 19 – July 2.
32. ———, November 3–30.
33. M. Freitag, University of Bath, Department of Mathematical Sciences, UK, April 10–21.
34. V. Garanzha, Russian Academy of Sciences, Federal Research Center of Computer Science and Control, Moscow, September 13–16.
35. N. Goerigk, Elektronische Fahrwerksysteme GmbH, Gaimersheim, February 6–10.
36. V. Guigues, Fundação Getúlio Vargas (FGV), School of Applied Mathematics, Rio de Janeiro, Brazil, February 5–9.
37. S. Hajian, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – December 31.
38. H. Hardering, Technische Universität Dresden, Institut für Numerische Mathematik, January 17–20.
39. L. Heltai, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, February 1 – April 30.
40. Ch. Hirsch, Ludwig-Maximilians-Universität München, Mathematisches Institut, July 23–28.
41. ———, October 9–12.
42. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, March 27–31.
43. J. Holley, Robert Bosch GmbH, April 1, 2017 – March 31, 2020.
44. K. Ito, North Carolina State University, Department of Mathematics, Raleigh, USA, May 1–13.
45. D. Ivanov, EFD Induction AS, Skien, Norway, May 7–12.
46. T. Keil, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – May 31.
47. G. Kitavtsev, University of Bristol, School of Mathematics, UK, May 20–23.
48. Y. Klochkov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, January 1 – December 31.
49. E. Knobloch, University of California, Department of Physics, Berkeley, USA, March 31 – April 5.
50. M. Kohlhase, Friedrich-Alexander-Universität Erlangen-Nürnberg, Informatik, Wissensrepräsentation und -verarbeitung, Erlangen, March 20–24.
51. M. Kraft, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, July 17 – August 14.
52. C. Kreisbeck, Universiteit Utrecht, Mathematical Institute, Netherlands, May 29 – June 2.
53. A. Kröner, Humboldt-Universität zu Berlin, Institut für Mathematik / CMAP, Ecole Polytechnique, Paris-Saclay, May 4 – September 30.

54. A. Kroshnin, Russian Academy of Sciences, Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, May 1–7.

55. Ch. Külske, Ruhr-Universität Bochum, Fakultät für Mathematik, May 23–26.

56. N.Z. Larbi Youcef, Università di Torino, Dipartimento di Matematica, Italy, December 11–15.

57. N. Lei, Dalian University of Technology, School of Software and Technology, China, September 13–17.

58. C. MacNamara, University of St Andrews, School of Mathematics & Statistics, UK, August 6–9.

59. B. Matejczyk, University of Warwick, Mathematics Institute, Coventry, UK, December 11–16.

60. St. Melchionna, University of Vienna, Faculty of Mathematics, Austria, March 1–8.

61. P. Mörters, Universität zu Köln, Mathematisch-Naturwissenschaftliche Fakultät, August 28 – September 1.

62. Ch. Mukherjee, Universität Münster, Fachbereich Mathematik und Informatik, April 1 – May 31.

63. D. Müller, Friedrich-Alexander-Universität Erlangen-Nürnberg, Informatik, Wissensrepräsentation und -verarbeitung, Erlangen, March 20–24.

64. ———, November 5–8.

65. L.O. Müller, Norwegian University of Science and Technology, Department of Structural Engineering, Trondheim, February 28 – March 3.

66. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, November 15–20.

67. J. Mura, Pontificia Universidad Católica de Chile, Centro de Imágenes Biomédicas, Santiago, January 31 – February 3.

68. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica (DMI), Italy, July 30 – August 11.

69. A. Naumov, Skolkovo Institute of Science and Technology (Skoltech), Center for Computational Data-Intensive Science and Engineering (CDISE), Moscow, Russian Federation, January 15–21.

70. ———, June 27 – July 2.

71. P. Nelson, Johannes Gutenberg-Universität, Institut für Mathematik, Mainz, June 5–9.

72. D. Nolte, Universidad de Chile, Center for Mathematical Modeling, Santiago, July 24 – August 23.

73. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, November 6–10.

74. Ch. Onyi, Nnamdi Azikiwe University Awka, Department of Mathematics, Awka, Nigeria, September 26 – December 31.

75. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, October 11–14.

76. M. Patriarca, University of Rome Tor Vergata, Electronic Engineering Department, Italy, August 15 – November 15.

77. T.d.P. Peixoto, University of Bath, Department of Mathematical Sciences, UK, August 25 – September 1.

78. G. Pitton, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, February 1 – March 31.

79. W. Polonik, University of California at Davis, Department of Statistics, USA, June 20 – July 15.

80. I.Y. Popov, St. Petersburg National Research University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russian Federation, January 30 – February 3.

81. F. Rabe, Jacobs University, Computer Science, Bremen, March 21–24.
82. C. Rautenberg, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – November 30.
83. L. Rebholz, Clemson University, Department of Mathematical Sciences, USA, October 15–21.
84. Y. Ren, Dalian University of Technology, School of Software Technology, China, August 31 – September 30.
85. E. Rocca, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 2–5.
86. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, May 14–19.
87. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, October 8 – November 8.
88. B. Schweizer, Technische Universität Dortmund, Fakultät für Mathematik, October 4–7.
89. O. Sekulovic, Crnogorski Telecom, Podgorica, Montenegro, October 8–15.
90. J. Sieber, University of Exeter, College of Engineering, Mathematics and Physical Sciences, UK, October 4–20.
91. D. Silvester, University of Manchester, Faculty of Science and Engineering, UK, April 3–7.
92. S. Simonella, Technische Universität München, Zentrum Mathematik, November 20–23.
93. A. Sobolevskiy, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, May 5–10.
94. Y. Sun, Humboldt-Universität zu Berlin, Institut für Mathematik, October 18, 2017 – September 30, 2018.
95. J. ten Thije Boonkkamp, Eindhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, March 27 – April 2.
96. I. Thompson, University of Bath, Department of Physics, UK, April 24–28.
97. R. Toader, University of Udine, DIMI, Italy, July 9–15.
98. A. Torcini, Université de Cergy–Pontoise, Laboratoire de Physique Théorique et Modélisation, France, February 10–19.
99. D. Turaev, Imperial College London, Department of Mathematics, UK, April 5–13.
100. V. Ulyanov, Lomonosov Moscow State University, Department of Mathematical Statistics, Probability Theory, Statistics, Russian Federation, January 15–21.
101. C. Visone, Università degli Studi del Sannio, Dipartimento di Ingegneria, Benevento, Italy, May 28–31.
102. J. Weed, Massachusetts Institute of Technology, Department of Mathematics, Cambridge, USA, April 25–28.
103. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, January 27 – February 1.
104. ———, April 20–30.
105. N. Zhivotovskiy, Skolkovo Institute of Science and Technology, Skoltech Center for Computational Data-Intensive Science and Engineering (CDISE), Moscow, Russian Federation, April 23–26.

A.11.2 Scholarship Holders

1. S. Aflatounian, K. N. Toosi University of Technology, Faculty of Electrical Engineering, Tehran, Iran, DAAD-IAESTE Fellowship (International Association for the Exchange of Students for Technical Experience), December 1, 2017 – January 31, 2018.

2. J.A. Brüggemann, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School, January 1 – October 31.
3. A. Fiebach, Berlin, EXIST Business Start-up Grant, Federal Ministry for Economic Affairs and Energy, June 1, 2017 – April 30, 2018.
4. K. Gärtner, Berlin, EXIST Business Start-up Grant, Federal Ministry for Economic Affairs and Energy, May 1, 2017 – April 30, 2018.
5. A. Jha, Freie Universität Berlin, Institut für Mathematik, New Delhi, India, Berlin Mathematical School, October 1, 2017 – December 31, 2018.
6. L. Kamenski, Berlin, EXIST Business Start-up Grant, Federal Ministry for Economic Affairs and Energy, May 1, 2017 – April 30, 2018.
7. T. Keil, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School, January 1 – May 15.
8. Ch. Onyi, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School, October 1 – December 31.
9. K. Papafitsoros, University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK, Humboldt Research Fellowship, April 1, 2016 – August 31, 2017.
10. H. Sun, Renmin University of China, Institute for Mathematical Sciences, Beijing, Humboldt Research Fellowship, February 1, 2017 – January 31, 2018.
11. A. Tobiás, Technische Universität Berlin, Institut für Mathematik, Berlin Mathematical School, January 1 – December 31.
12. P. Vagner, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, Erasmus+ Traineeship, February 1, 2017 – February 28, 2018.

A.11.3 External Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. L. Adamyan, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – December 31.
2. J.A. Brüggemann, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, Berlin Mathematical School, doctoral candidate, January 1 – October 31.
3. P. Das, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. D. Hömberg, European Industrial Doctorate project MIMESIS, doctoral candidate, January 1 – December 31.
4. K. Efimov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – September 1.
5. T. González Grandón, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. R. Henrion, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
6. J. Holley, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, Robert Bosch GmbH, doctoral candidate, April 1 – December 31.
7. A. Jha, Freie Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. V. John, Berlin Mathematical School, doctoral candidate, October 1 – December 31.
8. T. Keil, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, Berlin Mathematical School, doctoral candidate, January 1 – May 31.

9. E. Klochkov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 “High Dimensional Non Stationary Time Series Analysis”, doctoral candidate, January 1 – December 31.
10. Ch. Onyi, Humboldt-Universität zu Berlin, Mathematisch-Natutwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, Berlin Mathematical School, doctoral candidate, October 1 – December 31.
11. M. Patriarca, University of Rome “Tor Vergata”, supervisors: Dr. P. Farrell, Dr. J. Fuhrmann, doctoral candidate, August 15 – November 15.
12. Y. Reichelt, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. D. Hömberg, Berlin Mathematical School, doctoral candidate, February 1 – July 31.
13. S. Rösel, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, doctoral candidate, January 1 – February 7.
14. A. Stephan, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, Institut für Mathematik, supervisor: Prof. Dr. A. Mielke, Berlin Mathematical School, doctoral candidate, April 1 – December 31.
15. Y. Sun, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
16. A. Tobiás, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. W. König, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
17. A. Zeghuzi, Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, supervisor: Dr. M. Radziunas, BMBF program EffiLAS: PLUS project, doctoral candidate, January 1 – December 31.

A.12 Guest Talks

1. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, *Large deviations and concentration of scaling limits for weakly pinned integrated random walks*, June 7.
2. A. Ali, Universität Hamburg, Fachbereich Mathematik, *Global minima for semilinear optimal control problems*, May 9.
3. E. Arevalo, Pontificia Universidad Católica de Chile, Instituto de Física, Santiago, *Solitary waves in the nonlinear Schrödinger equation with complex potentials*, February 16.
4. B. Azmi, Karl-Franzens-Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, *On the stabilizability of infinite dimensional systems via receding horizon control*, May 5.
5. F. Baccelli, University of Texas at Austin, Department of Mathematics, USA, *Stochastic geometry and queuing in wireless networks*, July 10.
6. A.M. Badlyan, Technische Universität Berlin, Institut für Mathematik, *On the port-Hamiltonian structure of the Navier–Stokes equations for reactive flows*, January 26.
7. Ch. Ben Hammouda, King Abdullah University of Science and Technology (KAUST), Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, *Multilevel hybrid split-step implicit tau-leap*, July 11.
8. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, USA, *Hierarchy of PDE models of cell motility*, October 30.
9. Ch. Bick, University of Exeter, Department of Mathematics, UK, *From weak chimeras to switching dynamics of localized frequency synchronization patterns*, January 10.
10. R. Blossey, Université de Lille 1 & CNRS, Unité de Glycobiologie Structurale et Fonctionnelle (UGSF) CNRS UMR 8576, Villeneuve d'Ascq, France, *Beyond Poisson–Boltzmann: Charge correlation effects in DNA adsorption and transport through nanopores*, May 22.
11. A. Boitsev, St. Petersburg National University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russian Federation, *Boundary triplets, tensor products and point contacts to reservoirs*, November 15.
12. A. Bovier, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, *Adaptive dynamics, diploid models, and the escape from selection*, July 19.
13. E. Burnaev, Skolkovo Institute of Science and Technology, Center for Computational and Data-Intensive Science and Engineering, Moscow Region, Russian Federation, *Minimax approach to variable fidelity data interpolation*, March 28.
14. C. Butucea, Université Paris-Est Marne-la-Vallée, Laboratoire d'Analyse et de Mathématiques Appliquées, France, *Local asymptotic equivalence for quantum models*, May 3.
15. A. Ceretani, Humboldt-Universität zu Berlin, Institut für Mathematik, *Anomalous diffusion with free boundaries*, November 27.
16. D. Chae, Chung-Ang University, Seoul, Korea (Republic of), *On the blow-up problem for the incompressible Euler equation*, August 9.
17. D. Chapelle, Inria Saclay – Ile de France, Mathematical and Mechanical Modeling with Data Interaction in Simulations for Medicine, Palaiseau, France, *Biomechanical modeling of the heart, and cardiovascular system — From sarcomeres to organ/system, with experimental assessments and patient-specific clinical validations*, September 18.
18. E. Charkaluk, Ecole Polytechnique, Laboratoire de Mécanique des Solides (LMS) – UMR 7649, Palaiseau, France, *Fatigue of metallic additive manufactured structures: What can we learn from other manufacturing processes?*, November 21.

19. J. Chen, Zheijian University, Center for Engineering & Scientific Computation, Hangzhou, China, *Automatic and parallel mesh generation: Recent advances*, April 11.
20. D. Chetverikov, University of California at Los Angeles (UCLA), Department of Economics, USA, *On cross-validated lasso*, June 21.
21. M. Cicuttin, Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique, l'École des Ponts ParisTech, Marne-la-Vallée, France, *Implementation of discontinuous skeletal methods on arbitrary-dimensional, polytopal meshes using generic programming*, March 16.
22. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, *Numerical simulation of nonlocal delayed feedback controller for some new smart bioreactors*, December 5.
23. Ch. Clason, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, *Convex relaxation of hybrid discrete-continuous control problems*, March 29.
24. P. Colli, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, *About a non-smooth regularization of a forward-backward parabolic equation*, March 1.
25. F. Compte, Université Paris Descartes, UFR de Mathématiques et Informatique, Paris, France, *Laguerre basis for inverse problems related to nonnegative random variables*, February 1.
26. M. Cuturi, École Nationale de la Statistique et de l'Administration Économique, Centre de Recherche en Économie et Statistique, Malakoff, France, *A review of regularized optimal transport and applications to Wasserstein barycenters*, May 10.
27. F. Dassi, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, *The virtual element method in three dimensions*, January 26.
28. M. Demuth, Technische Universität Clausthal, Institut für Mathematik, *On eigenvalues of non-selfadjoint operators: A comparison of two approaches*, March 29.
29. F. den Hollander, Leiden University, Mathematical Institute, Netherlands, *Random walks on dynamic random graphs*, April 19.
30. G. Dong, Humboldt-Universität zu Berlin, Institut für Mathematik, *Regularization methods and nonlinear PDEs for solving inverse and imaging problems*, December 21.
31. A. Drewitz, Universität zu Köln, Mathematisches Institut, *The maximal particle of branching RW in random branching environment*, August 2.
32. M. Eikerling, Simon Fraser University, Department of Chemistry, Burnaby, Canada, *Theory and modeling of materials for electrochemical energy systems*, February 9.
33. J.C. Escanciano, Indiana University Bloomington, Department of Economics, USA, *Quantile-regression inference with adaptive control of size*, May 31.
34. I. Franovic, University of Belgrade, Institute of Physics Belgrade, Serbia, *Bistability, rate oscillations and slow rate fluctuations in networks of noisy neurons with coupling delay*, June 27.
35. M. Fromont-Renoir, Université Rennes 2, Équipe de Statistique de l'IRMAR, France, *Family-wise separation rates for multiple testing*, January 25.
36. S. Ganesan, Indian Institute of Science, Department of Computational and Data Sciences, Bangalore, *Stabilized three-field formulation of viscoelastic fluid flows*, June 1.
37. V. Garanzha, Russian Academy of Sciences, Federal Research Center of Computer Science and Control, Moscow, *Construction of quasi-isometric elastic deformations in mesh generation problems*, September 14.
38. A. Gassmann, Leibniz-Institut für Atmosphärenphysik e.V. an der Universität Rostock, Abteilung Theorie und Modellierung, Kühlungsborn, *Fluid dynamics on icosahedral staggered grids*, January 12.

39. J.-F. Gerbeau, Centre de Recherche INRIA de Paris, France, *Numerical methods for variability modeling and biomarkers design*, November 20.
40. D. Ghoshdastidar, Universität Tübingen, Fachbereich Informatik, *Two-sample hypothesis testing for inhomogeneous random graphs*, October 25.
41. I. Goldsheid, Queen Mary University of London, School of Mathematical Sciences, UK, *Invariant measure for random walks on random environments*, July 5.
42. C. Gräser, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Solving nonsmooth PDEs in Dune*, May 30.
43. V. Guigues, Fundação Getúlio Vargas (FGV), School of Applied Mathematics, Rio de Janeiro, Brazil, *Hypothesis testing and change point detection on controls of stochastic dynamical systems with independent state and observation noises belonging to spherical families*, February 7.
44. P. Gurevich, Freie Universität Berlin, Institut für Mathematik, *A short introduction to machine learning: Towards (un)certainty quantification*, May 23.
45. ———, *Rattling in hysteretic reaction-diffusion systems*, November 29.
46. L. Györfi, Budapest University of Technology and Economics, Department of Computer Science and Information Theory, Hungary, *The role of machine learning in the nonparametric prediction of time series*, February 15.
47. A. Hänel, Leibniz Universität Hannover, Institut für Analysis, *Spectral asymptotics for mixed problems and for crack problems on infinite cylinders*, February 1.
48. M. Hanss, Universität Stuttgart, Institut für Technische und Numerische Mechanik, *Fuzzy arithmetic and probability theory in uncertainty analysis – Unity in diversity*, June 26.
49. H. Hardering, Technische Universität Dresden, Institut für Numerische Mathematik, *Gradient flows in Riemannian manifolds space discretization by geodesic finite elements*, January 18.
50. S.W. Haugland, Technische Universität München, Physik-Department, Garching, *What can we learn about chimera states from minimal cluster dynamics?*, April 27.
51. S. Heidenreich, Physikalisch-Technische Bundesanstalt, Modellierung und Simulation, Berlin, *Uncertainty quantification for nanometrology*, January 10.
52. L. Heltai, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, *Immersed Finite Element Methods for interface and fluid structure interaction problems: An overview and some recent results*, March 28.
53. ———, *A numerical framework for optimal locomotion at low Reynolds numbers*, April 11.
54. T. Hulshof, University of Technology, Department of Mathematics and Computer Sciences, Eindhoven, Netherlands, *Higher order corrections for anisotropic bootstrap percolation*, February 23.
55. K. Ito, North Carolina State University, Department of Mathematics, Raleigh, USA, *Value function calculus and applications*, May 9.
56. C. Kirch, Universität Magdeburg, Fakultät für Mathematik, *Frequency domain likelihood approximations for time series bootstrapping and Bayesian nonparametrics*, May 24.
57. E. Knobloch, University of California, Department of Physics, Berkeley, USA, *Geostrophic turbulence and the formation of large scale structure*, April 4.
58. M. Kraft, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, *Moment projection method for solving population balance equations*, August 2.
59. A. Kröner, Humboldt-Universität zu Berlin, Institut für Mathematik / CMAP, Ecole Polytechnique, Paris-Saclay, *Optimal control of infinite dimensional systems*, May 4.

60. A. Kroshnin, Russian Academy of Sciences, Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, *Fréchet barycenters in the Monge–Kantorovich spaces*, May 2.
61. Ch. Kühn, Technische Universität München, Fakultät Mathematik, Garching, *Regularity structures and fractional diffusion*, April 19.
62. Ch. Külske, Ruhr-Universität Bochum, Fakultät für Mathematik, *Continuous spin models on annealed random graphs: Modifying the modified mean-field exponents*, May 24.
63. A. Kyprianou, University of Bath, Department of Mathematical Sciences, UK, *Applied probability and real-world impact*, June 23.
64. K.F. Lam, Universität Regensburg, Fakultät für Mathematik, *Diffuse interface models of tumor growth and optimizing cancer treatment times*, January 10.
65. N.Z. Larbi Youcef, Università di Torino, Dipartimento di Matematica, Italy, *Probabilistic models for large telecommunication systems*, December 13.
66. R. Lasarzik, Technische Universität Berlin, Institut für Mathematik, *Generalised solutions to the Ericksen–Leslie model describing liquid crystal flow*, November 8.
67. O. Lass, Technische Universität Darmstadt, Fachbereich Mathematik, *Nonlinear robust optimization and model order reduction with application to electric motor design*, May 9.
68. K.J.H. Law, Oak Ridge National Laboratory, Computer Science and Mathematics Division, and University of Tennessee, Mathematics Department, Knoxville, TN, USA, *Multilevel Monte Carlo for Bayesian inference*, July 28.
69. N. Lei, Dalian University of Technology, School of Software and Technology, China, *Quadrilateral and hexahedral mesh generation based on surface foliation theory*, September 14.
70. J. Linn, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Mathematische Methoden in Dynamik und Festigkeit, Kaiserslautern, *Simulation of flexible cables in car assembly*, March 14.
71. Ch. Löbbert, RWTH Aachen, Institut für Geometrie und Praktische Mathematik, *Parallel arithmetic for distributed tensors in the HT-format*, November 28.
72. J.-M. Loubes, Université Toulouse Paul Sabatier, Institut de Mathématiques de Toulouse, Equipe de Statistique et Probabilités, France, *Kantorovich distance based kernel for Gaussian processes: Estimation and forecast*, June 14.
73. D. Loukrezis, Technische Universität Darmstadt, Institut für Theorie Elektromagnetischer Felder, *Low-rank tensor decompositions for high-dimensional uncertainty quantification in electromagnetic field problems*, June 20.
74. G. Lube, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *Pressure-robust error estimates of exactly divergence-free FEM for time-dependent incompressible flows, Part I*, February 9.
75. M. Mäck, Universität Stuttgart, Institut für Technische und Numerische Mechanik, *Numerical implementation of fuzzy arithmetic in uncertainty analysis*, June 27.
76. B. Matejczyk, University of Warwick, Mathematics Institute, Coventry, UK, *Macroscopic models for ion transport in nanoscale pores*, December 14.
77. St. Melchionna, University of Vienna, Faculty of Mathematics, Austria, *A variational approach to symmetry, monotonicity and comparison for doubly-nonlinear equations*, March 3.
78. S. Merino-Aceituno, Imperial College London, Department of Mathematics, UK, *Kinetic theory to study emergent phenomena in biology: An example on swarming*, February 7.
79. P. Mörters, Universität zu Köln, Mathematisch-Naturwissenschaftliche Fakultät, *Reinforced branching processes*, August 31.

80. L.O. Müller, Norwegian University of Science and Technology, Department of Structural Engineering, Trondheim, *A local time stepping solver for one-dimensional blood flow*, March 2.
81. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, *Asymptotic analysis of models involving surface diffusion*, November 16.
82. J. Mura, Pontificia Universidad Católica de Chile, Centro de Imágenes Biomédicas, Santiago, *An automatic method to estimate 3D pulse wave velocity from 4D-flow MRI data*, February 2.
83. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica (DMI), Italy, *The evergreen Wigner transport equation*, August 2.
84. A. Naumov, Skolkovo Institute of Science and Technology (Skoltech), Center for Computational Data-Intensive Science and Engineering (CDISE), Moscow, Russian Federation, *Bootstrap confidence sets for spectral projectors of sample covariance*, January 18.
85. Th. Niendorf, Max-Delbrück-Center für Molekulare Medizin (MDC), Experimentelle Ultrahochfeld-MR, Berlin, *Explorations into ultrahigh field magnetic resonance – Where physics, mathematics, biology and medicine meet*, March 20.
86. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, *Quasi-optimal methods to approximate the incompressible Navier–Stokes equations*, November 7.
87. M. Pavelka, Charles University, Mathematical Institute, Prague, Czech Republic, *42=GENERIC — Unified Hamiltonian description of solids and fluids*, November 30.
88. T.d.P. Peixoto, University of Bath, Department of Mathematical Sciences, UK, *Statistical inference of network structure and dynamics*, August 28.
89. M. Pelger, Stanford University, Management Science & Engineering Department, USA, *Estimating latent asset-pricing factors*, January 11.
90. A. Pilipenko, Ukrainian National Academy of Sciences, Institute of Mathematics, Kiev, *On a selection problem for small noise perturbation of ODE in multidimensional case*, April 26.
91. G. Pitton, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, *Accelerating augmented and deflated Krylov space methods for convection-diffusion problems*, March 28.
92. W. Polonik, University of California at Davis, Department of Statistics, USA, *Statistical topological data analysis: Rescaling the persistence diagram*, July 12.
93. I.Y. Popov, St. Petersburg National Research University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russian Federation, *Tunneling through periodic arrays of quantum dots and spectral problems*, February 2.
94. K. Proksch, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, *Multiscale scanning in inverse problems – With applications to nanobiophotonics*, February 8.
95. J. Prüss, Martin-Luther-Universität Halle-Wittenberg, Institut für Mathematik, *Critical spaces for quasilinear evolution equations and applications*, June 21.
96. L. Rebholz, Clemson University, Department of Mathematical Sciences, USA, *On conservation laws of Navier–Stokes Galerkin discretizations*, October 19.
97. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *Corrector estimates for singularly perturbed boundary value problems with nonsmooth data*, January 11.
98. Y. Ren, Dalian University of Technology, School of Software Technology, China, *On tetrahedralisations containing knotted and linked line segments*, September 26.
99. E. Rocca, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, *Optimal control in diffuse interface models of tumor growth*, May 4.

100. ———, *Diffuse interfaces in complex systems*, June 15.

101. U. Römer, Technische Universität Darmstadt, Institut für Theorie Elektromagnetischer Felder, *Stochastic collocation with adjoint error control for uncertainty quantification in computational electromagnetics*, June 20.

102. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, *In between Energetic and Balanced Viscosity solutions of rate-independent systems: The Visco-Energetic concept, with some applications to solid mechanics*, May 17.

103. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, *Seismic waves and earthquakes in a global monolithic model*, November 1.

104. T. Schaeffter, Physikalisch-Technische Bundesanstalt, Medical Physics and Metrological Information Technologies, Berlin, *Advances in cardiac and quantitative MRI*, June 12.

105. M. Schäffner, Technische Universität Dresden, Institut für Wissenschaftliches Rechnen, *Stochastic homogenization of discrete energies with degenerate growth*, May 9.

106. St. Schmidt, Universität Würzburg, Institut für Mathematik, *SQP methods for shape optimization based on weak shape Hessians*, October 12.

107. P. Schröder, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *Pressure-robust error estimates of exactly divergence-free FEM for time-dependent incompressible flows, Part II*, February 9.

108. J. Schwientek, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Optimierung, Kaiserslautern, *Numerical methods for general(ized) semi-infinite optimization – Applied to gemstone cutting*, April 25.

109. D. Silvester, University of Manchester, Faculty of Science and Engineering, UK, *Accurate time-integration strategies for modelling incompressible flow bifurcations*, April 6.

110. S. Simonella, Technische Universität München, Zentrum Mathematik, *Correlations in the mean field dynamics: A random walk expansion*, November 22.

111. M. Slowik, Technische Universität Berlin, Institut für Mathematik, *Random conductance model in a degenerate ergodic environment*, May 9.

112. A. Sobolevskiy, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, *The Hamilton-Jacobi equation: Parallel transport in the 2-Wasserstein space and beyond*, May 9.

113. H. Stuke, Freie Universität Berlin, Institut für Mathematik, *Parabolic blow-up in complex time*, May 16.

114. T. Sullivan, Freie Universität Berlin, Institut für Mathematik, *Well-posedness of Bayesian inverse problems – Stable priors on quasi-Banach spaces*, January 17.

115. J. ten Thije Boonkkamp, Eindhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, *Complete flux schemes for conservation laws of advection-diffusion-reaction typ*, March 30.

116. I. Thompson, University of Bath, Department of Physics, UK, *Modelling device charge dynamics on the microscopic scale*, April 25.

117. R. Toader, University of Udine, DIMI, Italy, *Existence for dynamic Griffith fracture with a weak maximal dissipation condition*, July 12.

118. A. Torcini, Université de Cergy–Pontoise, Laboratoire de Physique Théorique et Modélisation, France, *Death and rebirth of neural activity in sparse inhibitory networks*, February 14.

119. D. Turaev, Imperial College London, Department of Mathematics, UK, *Energy equilibration in slow-fast systems*, April 11.

120. C. Visone, Università del Sannio, Dipartimento di Ingegneria, Benevento, Italy, *The applicative challenges of smart materials: From sensing to harvesting*, May 30.

121. J. Weed, Massachusetts Institute of Technology, Department of Mathematics, Cambridge, USA, *Optimal rates of estimation for the multi-reference alignment problem*, April 26.

122. S. Wolf, Technische Universität Berlin, Institut für Mathematik, *Tensor reconstruction*, September 19.

123. M.-Th. Wolfram, University of Warwick, Mathematics Institute, Coventry, UK, *Cross-diffusion systems with excluded volume effects*, June 17.

124. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Inverse problems and optimal control problems for fractional diffusion equations*, January 31.

125. ———, *Inverse problems for an integro-hyperbolic equation for the viscoelasticity*, April 25.

126. A. Zeghuzi, Ferdinand-Braun-Institut, Berlin, *Simulations of broad area high-power lasers with optical feedback*, June 15.

127. N. Zhivotovskiy, Skolkovo Institute of Science and Technology, Skoltech Center for Computational Data-Intensive Science and Engineering (CDISE), Moscow, Russian Federation, *Towards minimax optimal rates in classification and regression*, April 25.

128. H. Zidani, ENSTA ParisTech, Applied Mathematics Department, Palaiseau, France, *Multi-objective control problems under state constraints*, July 26.

129. A. Zubkova, Karl-Franzens-Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, *Homogenization of the generalized Poisson–Nernst–Planck system with nonlinear interface conditions*, October 24.

A.13 Software

AWC –Adaptive Weights Clustering (contact: V. Spokoiny, phone: +49 30/20372-575, e-mail: vladimir.spokoiny@wias-berlin.de)

AWC is an open source python package containing implementation of the novel non-parametric clustering algorithm Adaptive Weights Clustering. The method is fully automatic and does not require to specify the number of clusters or their structure. The procedure is numerically feasible and applicable for high-dimensional datasets.

More information: https://www.wias-berlin.de/software/awc/

AWS – Adaptive Weights Smoothing (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 **Laser**s. It integrates numerically the laterally extended dynamic traveling wave model (one- and two-dimensional partial differential equations), executes different data post-processing routines, and visualizes the obtained data.

More information: https://www.wias-berlin.de/software/balaser/

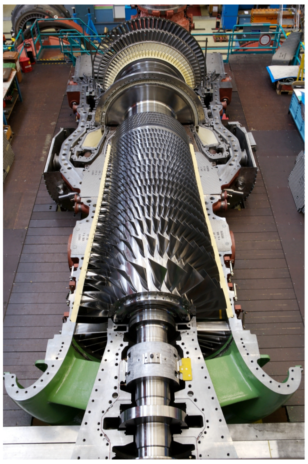
BOP (contact: P. Mathé, phone: +49 30/20372-550, e-mail: peter.mathe@wias-berlin.de)

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: https://www.wias-berlin.de/software/BOP/



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

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

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

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

Further information: https://www.wias-berlin.de/software/ClusCorr/

ddfermi (contacts: Th. Koprucki, phone: +49 30/20372-508, e-mail: thomas.koprucki@wias-berlin.de, J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de,)

`ddfermi` is an open-source software prototype which simulates the carrier transport in classical or organic semiconductors devices based on drift-diffusion models.

The key features are

- finite volume discretization of the semiconductor equations (van Roosbroeck system),
- thermodynamically consistent Scharfetter–Gummel flux discretizations beyond Boltzmann,
- general statistics: Fermi–Dirac, Gauss–Fermi, Blakemore and Boltzmann,
- generic carrier species concept,
- one-, two- and three-dimensional devices,
- C++-code based on `pdelib` and interfaced via Python,
- in-situ visualization.

Please find further information under https://www.wias-berlin.de/software/ddfermi/.

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

The program package `DiPoG` (**D**irect and **i**nverse **P**roblems for **o**ptical **G**ratings) provides simulation and optimization tools for periodic diffractive structures with multilayer stacks.

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

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

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

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

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

Detailed information: https://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 heat treatment for workpieces made of steel using single- and multi-frequency currents. It is the aim of the heat treatment to produce workpieces with hard, wear resistant surface and soft, ductile core. The boundary layer of the workpiece is heated up by induced eddy currents and rapidly cooled down by the subsequent quenching process. The resulting solid-solid phase transitions lead to a hardening of the surface of the workpiece.

WIAS-MeFreSim is based on the WIAS software pdelib. It solves coupled systems of PDEs consisting of Maxwell's equations, the heat equation and the equations of linear elasticity.

Fore more information see https://www.wias-berlin.de/software/MeFreSim/.

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

ParMooN is a flexible finite element package for the solution of steady-state and time-dependent convection-diffusion-reaction equations, incompressible Navier–Stokes equations, and coupled systems consisting of these types of equations, like population balance systems or systems coupling free flows and flows in porous media.

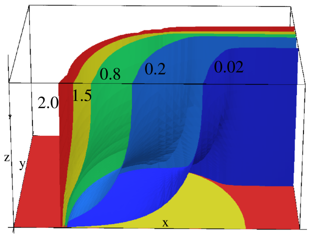
Please find more information under http://cmg.cds.iisc.ac.in/parmoon/.

Important features of ParMooN are

- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, non-conforming, discontinuous, higher-order, vector-valued, isoparametric, with bubbles)
- the use of implicit time-stepping schemes (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

ParMooN 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)



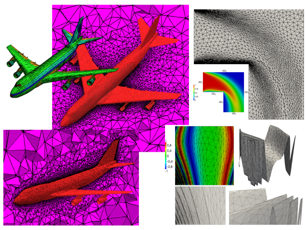
Concentration isosurfaces in a thin-layer flow cell (pdelib)

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

- iterative solvers for linear and nonlinear systems of equations
- sparse matrix structures with preconditioners and direct solver interfaces
- dimension-independent simplex grid handling in one, two, and three space dimensions
- finite volume-based solution of coupled parabolic reaction-diffusion-convection systems and pressure robust discretizations for Navier–Stokes
- finite element based solution of variational equations (especially thermoelasticity) with goal-oriented error estimators
- optimization tool box
- parallelization on SMP architectures
- graphical output during computation using OpenGL
- scripting interface based on the languages Python and Lua

- graphical user interface based on the FLTK toolkit
- modular build system and package manager for the installation of third-party software used in the code

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



Adapted tetrahedral meshes and anisotropic meshes for numerical methods and scientific computation

TetGen (contact: H. Si, phone: +49 30/20372-446, e-mail: hang.si@wias-berlin.de)

`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 https://www.wias-berlin.de/software/tetgen/.

WIAS-TeSCA (contact: H. Stephan, phone: +49 30/20372-442, e-mail: holger.stephan@wias-berlin.de)

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

The strategy of `WIAS-TeSCA` for solving the resulting highly nonlinear system of partial differential equations is oriented towards the Lyapunov structure of the system describing the currents of electrons and holes within the device. Thus, efficient numerical procedures for both the stationary and the transient simulation have been implemented, the spatial structure of which is a finite volume method. The underlying finite element discretization allows the simulation of arbitrarily shaped two-dimensional device structures.

`WIAS-TeSCA` has been successfully used in the research and development of semiconductor devices such as transistors, diodes, sensors, detectors, lasers, and solar cells.

The semiconductor device simulation package `WIAS-TeSCA` operates in a Linux environment on desktop computers.

WIAS is currently focusing on the development of a new generation semiconductor simulator prototype. Therefore, `WIAS-TeSCA` is in maintenance mode and is used for benchmarking of the new code and the support of running projects.

For more information please see https://www.wias-berlin.de/software/tesca/.

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

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

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

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

`dti` is a contributed package within the R-Project for Statistical Computing. The package contains tools for the analysis of diffusion-weighted magnetic resonance imaging data (dMRI). It can be used to read dMRI data, to estimate the diffusion tensor, for the adaptive smoothing of dMRI data, the estimation of the orientation density function or its square root, the estimation of tensor mixture models, the estimation of the diffusion kurtosis model, fiber tracking, and for the two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org). The multi-shell position-orientation adaptive smoothing (msPOAS) method for dMRI data is additionally available within the ACID toolbox for SPM (http://www.diffusiontools.com).

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