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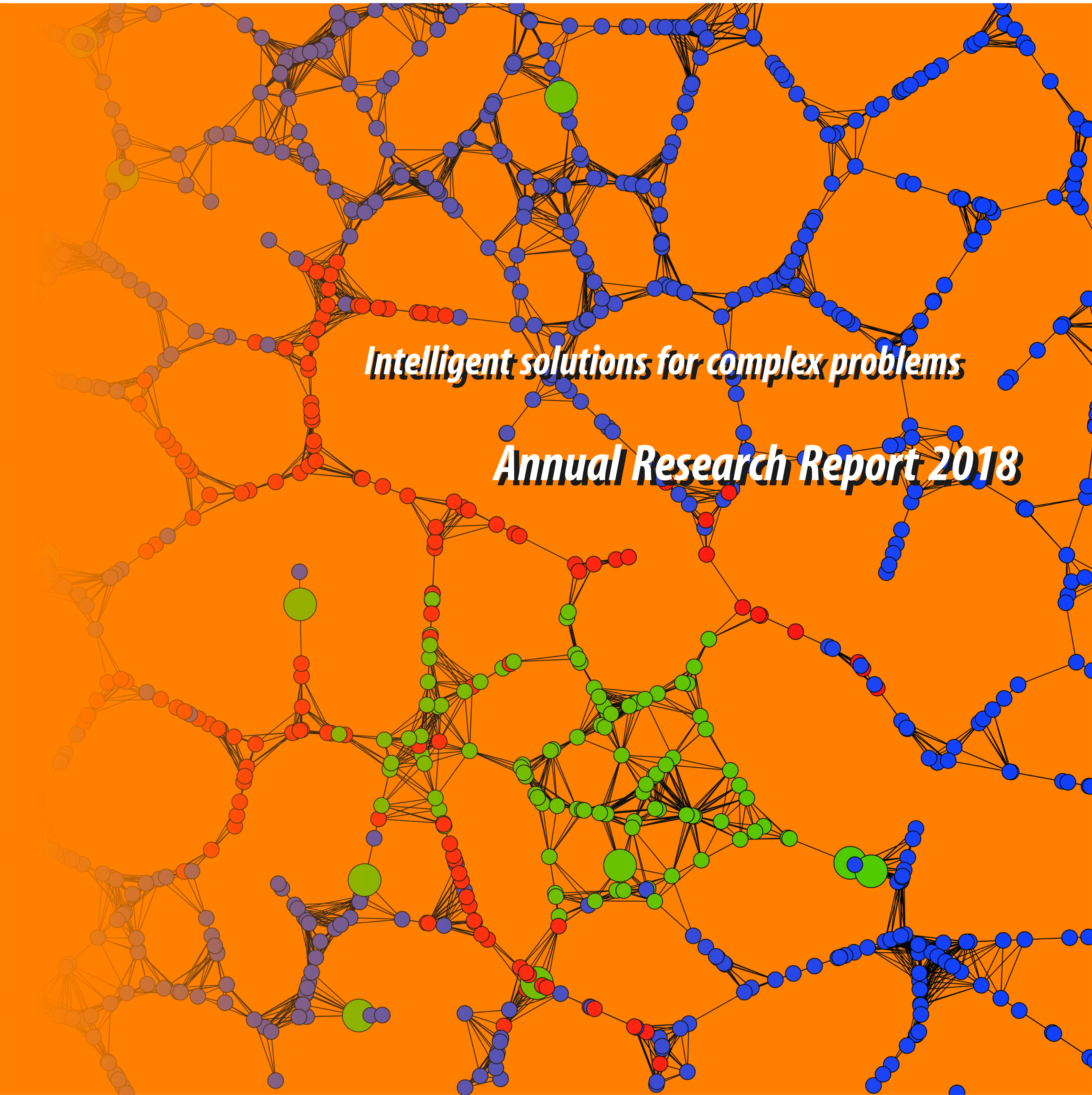

Intelligent solutions for complex problems

Annual Research Report 2018

Cover figure: Snapshot of the spatial distribution of a malware (red) over an ad-hoc communication system with many susceptible (blue) and immune (green) devices. In this model, the green devices even act as “white knights”, i.e., they are able to transmit their goodware to neighboring infected devices, making them immune as well.

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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 2018. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2018. Following six selected scientific contributions written for a broader public that highlight some results of outstanding importance, in the second part, a general introduction to WIAS is given, followed by the report of the IMU Secretariat, the essential results of the research groups, and statistical data.

Prof. Dr. Michael Hintermüller, Director

After its successful evaluation in 2017, the Senate of the Leibniz Association certified in March 2018 that WIAS does an internationally outstanding work in its field and that it produces extraordinary research and publication results. Another important event in 2018 was the acceptance of the proposal of the Berlin mathematicians for the next-generation excellence cluster "MATH+: The Berlin Mathematics Research Center" in the competition within the Excellence Strategy of the Federal Government and the Federal States of Germany. On September 27, 2018, we got the overwhelming official information that our proposal was among the successful ones. WIAS is proud to be among the five cooperation partners of MATH+. The cross-institutional and cross-disciplinary cluster of excellence concentrates on application-oriented basic mathematical research and ties in to the success of the Berlin Research Center MATHEON. The cluster will be supported by the German Research Foundation DFG for seven years and began its work in January 2019 with the WIAS Director Prof. Michael Hintermüller one of its spokespersons. WIAS has competed very successfully in the first round of project proposals within MATH+. As a consequence, 15 projects with PIs from WIAS started their research work in early 2019. MATH+ is one of the strategic scientific projects with a mid- to long-term impact. In particular, the Application Areas "Material, Light and Devices", "Energy and Markets" and the Emerging Fields "Integrated Physics-based Imaging" and "Particles and Agents" relate to topics on our Institute's long-term research agenda.

Berlin remains the center of world mathematics because WIAS remains the headquarters of the Secretariat of the International Mathematical Union (IMU). In July 2018, the General Assembly of the IMU in Sao Paulo took the final decision to continue the Secretariat of the IMU at WIAS that has been there since 2011. The vote was overwhelmingly positive and, in a plenary presentation, Professor John Toland, the former Director of the Isaac Newton Institute in Cambridge and Member of IMU's Executive Committee, praised the extraordinary quality of the Secretariat's work and its importance for the proceedings of the IMU. Its Secretary General, Professor Helge Holden, reinforced this statement also highlighting the political will in Germany to support this endeavor. In this framework, WIAS gratefully acknowledges the generous financial support provided by the Federal Ministry of Education and Research (BMBF) and by the Berlin Senate Chancellery who sponsor the IMU Secretariat at equal parts.

The newly implemented *Flexible Research Platform* 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. In 2018, the 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* worked under this umbrella.

Foreword

Like the previous years, 2018 has proven to be a busy and fruitful year for the institute with 98 preprints in the WIAS Preprint Series, 117 articles in refereed journals, one monograph, and 3.6 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 a very good level, continuing WIAS's successful track record.

After the successful founding of the M4Sim GmbH, WIAS has again obtained an EXIST Business Start-up Grant by the Federal Ministry for Economic Affairs and Energy of Germany for three young scientists, Dr. Johannes Neumann (WIAS), André Wilmes, Ph.D., and Abeed Visram, Ph.D., (both Imperial College London), for their planned spin-off "rDesign – Robust Topology-Optimization for SME in Industry 4.0".

In the WIAS-coordinated Leibniz Network "Mathematical Modeling and Simulation" (MMS), now thirty-two institutes from all sections of the Leibniz Association work together. On February 28 to March 2, 2018, the 3rd Leibniz MMS Days took place in Leipzig, supported by the member institutes TROPOS and IOM. Also the Leibniz MMS Summer School in September 2018 on Statistical Modeling and Data Analysis at the Mathematical Research Institute at Oberwolfach was a big success.

The Weierstrass Institute is committed to the implementation of policies and standards to achieve the goal of gender equality. In 2018, WIAS again retained the "audit berufundfamilie" (audit job and family) quality seal. New goals in this area are pursued 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 again 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, 45 additional co-workers (+ 9 outside WIAS; Dec. 31, 2018) could be financed from third-party funds.

Fourteen 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. A cornerstone of this cooperation is the fact that, in 2018, altogether six leading members of WIAS, including the director and his deputies, held WIAS-funded special chairs at the Berlin universities. But the highlight in this respect was also in 2018 the joint operation of the Research Center MATHEON "Mathematics for key technologies" located at the Technische Universität Berlin and in 2018 still funded by the "Einstein Foundation Berlin" in the framework of the "Einstein Center for Mathematics" (ECMath). From 2019 onwards, it will be supported in the framework of MATH+ (see above).

WIAS is committed to the success of the center by providing considerable financial and personal resources; several members of WIAS play key roles in the scientific administration of the MATHEON.

Another success story of the Berlin mathematics is the Berlin Mathematical School (BMS), now supported as BMS+ in the framework of MATH+. Here, collaborators of the mathematical institutions of Berlin supervise each year dozens of outstanding doctoral students from all over the world.

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 (CRCs), Priority Programs, and Research Training Groups of the German Research Foundation. Three in one sweep: The CRCs 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application* and 1114 *Scaling Cascades in Complex Systems* and the CRC/Transregio (TRR) 154 *Mathematical Modeling, Simulation and Optimization Using the Example of Gas Networks* got a positive appraisal and will be supported for another period of four years.

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 May 2019

M. Hintermüller

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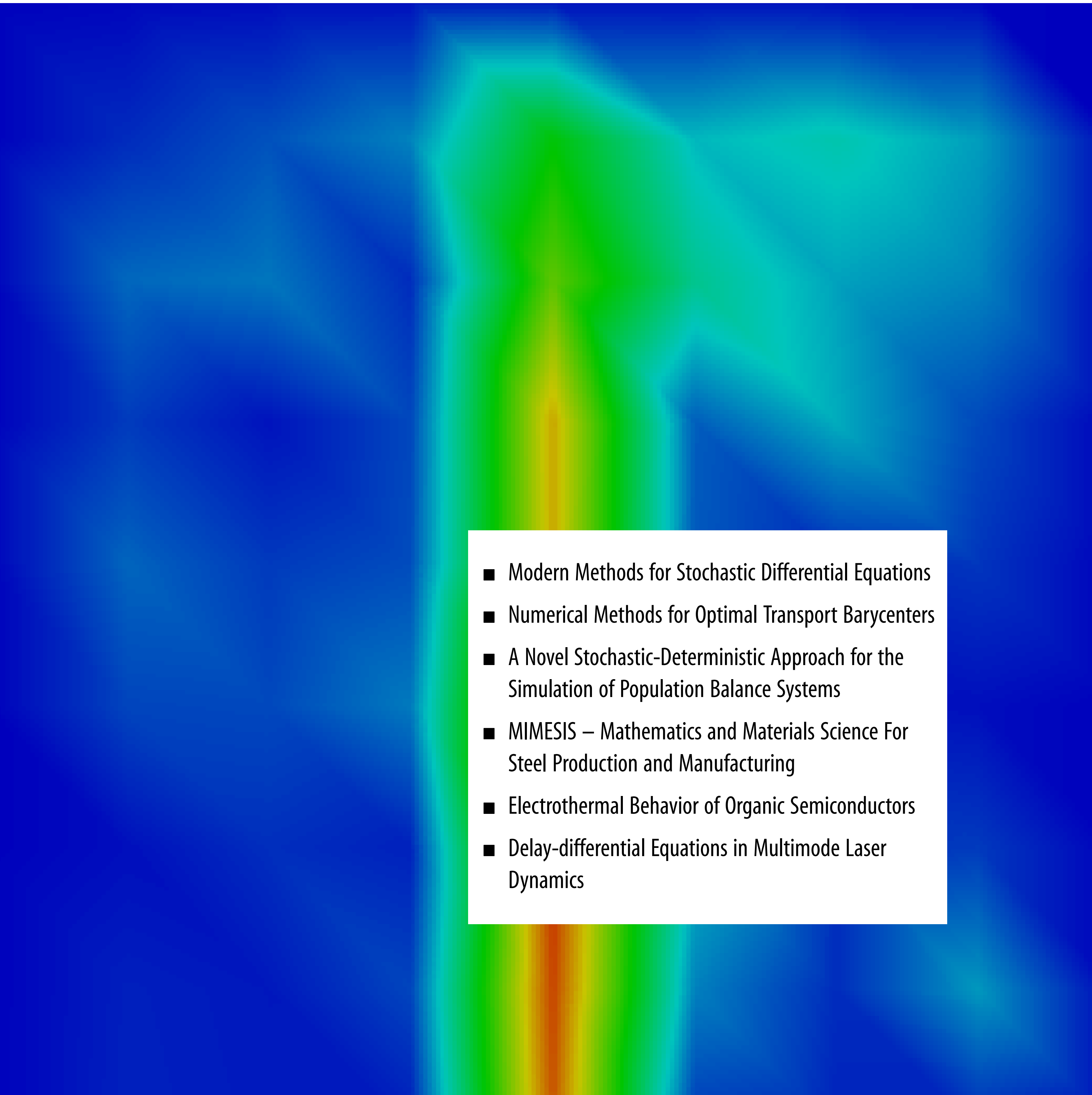
1 Scientific Highlights



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1.1 Modern Methods for Stochastic Differential Equations

Christian Bayer, Wolfgang König, Martin Redmann, John Schoenmakers, and Willem van Zuijlen,

Stochastic (partial) differential equations (S(P)DEs) belong to the most fundamental and ubiquitous concepts for the descriptions of physical processes under the influence of a large amount of microscopic randomness. They have been handled with extreme success for a number of decades using methods that have nowadays a classical status, like martingale descriptions, Malliavin calculus, or semigroup methods. Nevertheless, in 1998, a new idea was introduced to the theory by Terry Lyons, which is considered to have created a revolution and gave the theory a new perspective, which is currently growing a lot and does not seem to have an end in coming decades. This idea is based on a consideration of the input quantities in a pathwise way as (very non-regular) trajectories and to try to grasp the solution quantities as functions of them. This is possible via an abstract embedding into a large functional space with strong regularity properties in which, after an appropriate lifting, the solution can be seen as a quite regular function of the input quantities.

For the treatment of stochastic ordinary differential equations, the rough-path approach led to a considerable theoretical advancement, but also to very practical applications in numerics of SDEs, filtering (see below), machine learning, and other fields. For SPDEs, rough-path analysis fostered three strongly linked research approaches. First, rough-path theory can be directly applied to a large class of SPDEs, and provides pathwise solutions to many SPDEs that are difficult to handle with standard techniques of stochastic analysis. More recently, two further approaches, namely the method of *paracontrolled distributions*, and the theory of *regularity structures*, have been developed to specifically deal with certain classes of singular, nonlinear SPDEs, which are outside the reach of classical methods of stochastic analysis. For the development of the theory of regularity structures, a Fields Medal was awarded to Martin Hairer in 2014.

One of the world's hot spots in the research on these new methods is Berlin. This has been acknowledged in 2016 by the German Science Foundation DFG by instituting the research unit FOR 2402 entitled *Rough Paths, Stochastic Partial Differential Equations, and Related Topics* headed by one of the leading figures in this field, *Peter Friz* (Technische Universität Berlin and WIAS). The WIAS is an active part of this unit; two of its research groups (RG 5 and RG 6) participate in two of the five subprojects. Here, we report on their achievements of the first funding period.

Spectral properties of the parabolic Anderson model

The *heat equation with random potential* is the SPDE

$$\partial_t u = \Delta u + \xi \cdot u, \qquad u(0,\cdot) = \delta_0, \tag{1}$$

where ξ – called the potential – only depends on space and is random, and Δ is the Laplace operator. Since the operator on the right-hand side of (1), i.e., $\Delta + \xi$, is the well-known *Anderson operator* (a famous example of a random Schrödinger operator), this equation is also known as the *parabolic Anderson model (PAM)*. It has been studied in both continuous and discrete space. It describes the diffusion of heat in a random field of sinks and sources or alternatively the distribution of particle mass in a spatial branching process with random branching rates. While Δ, which drives the random propagation of the mass in space, has a smoothing effect on the solution, the term $\xi \cdot u$ causes local disorder; indeed, it exponentially increases or diminishes the mass, depending on the sign of ξ. One can interpret $u(t,x)$ as the amount of mass at time t at the space point x. The initial condition we want to consider is a unit mass at 0.

The model in (1) admits, under strong regularity assumptions on the input quantity ξ, particularly strong solution tools (like the Feynman–Kac formula and eigenvalue expansions). By these tools the results go far beyond the ubiquitous questions of existence, uniqueness, and regularity of the solutions, but also concern much deeper and more physical questions. For irregular ξ, (1) is therefore one of the prime examples of an SPDE to which the new methods are applied. The WIAS team is working at the forefront of such questions. The most interesting behavior of the solution to (1) is the effect of localization, called *intermittency*, after large times: The disorder dominates the smoothing in the sense that the bulk of the total mass is asymptotically concentrated in a few small "islands", which are far away from each other. A mathematical description of intermittency was introduced by [5], and it was shown there that this effect is present as soon as the potential ξ is non-trivially random. Since then, the asymptotics of the solution has been deeply investigated for a large number of random potential distributions, both in discrete and continuous space, and various tools have been developed. See [6] for a comprehensive survey.

Here, we study the PAM in continuous space in two dimensions. As a potential we would like to consider independent standard normally distributed random variables $\xi(x)$, indexed by $x \in \mathbb{R}^2$. However, this is not possible as ξ cannot be given the mathematical sense of a measurable function anymore. Therefore, we consider ξ to be white noise, which is a distribution, a generalized function. Furthermore, it is of such a low regularity that the product of ξ with u is a priori not defined. By naively trying to define $\xi \cdot u$ as the limit $\xi_\epsilon \cdot u$ for $\epsilon \downarrow 0$, with ξ_ϵ a mollification of ξ, one encounters that this causes a blow-up. The product can, however, be defined by using a renormalization procedure, which basically removes the blow-up factor. This procedure can be done using either the technique of regularity structures or the one of paracontrolled distributions.

We highlight here two works in progress that are crucial steps towards a deeper understanding of the behavior of the PAM for large times. Note that (1) reads $\partial_t u = Hu$ with $H = \Delta + \xi$ the Anderson operator, and so, formally, the solution should be given by $u(t,x) = \mathrm{e}^{tH} u_0(x)$. The main goal here is an asymptotic description of the total mass, $U(t) = \int u(t,x)\,\mathrm{d}x$, in terms of the principal part of the spectrum of H in large boxes.

Let us first start with describing spectral properties of H in large boxes. Romain Allez and Khalil Chouk (TU Berlin) [1] constructed a paracontrolled domain for the restriction of H to a box in $\mathbb{R}^2$ with periodic boundary conditions, on which it is a self-adjoint L^2-operator with a countable spectrum of eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots$. Within the FOR 2402, this was adapted in joint work of Khalil Chouk and Willem van Zuijlen to Dirichlet boundary conditions, by constructing a Dirichlet domain in the box $Q_R = (-R,R)^2$ on which the Anderson–Hamiltonian H_R is L^2-self-adjoint with a countable spectrum of eigenvalues $\lambda_1^R \geq \lambda_2^R \geq \cdots$. The main progress here consists of a detailed description of the asymptotic behavior of the eigenvalues λ_n^R for large R. Indeed, almost surely, in the limit as $R \to \infty$, it is shown that $\lambda_n^R \sim \rho_n \log R$, where ρ_n is a scalar represented by an explicit variational formula.

Heuristically, this implies the following for the large- t behavior of the total mass in a fixed box. By the above we may write $H_R = \sum_{n\in\mathbb{N}} \lambda_n^R \langle u_0, e_n^R\rangle e_n^R$, where e_n^R is an eigenvector corresponding to the eigenvalue λ_n^R , and the e_n^R 's are orthonormal. Let u_R be the solution to the PAM in the box $Q_R = (-R, R)^2$ with Dirichlet boundary conditions. Let $U_R(t) = \int u_R(t, x)\,\mathrm{d}x$ be the total mass of u_R at time t . Then we formally deduce that $U_R(t) = \langle u_R(t, \cdot), \mathbf{1}\rangle = \sum_{n\in\mathbb{N}} \mathrm{e}^{\lambda_n t}\langle u_0, e_n^R\rangle\langle e_n^R, \mathbf{1}\rangle$. Since λ_1^R is strictly the largest of the eigenvalues, one obtains $\frac{1}{t}\log U_R(t) \sim \lambda_1^R$, as $t \to \infty$, almost surely.

In order to obtain the asymptotic behavior of the total mass $U(t)$ of the solution to the PAM on $\mathbb{R}^2$, we couple large- t asymptotics with large- R asymptotics. Indeed, Wolfgang König and Willem van Zuijlen, in joint work with Nicolas Perkowski (HU Berlin), show that $\log U_{R_t}(t) \sim \log U(t)$ almost surely making the choice $R_t = t(\log t)^{10}$. From this and the above, using that $\log R_t \sim \log t$, we then derive the following main result:

$$\frac{\log U(t)}{t \log t} \sim \rho_1 \qquad \text{almost surely.}$$

Let us spend some words on the main step in the proof, the comparison of the infinite-space total mass $U(t)$ with the total mass in a large box, $U_R(t)$. For regular ξ , the main tool is the Feynman–Kac formula. Indeed, with $(B_s)_{s\in[0,\infty)}$ a Brownian motion starting from zero, and $\mathbb{P}$ its law, we have

$$U(t) = \mathbb{E}\left[\exp\left(\int_0^t \xi(B_s)\,\mathrm{d}s\right)\right],$$

and a version of that formula for $U_R(t)$ with restriction of the path $(B_s)_{s\in[0,t]}$ to Q_R . As white noise ξ is not a function but a distribution, this expression does not make sense. An innovative idea here is to use instead a partial Girsanov transform: With a stochastic process $\gamma = (\gamma_s)_{s\in[0,\infty)}$, we can represent

$$U(t) = \mathbb{E}_b\left[\exp\left(F((\gamma_s)_{s\in[0,t]})\right)\right],$$

and an analogous version for $U_R(t)$ with restriction of the path $(\gamma_s)_{s\in[0,t]}$ to Q_R . Here, F is a function and b is a distribution, both depending on ξ , and the coordinate process γ under the law $\mathbb{P}_b$ is determined by the SDE

$$\mathrm{d}\gamma_t = b(\gamma_t)\,\mathrm{d}t + \mathrm{d}B_t.$$

Even though b is a distribution, as it is of sufficient regularity, this SDE still has a weak solution, which is by now well-known from several works.

By means of these representations for $U(t)$ and $U_R(t)$, and since we have a good control on the function F , one is now left to control the probability of the event that the process γ leaves the large box Q_R before time t , with R replaced by $R_t = t(\log t)^{10}$. This in turn follows from new *heat-kernel bounds* for the density $\Gamma_t^b(x, y)$ of the transition probability $\mathbb{P}_b(\gamma_t \in \mathrm{d}y|\gamma_0 = x)$. Indeed, we prove the existence of a $c > 0$ and $M_b > 0$ such that for any $t > 0$ and $x, y \in \mathbb{R}^d$,

$$\frac{1}{c}\mathrm{e}^{-cM_b t}\,p(t, x-y) \le \Gamma_t^b(x, y) \le c\mathrm{e}^{cM_b t}\,p(t, x-y),$$

where p is the standard Gaussian kernel. New and important for us is that M_b is an explicit function of b, and c and M_b are independent of t. This ends the survey of the most recent achievements of Wolfgang König, Willem van Zuijlen (both WIAS), and Nicolas Perkowski (HU Berlin) on the parabolic Anderson model.

Numerics for rough PDEs

In another project of the FOR 2402 at WIAS, we develop numerical methods for rough partial differential equations. In the first phase of the project we focused on linear, parabolic partial differential equations driven by rough paths, i.e., paths that are even less regular than paths of the Brownian motion.

An important motivation for studying this class of equations comes from nonlinear filtering theory. As usual, we work on a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\geq 0}, \mathbb{P})$. Suppose that we are given a process X satisfying the (standard) SDE

$$\mathrm{d}X_t = \beta(X_t)\,\mathrm{d}t + \alpha(X_t)\,\mathrm{d}Z_t, \qquad X_0 \in \mathbb{R}^d, \tag{2}$$

where, for simplicity, we assume here that Z is a standard Brownian motion and $d = 1$. However, we do not observe the process X, but a perturbed process

$$W_t = \int_0^t h(X_s)\,\mathrm{d}s + U_t$$

for a Brownian motion U that is correlated with Z.

Our goal is to reconstruct X given our observation W as accurately as possible. Given W, we clearly cannot expect an exact resolution of X unless the driving processes Z and U are fully correlated. The proper probabilistic formulation of our goal is therefore to compute the *conditional distribution* of X given the information W. More precisely, let $\mathcal{F}_t^W := \sigma\left((W_s)_{0\leq s\leq t}\right)$ denote the filtration generated by the process W. Then our aim is to compute the measure-valued process π_t determined by

$$\int f(x)\,\pi_t(\mathrm{d}x) = \mathbb{E}^{\mathbb{P}}\left[f(X_t)\middle|\mathcal{F}_t^W\right]$$

for any test function f, where $\mathbb{E}^{\mathbb{P}}$ denotes the expectation with respect to $\mathbb{P}$. Note that π_t is, by definition, an $\mathcal{F}_t^W$-measurable random measure.

It turns out that π_t can be characterized as the solution of an SPDE driven by W. To this end, let us first "make W a Brownian motion" by a change of measures using the density

$$\xi_t := \left.\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{Q}}\right|_{\mathcal{F}_t} := \exp\left(\int_0^t h(X_s)\,\mathrm{d}W_s - \frac{1}{2}\int_0^t h(X_s)^2\,\mathrm{d}s\right).$$

We can express π_t in terms of a non-normalized conditional distribution V_t satisfying the *Kallianpur–Striebel formula*

$$\int f(x)\,V_t(\mathrm{d}x) = \mathbb{E}^{\mathbb{Q}}\left[f(X_t)\xi_t\middle|\mathcal{F}_t^W\right], \qquad \pi_t = \frac{V_t}{\int V_t(\mathrm{d}x)},$$

where $\mathbb{E}^{\mathbb{Q}}$ denotes the expectation with respect to $\mathbb{Q}$. If V_t has a *density* $v(t,\cdot)$ (with properly chosen initial value $v(0,\cdot)$), then it satisfies the *Zakai equation*

$$\mathrm{d}v(t,x) = \Big(\frac{1}{2}\partial_x^2\big[\alpha(x)^2 v(t,x)\big] - \partial_x[b(x)v(t,x)]\Big)\,\mathrm{d}t + \big(h(x)v(t,x) - \partial_x[\rho\alpha(x)v(t,x)]\big)\,\mathrm{d}W_t, \qquad (3)$$

where ρ denotes the correlation between U and Z.

Rough paths come into the picture in two ways: First, we can simply formally replace the Brownian motion W by a rougher process, e.g., by a fractional Brownian motion with Hurst index smaller than but close to $1/2$. More fundamentally, even in the above diffusion setting, note that we really need to solve (3) for a specific observation path W. In the multi-dimensional case, classical solution theory of SPDEs does not provide us with such a solution due to the inherent instability with respect to the noise. We can, however, construct pathwise, stable solutions as a function of a rough path $\mathbf{W}$ on W, see [4].

In [2], we propose a numerical method of solving the Zakai SPDE (and similar parabolic rough PDEs) pathwise, for a fixed (rough) path $\mathbf{W}$. This method, which is the first fully implemented and properly analyzed scheme for solving rough PDEs, is in an essential way based on the above motivation from filtering. Indeed, the method is based on a stochastic representation for v very similar to the above Kallianpur–Striebel formula, i.e., (in the simplest case)

$$v(t,x) = \mathbb{E}[g(X_t) \mid X_0 = x],$$

where X_t is the solution to a stochastic rough differential equation driven by a Brownian motion B and the rough path $\mathbf{W}$, which, at this point, is understood as a *deterministic* path. A solution in space x for fixed time t or in time and space (t,x) is then computed by regression. In more detail (and for fixed t), we are trying to approximate $v(t,x) \approx \sum_{k=1}^{K} \alpha_k \psi_k(x)$ so as to minimize the L^2-error (in space) with respect to some probability measure μ. To do so, we carry out the following program:

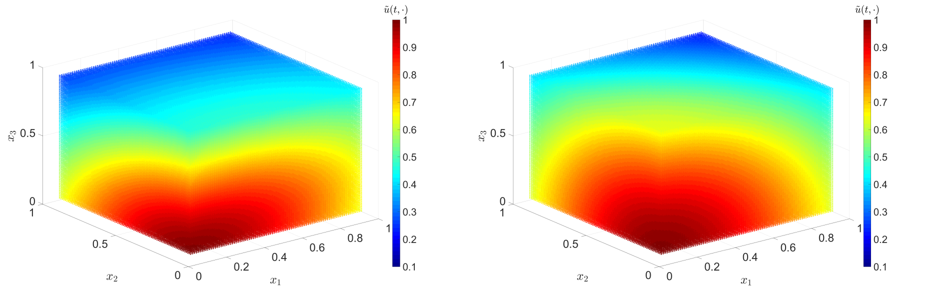

Fig. 1: *Three-dimensional numerical example from [2] for $t = 0.14$ and $t = 0.99$*

1. Simulate spatial samples $x^1, \dots, x^M$ with distribution μ;
2. for any such random starting value x^m, simulate a trajectory B^m of the driving Brownian motion and (approximately) solve X_t^m starting from $X_0^m = x^m$ (see [3] for the discretization method);
3. approximate $\alpha_k = \langle \psi_k , v(t,\cdot)\rangle_{L^2(\mu)} \approx \frac{1}{M}\sum_{m=1}^{M} \psi_k(x^m) g(X_t^m)$.

(In the last step, we assumed that the basis functions ψ_k are orthonormal w.r.t. μ.) The numerical approximation method sketched above is analyzed in [2]. In particular, we provide error rates for all the involved approximations.

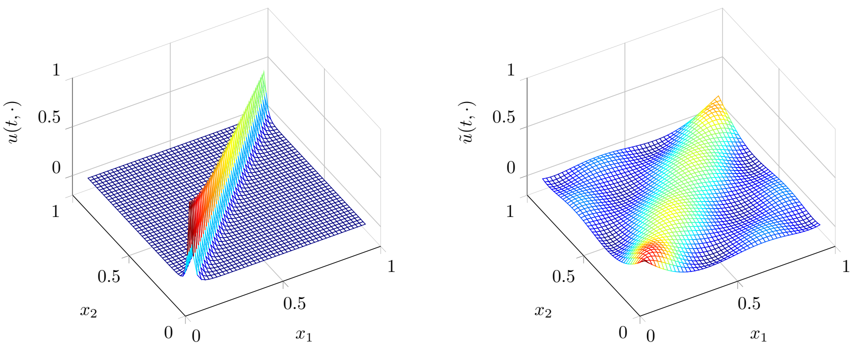

Fig. 2: *Two-dimensional numerical example from [2], exact vs. approximate solution.* $t = 0.14$ *and* $t = 0.99$

We end with a selection of our extensive numerical examples. In general, the numerical examples match with the theoretical results, but we find strong dependence of the observed errors on the driving trajectory $\mathbf{W}$. For instance, in Figure 2, the exact solution exhibits almost a singular shape, which is hard to approximate based on polynomial basis functions. On the other hand, other solutions of the same system driven by different rough path trajectories may lead to much smoother solutions, which are much easier to approximate.

Conclusion and outlook

The achievements of the WIAS-projects within the FOR 2402 have concerned the start of the first applications of modern methods for deriving first geometric properties of solutions of such SPDEs on one hand and of practically relevant properties on the other. One of the main goals in near future in the study of the parabolic Anderson model is a deeper analysis of geometric properties of all the principal eigenfunctions, in particular, their localization properties. A future goal on the numerical side is the development of simulation-based methods using rough-path analysis for deriving practical solutions of such SPDEs.

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1.2 Numerical Methods for Optimal Transport Barycenters

Darina Dvinskikh and Pavel Dvurechensky

Optimal transport (OT) distances between probability measures or histograms, including the earth mover's distance and Monge–Kantorovich, or Wasserstein, distance [6], have an increasing number of applications in statistics, such as unsupervised learning, semi-supervised learning, clustering, text classification, as well as in image retrieval, clustering, segmentation, and classification, and other fields, e.g., economics and finance or condensed matter physics.

Given a basis space and a transportation cost function, the OT approach defines a distance between two objects as a distance between two probability measures on a basis space. Consider an example of two grayscale images. In this case, the basis space can be defined as the pixel grid of this image. Then, for each pixel, the intensity can be seen as a mass situated at this pixel. Normalizing the intensity of each pixel dividing it by the total mass of the image, one obtains a discrete probability measure (or histogram) on the space of pixel grid. Then, the squared Euclidean distance between two pixels can be taken as a cost of transportation of a unit mass between these two pixels. Given two images, which are now modeled as probability measures, the goal is to transport the first image to the second. To do so, a transportation plan [5] is defined as a measure on the direct product of the basis pixel space by itself, i.e. a matrix with elements summing up to 1. Each row of this matrix corresponds to a pixel of the first image and tells what portion of mass is transported from this pixel to each pixel of the second image, see Figure 1. At the same time, each column of this matrix corresponds to a pixel of the second image and tells what portion of mass is transported to this pixel from each pixel of the first image. Note that this definition is symmetric as the same transportation plan can be used to transport the second image to the first one. Given squared Euclidean distance as transportation cost (i.e., for each pair of pixels, the cost of transporting a unit of mass from a pixel in the first image to a pixel in the second one) and transportation plan (i.e., for each pair of pixels, the mass which is transported from a pixel in the first image to a pixel in the second one), one can calculate the total cost of transportation of the first image to the second by summing individual costs for each pair of pixels and finding the total cost. Now, the transportation plan can be varied in order to find the minimum possible total cost of transportation. The square root of this minimum transportation cost is called *Wasserstein distance* on the space of probability measures. This is a particular case of optimal transport distance. Optimal transport theory proves that this minimum is attained and is indeed a distance which satisfies all the distance axioms.

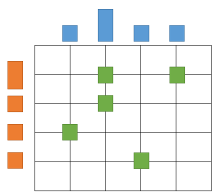

Fig. 1: *Transportation plan as coupling measure of two histograms*

Besides images, these probability measures or histograms can model other real-world objects like videos, texts, genetic sequences, protein backbones, etc. The success of OT approach in applications comes for the price of intense computations, as the computation of the Wasserstein distance between two histograms requires to solve a large-scale optimization problem, which complexity scales quadratically with the size of histograms. Despite this computational complexity OT distance captures complicated geometry of these objects (images, videos, texts...) well, that makes it suitable for finding the mean in different tasks, unlike simple Euclidean distance, see Figure 2

[0]Based on joint work [2] with Alexander Gasnikov, César A. Uribe and Angelia Nedić.

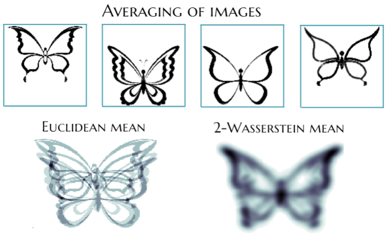

Fig. 2: *Barycenter of images with Euclidean distance vs Wasserstein distance*
Image courtesy: A. Suvorikova

As in the Euclidean space, when the mean object is defined as an object, minimizing the sum of Euclidean distances to all the objects in the set, the mean probability measure of a set of measures can be defined as a minimizer of the sum of squared Wasserstein distances to all the measures in the set. This mean object is called *Wasserstein barycenter*. If the objects in the set are randomly sampled from some distribution, theoretical results such as central limit theorem or confidence set construction [4] have been proposed, providing the basis for the practical use of the Wasserstein barycenter. However, calculating the Wasserstein barycenter of m measures is a computationally hard optimization problem which includes repeated computation of m Wasserstein distances. Moreover, in the large-scale setup, storage and processing of transportation plans, required to calculate Wasserstein distances, can be intractable for computation on a single computer. On the other hand, recent studies on distributed learning and optimization algorithms demonstrated their efficiency for statistical and optimization problems over arbitrary networks of computers or other devices with inherently distributed data, i.e., the data is produced by a distributed network of sensors or the transmission of information is limited by communication or privacy constraints, i.e., only limited amount of information can be shared across the network.

Motivated by the limited communication issue and the computational complexity of the Wasserstein barycenter problem for large amounts of data stored in a network of computers, we use state-of-the-art of computational optimal transport and convex optimization algorithms to propose a decentralized distributed algorithm to calculate an approximation to the Wasserstein barycenter of a set of probability measures. We solve the problem in a distributed manner on a connected and undirected network of agents oblivious to the network topology. Each agent locally holds a possibly continuous probability distribution, can sample from it, and seeks to cooperatively compute the barycenter of all probability measures exchanging the information with its neighbors. We adapt stochastic-gradient-type method and on each iteration each node of the network gets a stochastic approximation for the gradient of its local part of the objective, exchanges these stochastic gradients with the neighbors and makes a step. We show that as the time goes, the whole system comes to a consensus, and each node holds a good approximation for the barycenter.

Problem statement

Following [1], we consider the state-of-the-art technique of entropic regularization of OT with Kullback–Leibler divergence (KL), defining regularized Wasserstein distance between two probability measures μ and ν as

$$\mathcal{W}_\gamma(\mu,\nu) = \min_{\pi\in\prod(\mu,\nu)} \left\{ \int\int_{\mathcal{Y}\times\mathcal{Y}} \|x-u\|^2 d\pi(x,y) + \gamma\, KL(\pi,\theta) \right\}, \qquad (1)$$

where $\pi \in \prod(\mu, \nu)$ represents the constraint that π is in the set of probability measures $Prob(\mathcal{Y} \times \mathcal{Y})$ with marginals μ and ν, θ is the uniform distribution, γ is the regularization parameter.

For a given set of probability measures $\{\mu_1, \ldots, \mu_m\}$, the goal is to find a discrete approximation of their barycenter $p \in S_n(1)$, where $S_n(1)$ is the probability simplex. Then, the regularized Wasserstein barycenter in the semi-discrete setting is defined as the solution to the following convex optimization problem with the simpler notation $\mathcal{W}_{\gamma,\mu}(p) := \mathcal{W}_\gamma(\mu, \nu)$ for a fixed probability measure μ

$$\min_{p \in S_n(1)} \frac{1}{m} \sum_{i=1}^{m} \mathcal{W}_{\gamma,\mu_i}(p). \tag{2}$$

To solve this problem in the large-scale setting, i.e. when the number of measures m and the size of measures support n are large, and to be able to deal with the data μ_i, $i = 1, ..., m$, stored in a distributed network, we apply techniques developed in decentralized distributed optimization. We introduce a separate variable p_i for each distance in the sum and add additional constraint $p_1 = \cdots = p_m$. We suppose that there is a network of multiple agents, each holding a measure $\{\mu_1, \ldots, \mu_m\}$ and being able to sample from this measure. This network is represented by a fixed *connected undirected graph* $\mathcal{G} = (V, E)$, where V is the set of m nodes, and E is the set of edges. We assume that the graph $\mathcal{G}$ does not have self-loops. The network structure imposes information constraints, specifically, each node i has access to μ_i only and can exchange information only with its immediate neighbors, i.e., nodes j s.t. $(i, j) \in E$. We define the Laplacian matrix $\tilde{W} \in \mathbb{R}^{m \times m}$ of the graph $\mathcal{G}$ as

$$\forall i, j \in V \; \tilde{W}_{ij} = \{-1, (i, j) \in E; \; \mathrm{deg(i), i = j; \; 0, otherwise}\},$$

where $\deg(i)$ is the degree of the node i, i.e., the number of neighbors of the node. Finally, we define the communication matrix (also referred to as an interaction matrix) by $W := \tilde{W} \otimes I_n$ as well as matrix $\sqrt{W} := \sqrt{\tilde{W}} \otimes I_n$, where $\otimes$ denotes the Kronecker product of matrices. One can show that

$$\sqrt{W}\mathrm{p} = 0 \;\text{ if and only if }\; p_1 = \cdots = p_m,$$

where stacked column vector $\mathrm{p} = [p_q, \ldots, p_m]^T$, and equivalently rewrite problem (2) for a distributed setup as the maximization problem with linear equality constraint

$$\max_{\substack{p_1,\ldots,p_m \in S_1(n) \\ \sqrt{W}\mathrm{p}=0}} -\frac{1}{m} \sum_{i=1}^{m} \mathcal{W}_{\gamma,\mu_i}(p_i). \tag{3}$$

Dual approach to distributed optimization

The algorithmic approach is based on constructing a dual problem to (3). To construct it, we introduce a vector of dual variables $\boldsymbol{\lambda} = [\lambda_1^T, \cdots, \lambda_m^T]^T \in \mathbb{R}^{mn}$ for the constraint $\sqrt{W}\mathrm{p} = 0$ and write the Lagrangian dual problem for (3)

$$\min_{\boldsymbol{\lambda} \in \mathbb{R}^{mn}} \max_{p_1,\ldots,p_m \in S_1(n)} \left\{ \frac{1}{m} \sum_{i=1}^{m} \langle \lambda_i, [\sqrt{W}\mathrm{p}]_i \rangle - \mathcal{W}_{\gamma,\mu_i}(p_i) \right\} = \min_{\boldsymbol{\lambda} \in \mathbb{R}^{mn}} \frac{1}{m} \sum_{i=1}^{m} \mathcal{W}^*_{\gamma,\mu_i}([\sqrt{W}\boldsymbol{\lambda}]_i), \tag{4}$$

where $[\sqrt{W}\mathrm{p}]_i$ and $[\sqrt{W}\boldsymbol{\lambda}]_i$ denote the i-th n-dimensional block of vectors $\sqrt{W}\mathrm{p}$ and $\sqrt{W}\boldsymbol{\lambda}$ respectively, , and $\mathcal{W}^*_{\gamma,\mu_i}(\cdot)$ is the Fenchel-Legendre transform of $\mathcal{W}_{\gamma,\mu_i}(p_i)$. To make the following lemma simpler, we change the variables $\boldsymbol{\xi} = \sqrt{W}\boldsymbol{\lambda}$.

Lemma 1. For each fixed probability measure μ, $\mathcal{W}^*_{\gamma,\mu}(\cdot)$ is a smooth function explicitly expressed as an expectation of a function of additional random argument. Moreover, its gradient is Lipschitz-continuous w.r.t. the Euclidean norm and its l-th component is

$$[\nabla \mathcal{W}^*_{\gamma,\mu}(\xi)]_l = \mathbb{E}_{Y\sim\mu} \frac{\exp(([\xi]_l - c_l(Y))/\gamma)}{\sum_{\ell=1}^{n} \exp(([\xi]_\ell - c_\ell(Y))/\gamma)}, \; l = 1,\ldots,n,$$

where $Y \sim \mu$ means that random variable Y is distributed according to measure μ, and $c_l(Y)$ is the cost function at the point Y.

From Lemma 1 and the expression (4) for the dual objective, we can see that the *dual* problem (4) is a smooth stochastic convex optimization problem. Note that we not only need to solve the dual problem, but also need to reconstruct an approximate solution for the primal problem (3), which is the barycenter. Recently, an accelerated-gradient-based approach was shown [3] to give better results than the ubiquitous Sinkhorn's algorithm for Wasserstein distance. Moreover, accelerated gradient methods have natural extensions for the decentralized distributed optimization setting, but existing algorithms can not be applied to the barycenter problem in our setting of continuous distributions. Thus, we develop a novel accelerated primal-dual stochastic gradient method for a general smooth stochastic optimization problem, which is dual to some optimization problem with linear equality constraints. Let us illustrate the idea of this method applied to the Wasserstein barycenter problem.

Each node i has access to its own distribution μ_i and has access to its component $\mathcal{W}^*_{\gamma,\mu_i}(\xi)$ of the dual objective (4) via stochastic samples of its gradient $\widetilde{\nabla}\mathcal{W}^*_{\gamma,\mu_i}(\xi)$ defined using Lemma 1. Stochastic gradient descent step for problem (4) can be written separately for each variable ξ_i, $i = 1, \ldots, m$

$$\xi_i^{(k+1)} = \xi_i^{(k)} - \alpha \sum_{j=1}^{m} [W]_{ij}\, \widetilde{\nabla}\mathcal{W}^*_{\gamma,\mu_j}(\xi_j^{(k)}),$$

where k is the iteration number. The nice structure of this update is given by the structure of the matrix W, i.e., to calculate the step in variable ξ_i, stochastic approximations $\widetilde{\nabla}\mathcal{W}^*_{\gamma,\mu_i}(\xi)$ are only required from the neighbors of i, see the illustration in Figure 3. Acceleration makes the algorithm more complicated, but allows to obtain faster convergence rate. Averaging the stream of stochastic gradients $\widetilde{\nabla}\mathcal{W}^*_{\gamma,\mu}(\cdot)$, given in Lemma 1, through iterations, we obtain an approximation for the barycenter. For simplicity, we present the main theorem in the case of discrete probability measures μ_i, $i = 1, \ldots, m$, each having support size n.

Theorem 1. After $N = O\left(\frac{\sqrt{n}}{\varepsilon}\right)$ iterations and $O\left(\frac{mn^{2.5}}{\varepsilon}\right)$ arithmetic operations, the proposed algorithm outputs $p_1^{(N)}, \ldots p_m^{(N)} \in S_n(1)$, s.t.

$$\frac{1}{m}\sum_{i=1}^{m} \mathcal{W}_{\gamma,\mu_i}(p_i^{(N)}) - \frac{1}{m}\sum_{i=1}^{m} \mathcal{W}_{\gamma,\mu_i}(p^*) \le \varepsilon, \tag{5}$$

where p^* is the barycenter.

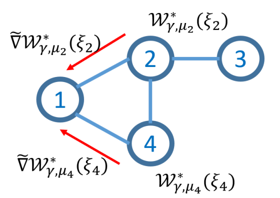

***Fig. 3:** Neighbors send their gradients to agent 1, so that it can make a step*

Figure 4 shows a simple example of an application of Wasserstein barycenter to medical image aggregation where we have 4 agents connected over a cycle graph, and each agent holds a magnetic resonance image (256×256). The idea is to reconstruct the brain from images with different angles of the head.

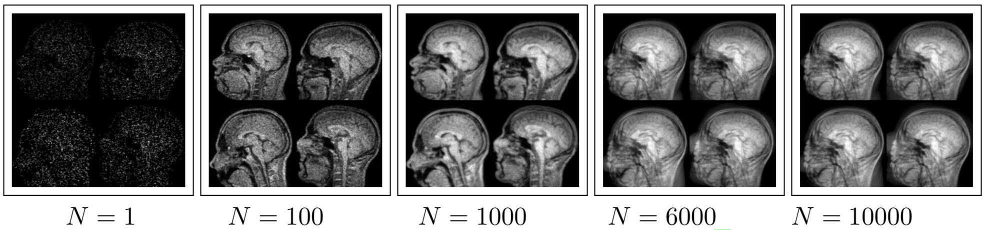

Fig. 4: *Barycenter of MRI images of human brains*

Conclusions and outlook

Optimal transport distances and barycenters provide a useful tool to analyze data of complicated nature, such as images, texts, protein sequences, videos, etc. However, these good practical results come for a price of intensive computations, which in the Big Data applications can not be performed on a single computer, and distributed computations should be used. For this reason we provided our distributed primal-dual accelerated gradient method based on the state-of-the-art entropy-regularized approach which allows to solve the Wasserstein barycenter problem even for large-scale setup: large set of measures having large size of support.

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1.3 A Novel Stochastic-Deterministic Approach for the Simulation of Population Balance Systems

Volker John and Robert I.A. Patterson

Introduction

Population balance systems (PBSs) model the behavior of particles in flows. In these models, the behavior of the particles in the mean is of interest. To this end, a function called *particle size distribution* (PSD) is introduced and a so-called *population balance equation* (PBE) is derived that models, e.g., the mean growth, transport, nucleation, and agglomeration (aggregation, collision growth) of particles. The PSD depends not only on time and space, as, e.g., the flow field or temperature field of the considered process, but it depends also on properties of the particles, so-called *internal coordinates*. Altogether, a PBS constitutes a system of partial differential and integro-partial differential equations, where the equations for the PSD are defined in a higher dimensional domain than the other equations. Applications that were considered in FG 3 in the past years came from chemical engineering and meteorology (droplets in clouds).

Within the DFG Priority Programme 1679 *Dynamic Simulation of Interconnected Solid Processes*, several methods for the numerical simulation of PBSs have been explored. In [1], a direct discretization of the PBE in the higher dimensional domain and an operator splitting scheme were compared. In the previous years, a completely different approach for solving the PBE has been studied, which combines the expertise of FG 3 for the simulation of problems from Computational Fluid Dynamics (CFD) and of FG 5 for the simulation of particle populations with stochastic simulation algorithms (SSAs).

Some features of the novel method

The CFD part of the studied applications consists of equations for the flow field (incompressible Navier–Stokes equations) and balance equations for the energy (temperature) and dissolved species (concentrations), which are of convection-diffusion type. These equations are simulated with deterministic methods, using, e.g., Large Eddy Simulation (LES) turbulence models and stabilized finite element methods of flux correction type. These equations are coupled with the PBE

$$\frac{\partial}{\partial t} f + \boldsymbol{u} \cdot \nabla f = \mathcal{C}(f) + \mathcal{G}(c, T, f) \quad \text{in } (0, t_{\text{end}}) \times \Omega \times [0, \infty), \tag{1}$$

where the sought function f $[1/\mathrm{m}^3\mathrm{kg}]$ is the particle number density. In (1), $\boldsymbol{u}$ $[\mathrm{m/s}]$ denotes the velocity field, T $[\mathrm{K}]$ the temperature, t_{end} $[\mathrm{s}]$ a final time, Ω the spatial domain, $\mathcal{C}(f)$ the coagulation term, and $\mathcal{G}(c, T, f)$ the growth term.

The solution of (1) is usually the most challenging part of the simulation of a PBS. Direct discretizations apply a stabilized finite difference or finite element method in the higher dimensional do-

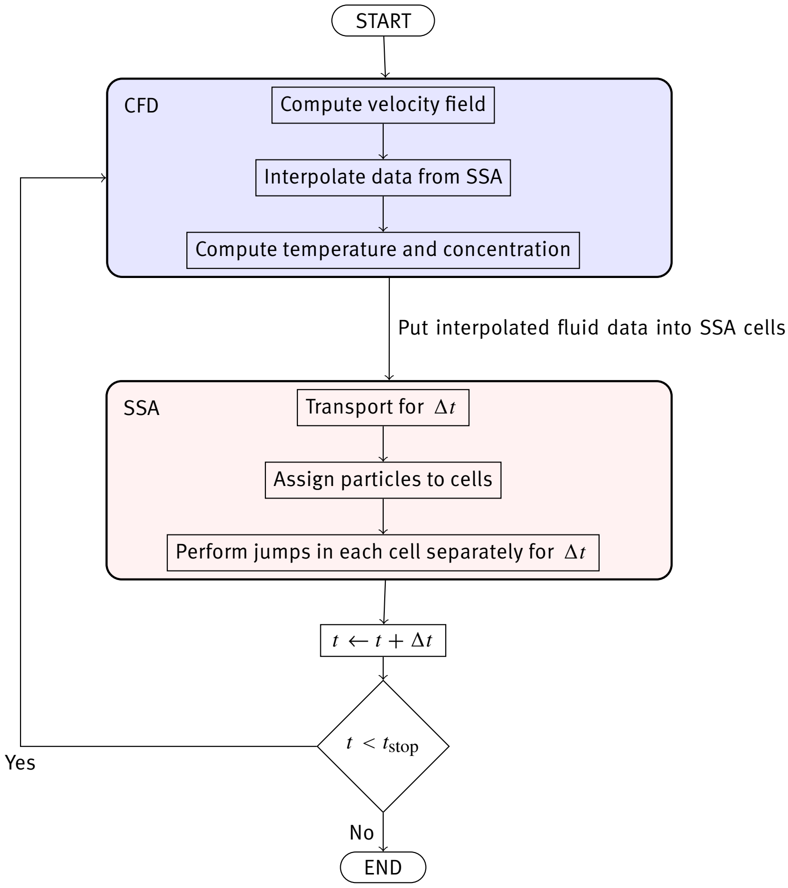

Fig. 1: *Schematic sketch of the coupled simulation via a splitting scheme*

main. Operator splitting schemes solve first an equation with respect to the spatial coordinate and then a problem with respect to the internal coordinate, thereby introducing a splitting error. In these deterministic methods for solving (1), the coagulation term is an integral of convolution type, whose efficient calculation is challenging.

In the novel method, an SSA is used for the numerical solution of (1), which is based on a method presented in [7]. In this algorithm, the behavior of the particles is modeled by stochastic (Markov) jump processes, concretely, the growth of particles, the coagulation of particles, and the insertion of particles entering the domain. It is based essentially on two sources: Bird's direct simulation Monte-Carlo algorithm for the Boltzmann equation [3] and Gillespie's stochastic algorithm for the simulation of collision growth phenomena in clouds [5]. While the Bird algorithm provides a way to deal with the convective transport part (by splitting), the Gillespie algorithm gives a tool to treat the coagulation part of the equation (by formulating a jump process). The domain is partitioned into cells and the physical particle population within each cell is approximated by an ensemble of computational particles. This approximation is justified by mathematical convergence proofs [6]. For a detailed description of the individual stochastic jump processes, see [2].

A sketch of the numerical scheme for coupling CFD and SSA is presented in Figure 1. In each discrete time, the computation is split into two steps. First, the deterministic CFD equations are solved

Table 1: *ASA flow crystallizer, quantities of interest at the outlet: (Number) mean particle diameter* $\bar{d}$ *and standard deviation* σ

Quantity	$\bar{d}$ [μm]		σ [μm]	
	experiment	simulation	experiment	simulation
Setup 1	243	238	65	85
Setup 2	214	215	50	73
Setup 3	192	189	49	56
Setup 4	166	176	44	54

with the in-house code ParMooN using the data from the SSA from the previous time instance. Then, the CFD data are interpolated via a custom C++ interface to the in-house Brush. As the second main step of the splitting scheme, the behavior of the particles is simulated.

There is a close coupling of the two parts. The velocity field enters the PBE, compare (1), and the coagulation kernel might depend on the temperature and the velocity field. The stochastically computed PSD appears in source and sink terms on the right-hand side of the energy and concentration balances.

Simulations of an ASA flow crystallizer: Proof of concept

A flow crystallizer consists mainly of a long, thin tube that is usually coiled up for practical reasons. A three-component dispersion is pumped into the tube at the inlet. The dispersion contains a solvent, a solute, and seed crystals, which consist of the same material as the solute; it is warm and highly saturated. As the dispersion flows through the tube, crystal sizes change due to nucleation, surface attachment growth, particle collision growth, or particle breakage. Flow crystallizers are a promising technology in pharmaceutical production. They allow for a regular particle growth that can be accurately controlled. Regular shape and size are desirable properties of crystals that are used in medicines, as crystal morphology influences medicinal effects. From a technical point of view, flow crystallizers are interesting for two more reasons. Firstly, they can be operated continuously. Secondly, scale-up from laboratory to industrial production is relatively easy.

The flow crystallizer that was in the focus of our simulations was described in [4]. The crystalline model substance was acetylsalicylic acid (ASA $=$ aspirin) and the solvent was almost pure ethanol (EtOH). In the experimental setup, as described in [4], the crystallization takes place in a $15\,\mathrm{m}$ long polysiloxane tube that is coiled up. The inner diameter of the tube is $2\,\mathrm{mm}$. Experimental data for quantities of interest for four setups are listed in Table 1.

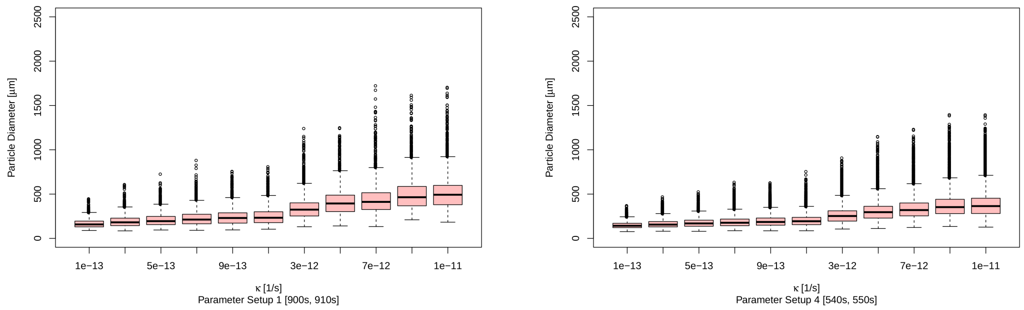

Fig. 2: *Simulated flow crystallizer PSDs at the exit of the crystallizer for different coagulation parameters κ. Boxes indicate the first quartile, median and third quartile of the particles, whiskers the main range; circles are outliers.*

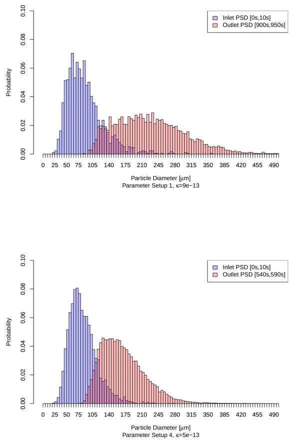

Fig. 3: *ASA flow crystallizer, simulation results for two setups, best coagulation parameter κ, PSDs at inlet and outlet are shown*

The setup of the numerical simulations applied several simplifications compared with the experimental setup. The most important one was that the tube was straightened out such that it was possible to pursue an axisymmetric 2D approach. The flow field has the Hagen–Poiseuille profile. As usual in applications, an appropriate model for the coagulation kernel had to be found. It turned out that the constant kernel with an appropriate choice of the coagulation parameter κ could be used successfully. Results for different values of κ for one setup are presented in Figure 2. For the two setups 1 and 2, $\kappa_1 = 9 \cdot 10^{-13}$ $1/\mathrm{s}$ and $\kappa_2 = 10^{-12}$ $1/\mathrm{s}$ proved to be the best choices. For the other setups, the best parameters were half an order of magnitude smaller, $\kappa_3 = 6 \cdot 10^{-13}$ $1/\mathrm{s}$ and $\kappa_4 = 5 \cdot 10^{-13}$ $1/\mathrm{s}$. Computational results that were obtained with these κ are given in Table 1. One notices that the mean diameter could be hit quite well. The standard deviation of the computed PSDs is about 1.1 to 1.5 times as high as the standard deviation of the experimental data. The change of the PSD from the inlet to the outlet is illustrated in Figure 3.

Simulations of a fluidized bed crystallizer

Fluidized bed crystallizers are crystallization devices that are used in chemical engineering in order to grow crystal fractions into larger sizes. A photograph of a fluidized bed crystallizer is supplied in Figure 4. The central unit of the system is a bulgy vessel, here it has the form of an upside-down bottle of 50 cm height. The vessel is part of a closed circuit of a streaming suspension, which contains those chemical ingredients that are necessary to excite the desired crystal growth mechanisms. The flow enters at the bottom and exits through a filter at the top, entering a system of tubes and pumps, leading it back in at the bottom. In contrast to the tube crystallizer, collision growth is mainly responsible for the crystal size gain. Therefore, the resulting particles are aggregates, bringing along the distinct properties of crystal aggregates: greater surface, higher porosity, and in general less regular shapes than monocrystals gained by surface attachment growth. The main reason for particle collision growth inside a fluidized bed crystallizer is the non-laminar velocity field. It is responsible for particles following non-aligned trajectories, resulting in many collisions of particles of different sizes in various angles. A certain percentage of those collisions are “effective” in the sense that a solid bridge between two crystals gets formed: an aggregate is born.

The computational domain, Figure 5, comprises the inner part of the crystallization vessel. Since the flow field is turbulent, a Smagorinsky LES model was used. A snapshot of the velocity can be seen in Figure 6.

Fig. 4: *An experimental fluidized bed crystallizer, built up by the Chair for Process Systems Engineering at Otto-von-Guericke Universität Magdeburg*

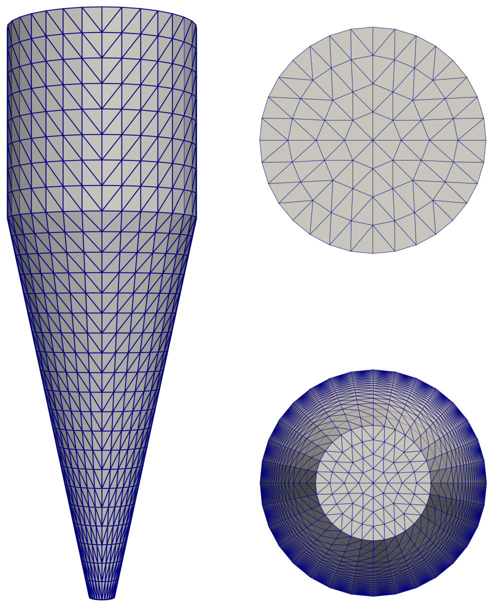

Fig. 5: *Fluidized bed crystallizer, geometry and mesh used in the simulations. The inlet is cut off, the domain Ω_x is regularly decomposed into 10752 tetrahedra of almost the same height. Left: Front view. Right: Top and bottom view.*

Important new aspects of this application, compared with the tube crystallizer, are that collisions of particles with the wall occur and that the sedimentation of particles has to be taken into account. Particles colliding with the wall are reflected. The developed reflection algorithm is described in detail in [2]. It is restricted to convex domains. Concerning sedimentation, a model for spherical particles, which was appropriately scaled, was applied. The Brownian kernel was used for the coagulation term.

Numerical results for the development of the average particle diameter according to the sample height (z-coordinate) in the crystallizer are displayed in Figure 7. It can be seen that at different heights of the crystallizer, different average particle diameters occur, where the largest particles are close to the bottom ($z = 0$). This situation is exactly the situation longed for in practice, since it enables to harvest particles of desired sizes at certain heights of the crystallizer.

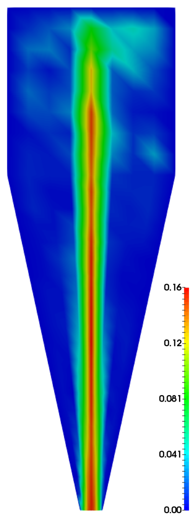

Fig. 6: *Fluidized bed crystallizer, flow field (norm of the velocity in $\frac{m}{s}$) in a vertical cut plane after 200 s*

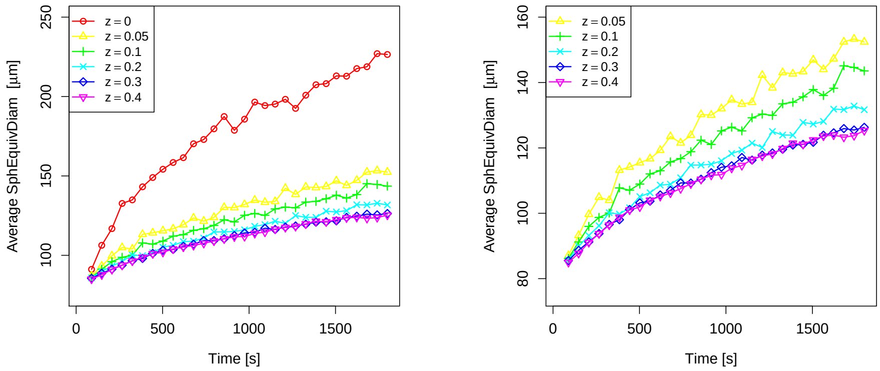

Fig. 7: *Fluidized bed crystallizer, temporal development of the spatially averaged sphere equivalent particle size diameter in different heights in the crystallizer device. Height z is given in m above the inlet. The right picture shows details of the left one (without the particles directly above the inlet).*

Conclusions and outlook

The numerical results of the batch crystallizer still have to be assessed against experimental data, which have been obtained from our collaborators in the DFG project from the University of Magdeburg. From the modeling point of view, more sophisticated models for the agglomeration kernel and the sedimentation are needed. In future, applications with more complex particles shall be studied, a situation for which the used SSA is designed. For increasing the efficiency of the simulations, an MPI parallelization of the SSA method and the interface is planned.

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1.4 MIMESIS – Mathematics and Materials Science For Steel Production and Manufacturing

Najib Alia, Prerana Das, Dietmar Hömberg, and Volker John

Introduction

Almost all manufacturing sectors, from construction to transport to consumer goods, are largely based on the utilization of steels. Steel products often compete favourably with alternative material solutions in cost efficiency and life cycle analyses. The last fifteen years have seen the development of ever more refined high-strength and multiphase steels with purpose designed chemical compositions allowing for significant weight reduction, e.g., in automotive industry. The production of these modern steel grades needs a precise process control, since there is only a narrow process window available in which the desired physical properties are defined. In combination with component walls getting thinner and thinner, these new steels make also new demands on a more precise process control in metal manufacturing processes, such as welding and hardening.

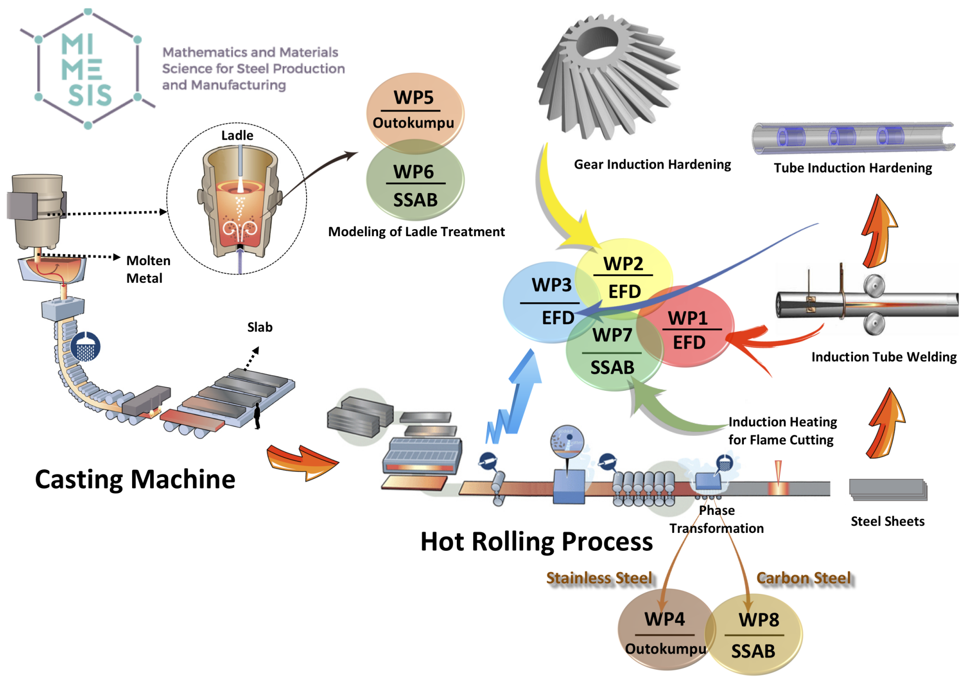

Fig. 1: *MIMESIS – Ph.D. projects in a nutshell*

Improved and optimized process control requires quantitative mathematical modeling, simulation, and optimization of the complex thermal cycles and thermal gradients experienced by the processed material. Such models require an understanding of the behavior of the materials from a materials science and phase transformations perspective. Unfortunately, it is almost impossible for companies to find graduates combining deep knowledge in materials science with expertise in mathematical modeling, simulation and optimization.

To fill this gap, five partners from steel production (Outokumpu and SSAB in Finland) and steel manufacturing (EFD Induction in Norway), from materials science (University of Oulu, Finland) and applied mathematics (WIAS) established the European Industrial Doctorate program on *"Mathematics and Materials Science for Steel Production and Manufacturing (MIMESIS)"*, where eight Ph.D. projects are jointly carried out. The students spent at least 18 months with an industry partner, thereby encouraging inter-sectoral mobility. Finally, the project has a clear interdisciplinary makeup: Four Ph.D. students are from materials science and four from mathematics.

The research is focussed on three major topics along the process chain for steel production and manufacturing. Two theses are related to secondary metallurgy in the ladle considering computational fluid dynamics models of ladle treatments (WP5) and optimal control of ladle stirring (WP6, see the subsection on optimal control of ladle stirring), and two theses are concerned with phase transformations during steel production (WPs 4&8). Two theses concern the induction hardening process: One is on the hardening of helical and bevel gears by an optimized single or multi-frequency approach, and the other is a novel idea about the hardening of the inner surface of pipes (WPs 2&3). One thesis studies a prototype set-up for inductive pre- and post-heating in the thermal cutting of steel plates and one is related to high-frequency welding of steel tubes (WPs 1&7). The latter will be discussed in more detail in the subsection on modeling and simulation of tube welding.

A specific highlight of the programme were customized three-month courses on steelmaking, physical simulation and testing of steels in Oulu and on numerical simulation and optimization in Berlin. Additionally, the early stage researchers also had tailored on-site industrial trainings offered by three industrial partners.

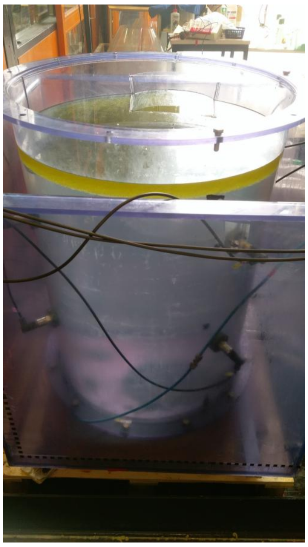

Fig. 2: *Photo of the experimental ladle in the laboratory of the University of Oulu*

Optimal control of ladle stirring

Ladle stirring is a process of steel-making where liquid steel is stirred by a gas injected from the bottom of the tank (ladle). The objective of the project is to improve the control of ladle stirring to enhance the cleanliness of liquid steel. The objective will be reached by developing a numerical model together with vibration measurement systems to monitor the actual stirring and optimize it. Better control of stirring gives a possibility to reduce the formation of non-metallic inclusions and to optimize the treatment time and gas consumption during the process.

Numerical model of a laboratory-scale ladle stirring. Making measurements during ladle stirring in real industrial conditions is a complex task due to the extreme environment. It is, therefore, usual to reproduce the process in laboratory conditions by using water instead of liquid steel and air instead of argon gas (see Figure 2).

A numerical model is developed in order to study and optimize mathematically the stirring flow. The flow is computed using the single-phase incompressible Navier–Stokes equations for the liquid steel and a buoyancy force for the gas phase [1] (see Figure 3). In addition, the Smagorinsky turbulent viscosity is applied to resolve the turbulence of the flow (Reynolds number $\sim$ 100,000). The model is solved with the in-house code ParMooN developed by RG 3 *Numerical Mathematics and Scientific Computing* [2].

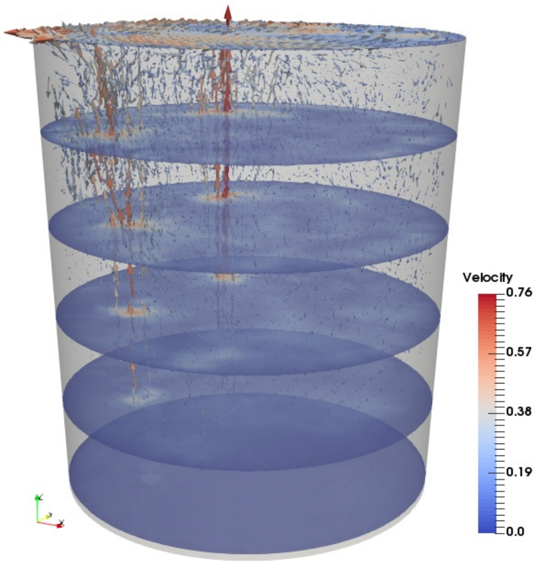

Fig. 3: *Numerical ladle stirring: Snapshot of the velocity field computed with* ParMooN *with the Smagorinsky turbulent model*

One reason of simulating a laboratory-scale ladle rather than an industrial one is the availability of experimental measurements. They can indeed be advantageously used to adjust numerical parameters, such as the turbulent viscosity constant, and to validate the model (see Figure 4). The results obtained so far show how simplified modeling assumptions (two-phase flows reduced to a single-phase flow) can lead to reasonable results.

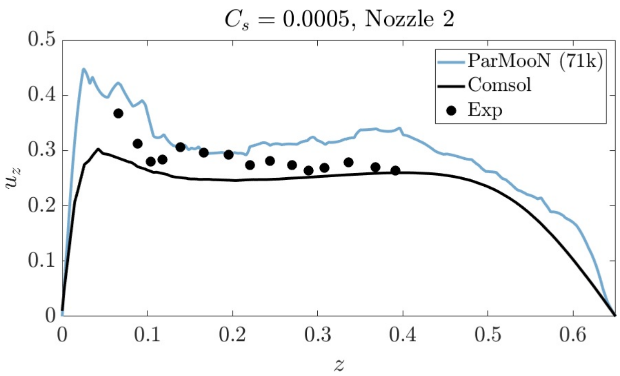

Fig. 4: *Validation of the numerical flow model: Comparison of the vertical velocity component between numerical results and experimental measurements*

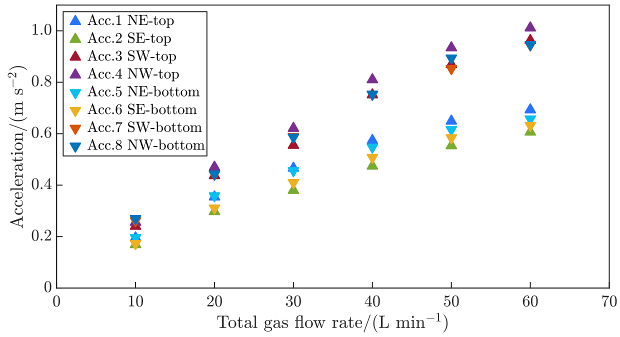

Fig. 5: *Evolution of RMS values of vibrations with gas flow rate*

After validating the numerical model, the objective is to formulate and to solve an optimal control problem to make the stirring more efficient. Several control parameters are considered, e.g., the intensity of the gas flow rate, its evolution in time, or the position of the nozzles. The solution can then be used in combination with vibrations measurements to make the operations more efficient and easier to control for the operators.

Experimental vibrations measurements. In this project, in addition to the numerical investigation, an experiment was conducted using vibrations sensors on the ladle wall. Since it is of industrial interest to use the vibrations to monitor and control automatically the process, it is of importance to study the vibrations signals measured by accelerometers, the relationship between the mixing intensity in the steel bath and the vibrations level, the effect of the sensors' positions on the signals, etc. It is shown, for example, that the vibrations increase significantly with the injected gas flow rate (see Figure 5). Moreover, the position of the accelerometers has an influence on the measured signal. By placing several sensors at relevant positions, it is possible to describe precisely the mixing intensity in the ladle, as well as stirring problems, such as gas nozzle clogging or loss of stirring efficiency.

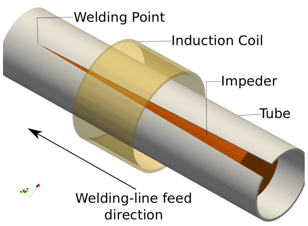

Fig. 6: *High-frequency induction welding of a steel tube*

Modeling and simulation of tube welding

High-frequency induction welding is widely used, especially in the production of superior quality oil and gas pipes and structural tubes. A steel strip is cold-formed into a tubular shape in a continuous roll forming mill. The strip edges are electromagnetically heated and joined mechanically by pushing the strip edges against each other to form the longitudinally welded tube (see Figure 6).

The welded joint, as seen in the transverse cross section of a welded tube, is a very narrow zone compared to the tube diameter. The strip edges are heated to almost melting temperature and are pushed against each other in the viscoplastic state to form the welded joint where crystallographic texture and microstructural changes appear.

The electromagnetic heating of the tube is analogous to transformer theory. The coil is the primary current source, the strip is where the current is induced, and the impeder acts as a magnetic core. The entire setup, coil current and frequency determine the amount of the induced current in the tube.

High-frequency alternating current is supplied to the induction coil. This induces eddy currents in the strip under the coil. The induced current can follow the principal paths indicated in Figure 7 to complete the circuit. Along the strip edges, it can flow downstream from the coil towards the welding point or away from the coil in the upstream direction. At any strip cross section, the current can follow a path either along the outer circumference or the inner circumference. The goal of high-frequency induction welding is to maximize the current density in the strip edge downstream, towards the welding point.

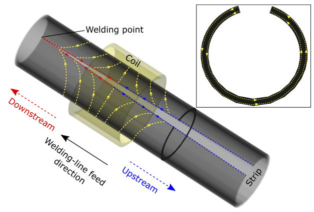

Fig. 7: *Schematic current path in the tube*

The relative positioning of the strip, induction coil, and impeder is very important to obtain an efficient heating process. The geometric shape of the opening between the strip edges is usually a Vee shape. Sometimes it is distorted by spring-back due to the mechanical forming of the strip. This also affects the current distribution. Further important process parameters are the coil current and welder frequency.

For a better understanding of the complex interactions between the above parameters, numerical simulation is an indispensable tool. In [3], we present the first comprehensive simulation approach for high-frequency induction welding in 3D. Its main novelties are a new analytic expression for the space-dependent velocity of tubes accounting for arbitrary Vee-angle and spring-back and a stabilization strategy, which allows us to consider realistic welding-line speeds.

Mathematical model and numerical realization. The mathematical model comprises a harmonic vector potential formulation of Maxwell's equations and a quasi-static, convection-dominated heat equation coupled through the Joule heat term and nonlinear constitutive relations.

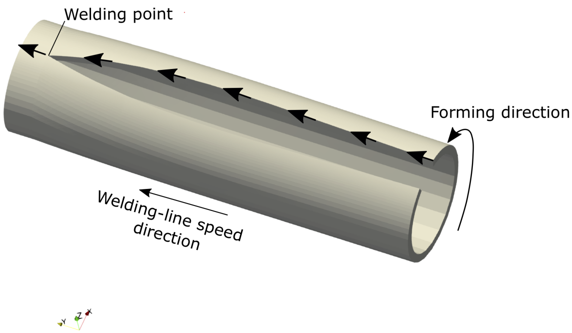

Fig. 8: *Local velocity to represent feed velocity and forming*

An important effect that needs to be accounted for is the computation of velocity in the strip. After the welding point is reached, the velocity has only a component in the feeding direction, while before, the velocity varies locally with non-vanishing radial and angular components. To obtain the correct temperatures especially close to the strip edge, it is crucial to use the correct locally varying velocity for the simulation. Figure 8 shows the resulting local velocity vectors for selected points on the strip opening for a spring-back tube opening. Instead of a constant velocity solely in y-direction one can see that now the velocity follows the contour of the opening; for details, we refer to [3].

The heat equation is discretized by linear nodal finite elements. To account for high speeds somewhere in the range of 40m/min to 200m/min, the Streamline Upwind Petrov Galerkin (SUPG) method is used. The discretization of Maxwell's equations is done with Nédélec elements of lowest order. The magnetization depends both on the temperature and the magnetic field. For fixed temperature this nonlinearity is resolved numerically based on an averaging approach [4]. The coupled system is iteratively decoupled and solved using a fixed-point iteration.

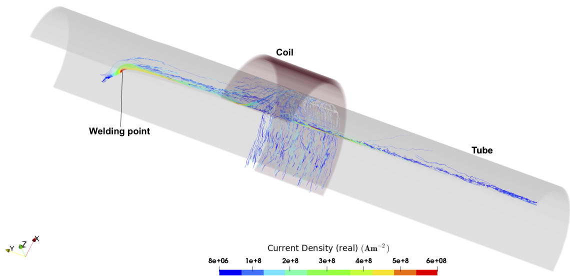

Fig. 9: *Current path in the tube*

Simulation results. Figure 9 shows the current density distribution in the strip edge with current concentration both in the downstream and upstream directions and a maximum close to the weld point. Examples of temperature distribution in the welded strip are depicted in Figure 10 for two different Vee-openings and a spring-back distorted opening. The strip edges are heated to very high temperatures because of Joule heating from eddy current concentration. The velocity function incorporates the mechanical forming of the strip into a tube in addition to the welding-line velocity.

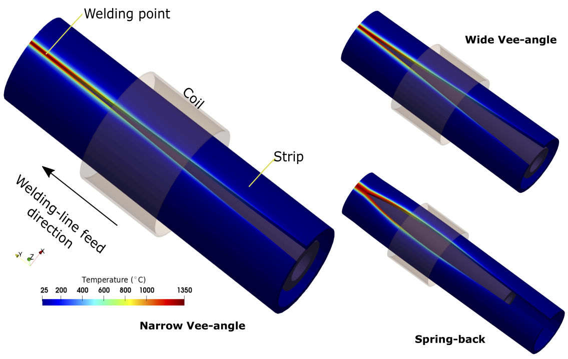

Fig. 10: *Temperature distribution in the tube for different openings*

Conclusion and outlook

Concerning the optimization of ladle stirring, the project revealed how complex the industrial problem is, and how important it is to decompose the different issues into different steps and work on simplified aspects of the problem, e.g., laboratory-scale experiment instead of real ladle and single-phase flow instead of multiphase flows. The experimental vibrations measurements have led to innovative ideas which were not considered so far in the industry, namely, use of several sensors simultaneously and at different positions to have a more precise knowledge of the actual stirring in the ladle.

The next step consists of implementing such ideas in the industrial process. Several opportunities appear from the perspective of applied mathematics: Modeling and computation of the fluid-structure interaction to predict the vibrations level of the ladle, or application of deep learning techniques to analyze the big amount of data measured by the vibrations to find out the vibrations level corresponding to optimal stirring.

For high-frequency induction welding a three-dimensional model has been developed. It is a nonlinearly coupled system of Maxwell's equations and the heat equation. The results show a temperature distribution in the strip edges that develops as expected from previous studies and visual observations of the process. A wider Vee-angle results in a wider heat-affected zone. Increasing the frequency reduces the width of the heat-affected zone.

This new three-dimensional simulation tool will provide a basis for an optimization of the design of the welder, especially with respect to the dimensioning of induction coil, impeder, and the configuration of these relative to the steel strip. Future work will include the study of the mechanics of the material squeeze-out when the strip edges are joined together after heating.

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1.5 Electrothermal Behavior of Organic Semiconductors

Duy-Hai Doan, Jürgen Fuhrmann, Annegret Glitzky, and Matthias Liero

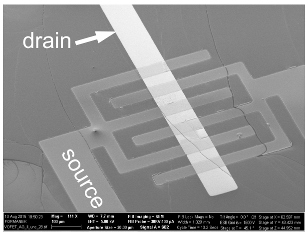

Fig. 1: *Organic thin-film transistor developed at IAPP*

Organic electronics is a future-oriented green technology using carbon-based semiconductor materials. Such materials can lead to innovative electronic components with fine-tuned properties and promise more sustainable, eco-friendly electronic technologies. The potential for greater sustainability extends across the entire life cycle of organic electronics, beginning with the use of materials that are synthesized rather than mined from the earth, over low temperature production of devices, and ending with potentially biodegradable or recyclable devices.

Presently, organic semiconductors are already used in photovoltaics, in smartphone displays, as sensors in cameras, and increasingly in TV screens. The technological adaption to other applications such as advanced lighting applications and thin-film transistors is still at an early stage. However, the fast pace in the development of new organic materials with fine-tuned properties yields the potential for smart 3D vertical structures with desired electronic behavior.

Innovative lighting applications can also profit from the fascinating properties of organic light-emitting diodes (OLEDs), e.g., large-area surface emission, semi-transparency, and mechanical flexibility. Since lighting requires a much higher brightness than displays, also higher currents occur. These cause substantial Joule self-heating accompanied by unpleasant brightness inhomogeneities of the OLED panels. An explanation for these inhomogeneities starts with the observation that the charge-carrier transport in organic semiconductors is realized by hopping between adjacent molecules, which is a temperature-activated process. In connection with Joule self-heating this leads to a strong positive feedback between (i) power dissipation, (ii) temperature, (iii) conductivity, and (iv) current flow. This results in complicated nonlinear behavior such as S-shaped current-voltage relations with regions of negative differential resistance (NDR) and hysteresis phenomena, see [3].

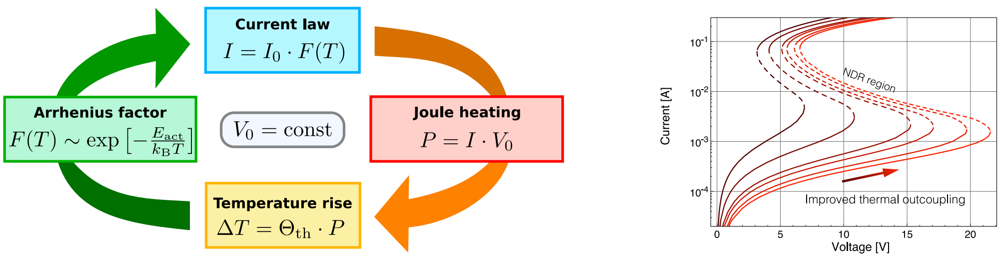

Fig. 2: *Left: Electrothermal feedback loop.*
Right: Simulated S-shaped current-voltage relations for different thermal outcoupling.

In a simplified model (see Figure 2 left), a constant voltage V_0 induces a current I in the device, which in turn is related to a power dissipation P by Joule self-heating. In proportion to the thermal resistance Θ_{th}, the temperature T of the structure increases. Assuming an Arrhenius-like conductivity-temperature law $F(T)$ with an activation energy E_{act}, this leads to a higher current. A feedback originates that can be treated analytically in this simplified setting. The process converges to a stable solution since $F(T)$ saturates. In experimental situations, the destruction of devices due to material degradation can be observed for sufficiently high applied voltages.

The activities on modeling, analysis, and simulation of organic semiconductor devices at WIAS are accompanied by a long-term close collaboration with the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) at TU Dresden. The research was funded by the ECMath-MATHEON projects SE2 "Electrothermal modeling of large-area light-emitting diodes" and SE18 "Models for heat and charge-carrier flow in organic electronics".

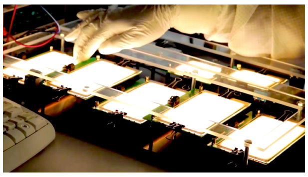

Fig. 3: *OLEDs at IAPP*

First, the electrothermal behavior of organic semiconductors was described by the above simplified model for the total current flow coupled to a global heat balance. Next, this model was extended in [3] by considering spatially resolved electrothermal circuit models where the current and heat flow between electrically and thermally coupled resistors was balanced to explain the brightness inhomogeneities in large-area OLEDs at high power. This circuit model reproduces the experimentally observed S-shaped NDR behavior. Additionally, a new operation mode, called "switched-back" mode, where local currents are even decreasing was discovered.

p-Laplace thermistor models

Motivated by the successful circuit model approach in [3], a thermistor model based on partial differential equations (PDEs) was introduced in Liero et al. ZAMP 2015 offering more flexibility with respect to device geometry and material variations. In this PDE thermistor model, the balance equation for the total current, driven by a potential φ, is coupled to the heat equation:

$$-\nabla \cdot j_{\text{tot}}(x, T, \nabla\varphi) = 0, \qquad -\nabla \cdot \big(\lambda(x)\nabla T\big) = H(x, T, \nabla\varphi)\,, \tag{1}$$

with electrical current density j_{tot}, heat conductivity λ, and Joule heat term H. The special features of the model are a non-Ohmic conductivity law as well as an Arrhenius-like temperature law incorporated by a power law in the function j_{tot} and a temperature factor, respectively,

$$j_{\text{tot}}(x, T, \nabla\varphi) = \kappa_0(x)F(x, T)|\nabla\varphi|^{p(x)-2}\nabla\varphi, \quad F(x, T) = \exp\Big[-\frac{E_{\text{act}}(x)}{k_B}\Big(\frac{1}{T} - \frac{1}{T_a}\Big)\Big].$$

Here, $T_a > 0$ and k_B denote the fixed ambient temperature and Boltzmann's constant. The quantitites κ_0, p, and E_{act} are material-dependent effective conductivity, power law exponent, and activation energy, respectively, which can be extracted from measurements. The first equation in (1) is of $p(x)$-Laplacian type with discontinuous but piecewise constant exponent p. In particular, one has to set $p(x) \equiv 2$ in Ohmic materials such as electrodes and different values $p(x) > 2$ in organic layers. The Joule heat term in the second equation of (1) takes the form

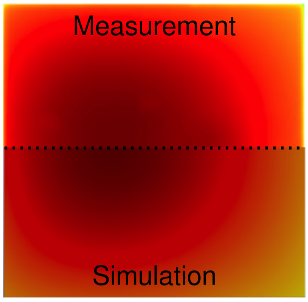

Fig. 4: *Inhomogeneous luminance in large-area OLED*

$$H(x, T, \nabla\varphi) = \eta(x, T, \nabla\varphi)\, j_{\text{tot}} \cdot \nabla\varphi\,,$$

where $\eta(x, T, \nabla\varphi) \in [0, 1]$ is the light-outcoupling factor. The system is complemented by suitable boundary conditions to model the electrical contacts and heat transfer into the environment.

From a mathematical point of view, the system in (1) is challenging for two reasons: First, the treatment of the $p(x)$-Laplacian with discontinuous $x \mapsto p(x)$ requires the notion of non-standard Lebesgue and Sobolev spaces. Second, the right-hand side H of the heat equation is not integrable enough for classical ellipticity theory. Thus, the concept of entropy solutions was used to verify the solvability of the $p(x)$-Laplace thermistor system (1). In two spatial dimensions, higher integrability of solutions was established (see [1] and the references therein).

Using a hybrid finite-volume / finite-element scheme, which preserves the maximum principle for the current flow equation and the positivity of temperature, the system was implemented in a software tool. Through the use of path-following methods (Figure 10), the tool is able to reproduce the experimentally observed electrothermal behavior of organic LEDs with the typical S-shaped current-voltage relations (see Figure 2 right and [6]). Also the appearance of inhomogeneous current distributions (and, hence, brightness inhomogeneities in large-area OLEDs) due to self-heating is captured, see Figure 4. In the simulations, we considered large OLED panels, where the OLED stack is positioned on a glass substrate and covered from above by a transparent, electrically conducting electrode, contacted at the edges. The simulations show that zones with NDR emerge, where, locally, voltages are decreasing and currents are increasing (Figure 5b). These zones spread through the device with increasing external current towards the contacts. Once the contacts are reached, the current-voltage curve of the device shows NDR.

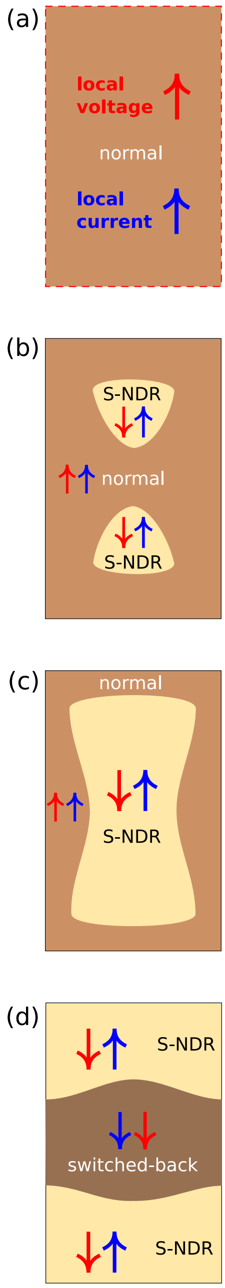

Fig. 5: *Propagation of operation modes in large-area OLED panel: Red and blue arrows indicate increase or decrease of local voltages and currents*

Moreover, the simulations predict the appearance of a new effect related to the electrothermal interplay in large-area OLEDs: Eventually, zones close to the contacts have locally decreasing voltages under growing external current (Figure 5c). However, the lateral heat conduction by the substrate is not high enough to sufficiently warm up central zones of the panel. Then, the growing temperature factor in the conductivity cannot compensate the declining voltage drop in these zones, and the local differential resistance in the central zones has again a positive sign. Since the zones between them and the outer contacts show declining local voltages due to the NDR, local voltages *and* local currents decrease (Figure 5d). For that reason, we call them *switched-back zones*.

This effect has recently been proven experimentally by our partners at IAPP. The fact that the luminance of the OLED lighting panel saturates and even decreases in the center is directly connected to this switched-back effect and the decrease of the local currents there. The presence of switched-back zones also explains why local NDR is observed first farthest away from the edges. In order to have a transition from the normal regime to the switched-back regime, it is inevitable for a certain zone of the device to pass through the NDR regime.

Energy-drift-diffusion models for organic semiconductors

In the empirical thermistor model, electronic details such as electron and hole flow, charge carrier polarization, recombination, and energy barriers at material interfaces are neglected. To be more predictive with respect, e.g., to the diode behavior of advanced OLED concepts or current paths in small-scale devices like organic transistors, a refined description incorporating electron and hole currents, recombinations, and heterostructures is needed. The starting point is an adapted van Roosbroeck system consisting of continuity equations for the electron and hole densities n_e and n_h which are self-consistently coupled to a Poisson equation for the electrostatic potential ψ,

$$\begin{aligned} -\nabla\cdot(\varepsilon\nabla\psi) &= q(C-n_e+n_h), \\ q\partial_t n_e - \nabla\cdot j_e &= -qR, \qquad j_e = -qn_e\mu_e(T,n_e,|\nabla\psi|)\nabla\varphi_e, \\ q\partial_t n_h + \nabla\cdot j_h &= -qR, \qquad j_h = -qn_h\mu_h(T,n_h,|\nabla\psi|)\nabla\varphi_h. \end{aligned} \tag{2}$$

The driving forces in the carrier fluxes are the gradients of the quasi-Fermi potentials $\varphi_{e,h}$. In organic semiconductors, the energy levels are Gaussian-distributed centered at $E_{e,h}$ with disorder parameter $\sigma_{e/h}$ such that the carrier densities $n_{e/h}$ are related to the quasi-Fermi potentials $\varphi_{e/h}$ by Gauss–Fermi integrals, e.g.,

$$n_e = N_{e0}\mathcal{G}\Big(\frac{q(\psi-\varphi_e)-E_e}{k_BT}\Big) = \frac{N_{e0}}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp\Big(-\frac{x^2}{2}\Big)\frac{1}{\exp\big(\frac{\sigma_e x}{k_BT}-\frac{q(\psi-\varphi_e)-E_e}{k_BT}\big)+1}\,\mathrm{d}x, \qquad (3)$$

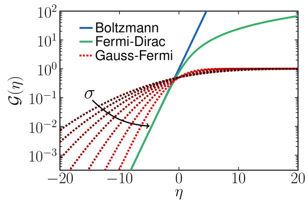

***Fig. 6:** Statistical relation in comparison to Boltzmann and Fermi-Dirac statistics*

see Figure 6. In contrast to classical semiconductors with Boltzmann statistics, this leads to a generalized Einstein relation and results in a nonlinear diffusion enhancement in the relation between drift and diffusion current [2]. The mobility functions $\mu_{e,h}$ for organic semiconductor materials with Gaussian disorder are increasing with respect to temperature, carrier density, and electrical field strength. These dependencies were obtained from numerically solving the master equation for hopping transport in a disordered energy landscape, see Kordt et al., Adv. Funct. Mater. 2015.

Existence and boundedness of stationary solutions for problem (2) in any spatial dimension were verified by Schauder's fixed point theorem. Moreover, in two spatial dimensions, the existence of global weak solutions of the instationary problem was proven by considering a problem with regularized state equations. Its solvability was shown by time discretization and passage to the time-continuous limit. Positive lower a priori estimates for the densities of solutions for the regularized problem that are independent of the regularization level ensure the existence of solutions to the original problem, see [5].

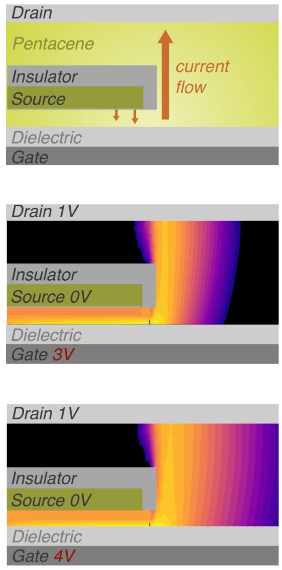

***Fig. 7:** Simulated current density for opening the channel of a vertical organic field effect transistor*

Within the WIAS device simulation tool `ddfermi`, the implementation of the van Roosbroeck system with Gauss-Fermi statistics (3) and typical charge-carrier mobility functions was realized using a finite volume method and a generalized Scharfetter–Gummel scheme [2]. Whereas Figure 8 shows the influence of the disorder parameter σ_e on the electrostatic potential and charge carrier density in a resistor structure, Figure 7 presents simulations for a vertical organic field effect transistor.

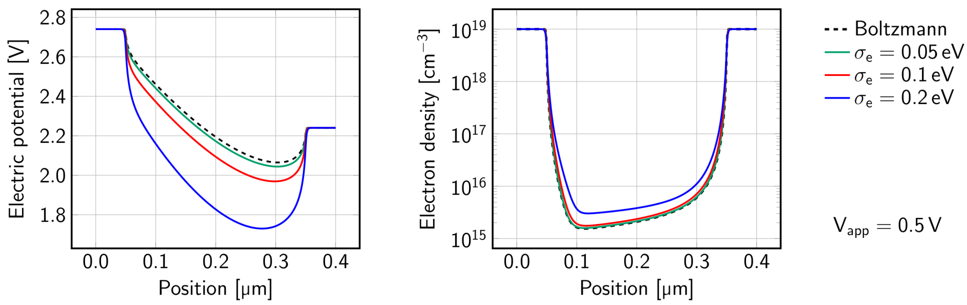

***Fig. 8:** Organic resistor structure: effects of the disorder parameter*

As demonstrated by the (coarser) thermistor model (1), organic devices show a strong interplay of current and heat flow. To include this effect in the drift-diffusion context, the van Roosbroeck system (2) is coupled to a heat equation balancing the produced Joule and recombination heat

$$-\nabla\cdot(\lambda\nabla T) = H, \qquad H = H(j_n, j_p, R). \qquad (4)$$

For the stationary problem energy-drift-diffusion system (2), (4) the existence of solutions is proven by an iteration scheme and Schauder's fixed point theorem. The underlying solution concept is related to weak solutions of the van Roosbroeck system and entropy solutions of the heat equation. Additionally, for two spatial dimensions, higher regularity of solutions could be established.

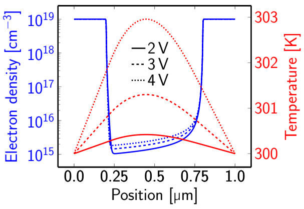

Fig. 9: *Electron density and produced Joule heat in a cooled resistor structure*

As a first step in the discretization of (2), (4), a one-way coupling was implemented, where the temperature rise is neglected in the electric subsystem (2). Figure 9 shows the simulated electron density as well as the increase of temperature due to current flow for a resistor structure for several applied voltages. Next, the temperature effects have to be self-consistently included.

Conclusions and outlook

As for the thermistor model (1), path following techniques (Figure 10) are mandatory for reproducing S-shaped current-voltage characteristics, which are observed in organic resistors, LEDs, transistors, and solar cells. These methods will be used to study the ability of the energy-drift-diffusion model (2), (4) to qualitatively and quantitatively capture the electrothermal behavior including S-shaped current-voltage characteristics with regions of NDR for organic devices. The crucial point is to estimate the parameter range for the occurrence of this phenomenon.

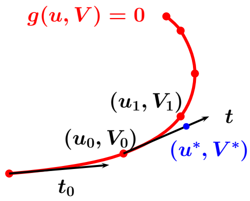

Fig. 10: *Illustration of predictor-corrector method for path following*

The theoretical results and the simulation tool under construction allow to investigate real structures and novel device concepts from our cooperation partner IAPP (see [4, 6]) and to contribute to the applied research in the field of organics. Our results form a solid base for the treatment of hybrid models for the electrothermal description of organic semiconductor devices that combine energy-drift-diffusion and coarser thermistor systems for device subregions with the goal to be as accurate as necessary but as computationally inexpensive as possible.

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1.6 Delay-differential Equations in Multimode Laser Dynamics

Andrei G. Vladimirov and Alexander Pimenov

Since 1960, when the first laser was built, many scientific, military, medical, and commercial laser applications have been developed. Furthermore, due to unique properties of laser light sources, such as high coherence and monochromaticity, as well as an ability to reach extremely high output powers in a narrow spectral domain, the field of laser applications is constantly expanding nowadays.

A typical laser consists of three main components: active medium with population inversion, a pump source to create population inversion, and an open optical cavity. The laser cavity provides a feedback mechanism for the laser field, which is necessary for the achievement of laser generation and, in addition, it selects a set of modal frequencies that can be excited in the laser. For example, in the simplest Fabry–Pérot cavity consisting of two plane mirrors separated by the distance L, the allowed longitudinal modes are those satisfying the condition that the mirror separation distance L is equal to an exact multiple of half the wavelength λ_q : $L = q\lambda_q/2$, where q is an integer number. Since the bandwidth of the laser active medium is usually much larger than the frequency separation of the longitudinal laser modes, many lasers operate simultaneously in multiple longitudinal modes.

Although multimode laser operation is undesirable in many cases when different methods are applied to select only a single longitudinal mode, there exist very important applications where multimode lasers are used. This primarily concerns the so-called *mode-locking of lasers*, which corresponds to the generation of many longitudinal modes with exactly equidistant frequencies and some fixed phase relations between the modes. Mode-locked (ML) lasers emit a periodic sequence of short optical pulses suitable for various practical applications including spectroscopy, medicine, metrology, optical telecommunications, etc. [1]. Furthermore, an ML regime is associated in the frequency domain with the so-called *optical frequency comb*, consisting of a discrete set of equally spaced frequency lines. Optical frequency combs are used in numerous scientific and practical applications, including high-precision spectroscopy, metrology, medicine, optical clocking. In 2005, Theodor Hänsch received a Nobel Prize for Physics for his scientific contributions to the development of laser-based precision spectroscopy, including the optical frequency comb technique. Since then low-noise optical frequency combs generated by ultra-short pulse ML lasers have revolutionized such fields of science and technology as high-precision spectroscopy, metrology, and photonic analog-to-digital conversion. In this article, we discuss an efficient approach for the theoretical modeling of ML and other types of multimode lasers, based on the use of delay-differential equations.

Mode-locked semiconductor lasers

Among various types of ML lasers, monolithic multisection passively ML semiconductor lasers are of particular interest, see Figure 1. These lasers containing gain and saturable absorber sections emit picosecond and subpicosecond optical pulses with high repetition rates suitable for numerous applications, such as data communications, optical clocking, high-speed optical sampling, all-optical clock recovery, and microscopy.

A standard theoretical approach to the modeling of monolithic multi-section ML semiconductor lasers is based on the use of the so-called *travelling wave equations* governing the temporal and spatial evolution of complex electric envelopes of the two counter-propagating waves in the laser cavity and carrier density in the laser sections. This set of partial differential equations must be supplied with proper boundary conditions on the laser facets and solved numerically with the help of specially designed software. Another well-known approach to model ML lasers is based on the so-called *Haus master equation* [1]. Haus master equations are much more simple than the traveling wave model and under certain simplifying assumptions yield an analytical expression for an ML pulse in the form of a hyperbolic secant. However, the derivation of the Haus master equation is based on the small gain and loss approximation, which is hardly satisfied for semiconductor lasers. This, in particular, explains why a simple master equation fails to reproduce the asymmetry of the ML pulses emitted by semiconductor lasers. Furthermore, the form of the Haus master equations can depend on the ratios of the gain and absorber relaxation rates to the cavity decay rate. For example, two different models were proposed by Haus to describe ML lasers with the slow and fast saturable absorbers.

To get rid of the shortcomings of the Haus master equation approach, the delay-differential equation (DDE) model of an ML laser was derived in [2] from the traveling wave equations using the so-called *lumped element* approach. Similarly to the Haus master equations, the DDE model assumes unidirectional lasing in a ring cavity. However, the DDE ML model is free from the small gain and loss approximation and remains valid for any values of the gain and absorber relaxation times. The DDE model governing the time evolution of the electric field envelope $A(t)$ at the entrance of the absorber section, saturable gain $G(t)$, and saturable loss $Q(t)$, associated with the gain and absorber sections, respectively, reads

Fig. 1: *Monolythic semiconductor laser, Ronald Kaiser, Bernd Hüttl, HHI Berlin*

$$\gamma^{-1}\frac{dA}{dt} + A = \sqrt{\kappa}\, e^{(1-i\alpha_g)G/2-(1-i\alpha_q)Q/2-i\varphi} A(t-T), \quad (1)$$

$$\frac{dG}{dt} = g_0 - \gamma_g G - e^{-Q}\left(e^{G}-1\right)|A(t-T)|^2, \quad (2)$$

$$\frac{dQ}{dt} = q_0 - \gamma_q Q(t) - s\left(1-e^{-Q(t)}\right)|A(t-T)|^2. \quad (3)$$

Here, γ is the spectral width of the Lorentzian filter, $\kappa < 1$ is the attenuation factor responsible for non-resonant linear losses in the semiconductor medium and due to the output of laser radiation from the cavity. g_0 and q_0 are the linear gain (pump) and linear loss parameters. $\gamma_{g,q}$ and $\alpha_{g,q}$ denote, respectively, carrier relaxation rates and linewidth enhancement factors in the gain and absorber sections, s is the ratio of the saturation intensities in the gain and absorber sections. Finally, the delay parameter T is equal to the cold cavity round trip time, and φ is the phase shift per round trip. The DDE ML model (1)–(3) has proven to be a powerful tool for the analysis of the dynamical regimes in monolithic ML semiconductor lasers. In the last few years, modifications of this model were used to study various timing-jitter reduction techniques that are crucial for the application of ML lasers in future optical communication networks.

The DDE model (1)–(3) is much simpler than the corresponding traveling wave models. It can be integrated using standard software. Moreover, under certain simplifying approximations the DDE ML model can be studied analytically. Some results of the analytical analysis of the DDE model (1)–(3) are presented in the left panel of Figure 2, where the stability domain of the fundamental ML regime with a single pulse per cavity round trip time is shown in green color. This domain looks qualitatively very similar to the experimentally measured stability domain of the ML regime in a monolithic semiconductor ML laser shown in the right panel of Figure 2.

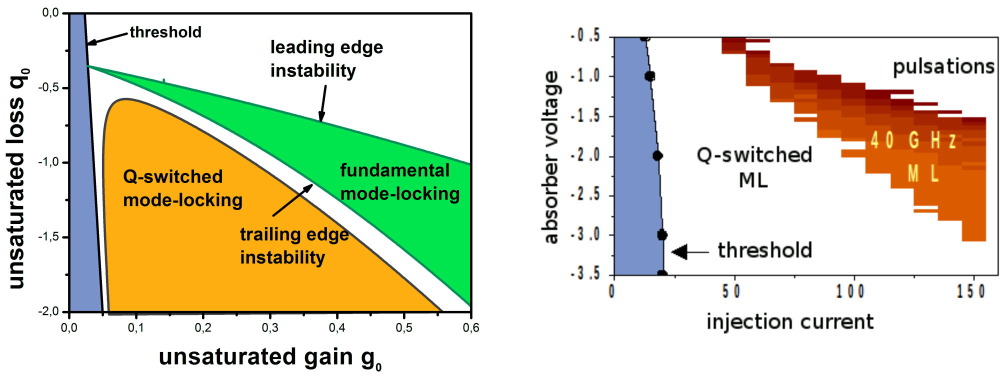

Fig. 2: *Left: Regions of stability of various regimes of the ML laser obtained analytically: laser off state (blue), Q-switched ML (yellow), fundamental ML (green). Right: Regions of stability of the same regimes measured experimentally by Ronald Kaiser and Bernd Hüttl in Heinrich Hertz Institute in Berlin.*

Close to the codimension-two point where the green cone touches the laser threshold line, see left panel of Figure 2, the DDE ML model can be reduced to one of the Haus master equations, a PDE model, which was derived earlier from physical considerations. The form of these equations, however, depends on the ratios of carrier and cavity decay rates in the gain and absorber sections. In particular, the Haus master equations derived by Kolokolnikov and co-authors were obtained for the case of slow gain and fast absorber relaxation. Furthermore, Haus master equations are based on the small gain and loss approximation, which is hardly valid for semiconductor lasers.

Long cavity frequency swept laser

Frequency swept sources have greatly improved the acquisition speed and the sensitivity of optical coherence tomography. In particular, the frequency swept laser studied experimentally in the group of Guillaume Huyet in the Tyndall National Institute in Cork is shown schematically in Figure 3. It includes three basic components: a semiconductor optical amplifier (SOA) acting as a gain element, a fast tunable filter, and a long fiber delay line. When the central frequency of the tunable filter is swept with the period close to the cavity round trip time T, the so-called *Fourier domain ML* regime can develop, which is characterized by periodically swept frequency of the output radiation.

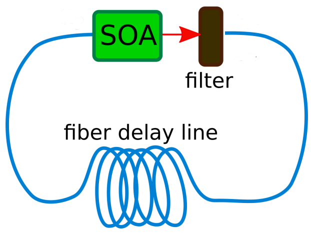

Fig. 3: *Frequency swept FDML laser*

A DDE model of the FDML laser proposed in [3] was successfully applied to explain the asymmetry of the laser output with respect to the filter sweep direction in the normal dispersion regime. An important drawback of this model is, however, that it does not account for chromatic dispersion of the fiber delay line. This is why the model of [3] does not agree with the experiments, which show the absence of output asymmetry when the dispersion of the fiber delay line is anomalous. Therefore, to model the dynamics of a frequency swept ring laser, we have upgraded the DDE FDML model by assuming that the chromatic dispersion is created by a Lorentzian absorption line strongly detuned from the lasing transition. The resulting distributed DDE model governing the time evolution of the electric field envelope $A(t)$ and saturable gain $G(t)$ has the form [4]:

$$\begin{aligned} \gamma^{-1}\frac{dA}{dt}+[1-i\Delta(t)]\,A &= \sqrt{\kappa}e^{(1-i\alpha)G/2+i\varphi}\,[A(t-T)+P(t-T)]\,, &(4)\\ \frac{dG}{dt} &= \gamma_g\left[g_0-G-(e^G-1)\,|A(t-T)+P(t-T)|^2\right], &(5)\\ P(t) &= -\sigma L\int_{-\infty}^{t}e^{-(\Gamma+i\Omega)(t-s)}\frac{J_1\left[\sqrt{4\sigma L(t-s)}\right]}{\sqrt{\sigma L(t-s)}}A(s)ds, &(6)\end{aligned}$$

where T is the cavity round trip time, γ describes the spectral width of the filter, σ is the dispersion strength, L is the delay line length, Γ and Ω describe the spectral width and central frequency of the Lorentzian absorption line. The parameters κ and φ describe, respectively, linear attenuation and phase shift per cavity round trip, α is the linewidth enhancement factor, γ_g is the carrier relaxation rate, and g_0 is the pump parameter. Finally, the parameter $\Delta(t)$ describes the position of the periodically swept central frequency of the filter.

The simplest solutions of (4)–(6) are the so-called *continuous wave* (CW) solutions corresponding to time independent laser intensity, $A(t)=A_0e^{i\omega t}$, $P(t)=P_0e^{i\omega t}$, and $G=G_0$. These solutions correspond to different longitudinal modes of the laser. Using the approach of [5] linear stability analysis of the CW solutions can be performed in the large delay limit $\gamma T \gg 1$, when the eigenvalue spectrum is separated into discrete and pseudo-continuous parts. In the large delay limit eigenvalues belonging to the pseudo-continuous spectrum can be represented in the form:

$$\lambda = i\lambda_0+\frac{\lambda_1}{\gamma T}+\mathcal{O}\left(\frac{1}{\gamma^2T^2}\right)$$

with real λ_0. By substituting this relation into the characteristic equation and keeping only zero order terms in $(\gamma T)^{-1}$, it is possible to express λ_1 as a function of λ_0. The dependence $\mathrm{Re}\,\lambda_1(\lambda_0)$ gives the two branches of pseudo-continuous spectrum determining the stability of CW solutions. The branches responsible for the development of long wavelength modulational and short wavelength Turing-type instabilities are shown in the left panel of Figure 4.

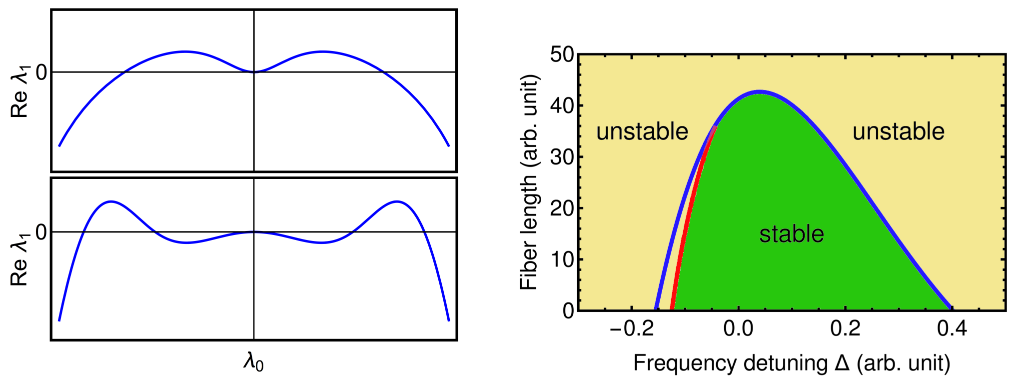

Fig. 4: *Left: Branch of pseudo-continuous spectrum after modulational (top) and Turing-type (bottom) instability. Right: CW regime stability domain (green area). Blue (red) line indicates modulational (Turing-type) instability.*

A modulational instability of the CW regime takes place when the pseudo-continuous spectrum branch, which is tangent to the axis $\mathrm{Re}\,\lambda_1 = 0$, changes its curvature from negative to positive at the point $\lambda_0 = 0$, see top figure on left panel of Figure 4. Another type of instability takes place when a branch of pseudocontinuous spectrum crosses the axis $\mathrm{Re}\,\lambda_1 = 0$ at $\lambda_0 = \pm\lambda_0^*$, where $\lambda_0^* > 0$. It is seen from the right panel of Figure 4 that when the dispersion is sufficiently weak the stability range of CW solutions is asymmetric and is limited by different bifurcations, corresponding to modulational and Turing-type instabilities. This explains the experimentally observed asymmetry of the output characteristics with respect to the sweep direction [4]. On the other hand, when the anomalous dispersion is sufficiently large, all CW regimes are unstable with respect to modulational instability, and the laser demonstrates chaotic pulsations for both sweep directions. The necessary condition for the modulational instability of CW solutions can be derived analytically in the large delay limit:

$$\alpha L D_2 < -\frac{1}{\gamma^2}, \quad D_2 = \mathrm{Im}\,\frac{\mathrm{d}^2}{\mathrm{d}\nu^2}\left(\frac{-\sigma}{\Gamma + i(\Omega+\nu)}\right), \tag{7}$$

where D_2 is the second-order dispersion coefficient per unit length. This condition resembles the modulational instability criterion for the complex Ginzburg–Landau equation.

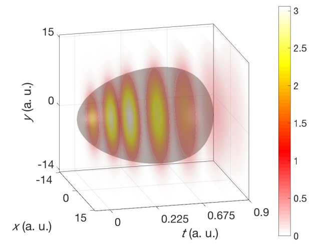

Fig. 5: Light bullet solution of (8–10)

Optical bullets

So-called *light bullets* (LBs) are pulses of electromagnetic energy that are localized both in space and time and preserve their shape in the course of propagation. Since the first theoretical prediction of LBs by Yaron Silberberg in 1990, their experimental observation remains one of the challenging problems in nonlinear optics. The formation of LBs was predicted theoretically in various optical systems, such as optical parametric oscillators, bistable cavities with an instantaneous response of the active medium, and more recently by Julien Javaloyes in a broad area passively ML laser operated in the long cavity regime. To describe the generation of LBs in this laser we have proposed a generalization of the DDE model (1)–(3) taking into account transverse diffraction of the laser field:

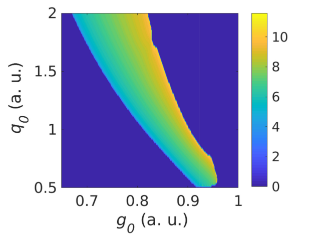

Fig. 6: Domains of existence of stable LBs. The color code represents the energy of the pulse.

$$\gamma^{-1}\frac{dA}{dt} + A = \frac{\sqrt{\kappa}e^{i\phi}}{2\pi i}\iint_{-\infty}^{+\infty} e^{\frac{i}{2}(x-x')^2+\frac{i}{2}(y-y')^2} e^{\frac{1-i\alpha_g}{2}G(x',y',t)-\frac{1-i\alpha_q}{2}Q(x',y',t)} A(x',y',t-T)dx'dy', \tag{8}$$

$$\frac{dG}{dt} = g_0 - \gamma_g G - e^{-Q}(e^G - 1)\,|A(x,y,t-T)|^2, \tag{9}$$

$$\frac{dQ}{dt} = q_0 - \gamma_q Q - s(1-e^{-Q})\,|A(x,y,t-T)|^2. \tag{10}$$

Here, $A(x,y,t)$, $G(x,y,t)$, and $Q(x,y,t)$ are the transverse distributions of the electric field envelope, saturable gain, and saturable loss, respectively. The parameters are the same as in (1)–(3).

In [6], the DDE model (8)–(10) was studied with the help of direct numerical integration, which involves the time propagation of the Fourier-transformed electrical field $\hat{A}(\xi,\chi,t)$ using the spatial Fourier transform of (8) and the propagation of the quantities $G(x,y,t)$, $Q(x,y,t)$ using the inverse Fourier transform of $\hat{A}(\xi,\chi,t)$. Moreover, we have developed a special spectral method based on the functional mapping that allowed us to calculate the LB solution on a time interval much shorter than the cavity round trip time T and, hence, to reduce the amount of calculations considerably. The profiles of two-dimensional LB solutions are presented in Figure 5. The stability domain of the LB solution calculated with the help of the functional mapping method is shown in Figure 6. The theoretical analysis of the LBs formation in the nonlocal DDE model (8)–(10) demonstrates their robustness in the parameter space and provides useful practical guidelines for their future experimental observation.

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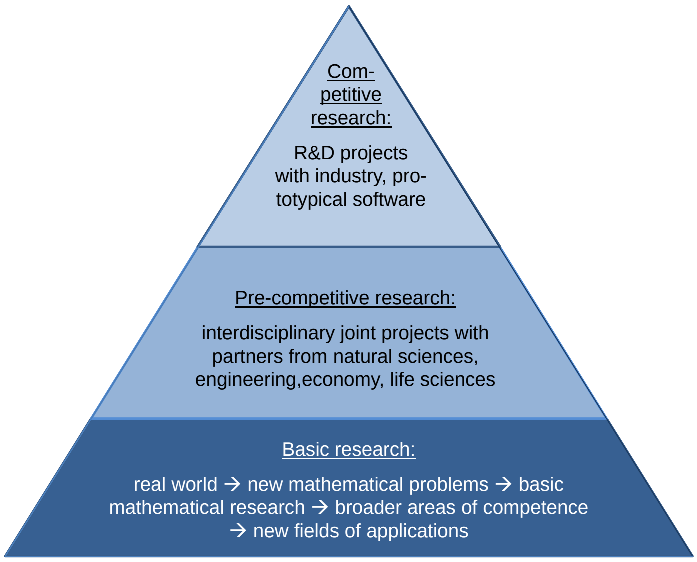
2 WIAS in 2018

- 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.

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, currently, one trainee to become a "mathematical technical software developer".

WIAS promotes the international collaboration in applied mathematics by organizing workshops and running guest 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 thirty-two 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 "3rd Leibniz MMS Days" took place from February 28 to March 2, 2018, in Leipzig; see page 121.

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. In September 2018, the DFG decided to provide funding for MATH+, the Berlin Mathematics Research Center, an interdisciplinary Cluster of Excellence and cross-institutional venture of FU Berlin, HU Berlin, and TU Berlin, WIAS, and Zuse Institute Berlin (ZIB). Michael Hintermüller is a founding member (PI) of MATH+, a co-speaker of the center and a Scientist-In-Charge of MATH+' Emerging Field *Model-Based Imaging*. MATH+ came into operation in 2019. Its structure integrates and merges the Research Center MATHEON, which was funded from 2002 to 2014 by the DFG and subsequently by the Einstein Center for Mathematics ECMath, the Berlin Mathematical School (BMS), and others.

MATH+

2.2 Structure and Scientific Organization

2.2.1 Structure

In 2018, 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 58), 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:

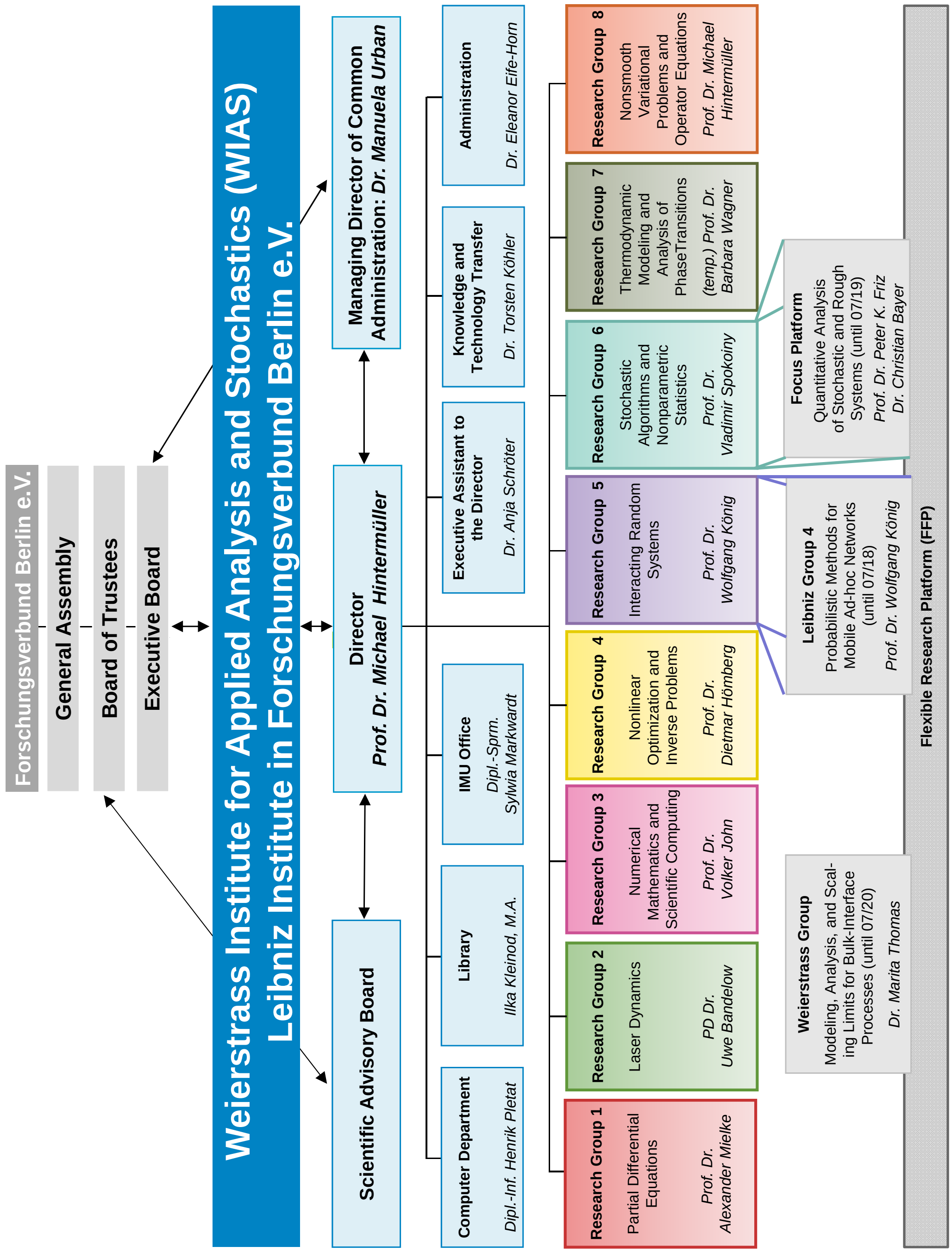
RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing
RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase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

Flexible Research Platform:

LG 4. Probabilistic Methods for Mobile Ad-hoc Networks (until 7/2018)
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 2018.

[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. Dr. Michael Hintermüller
Managing Director of Common Administration: Dr. Manuela Urban
Computer Department
Dipl.-Inf. Henrik Pletat
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
Dr. Eleanor Eife-Horn
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 07/18)
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 2018 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 2018 in the interdisciplinary solution process described above (dark blue: over 20% of the group's working time, light blue: up to 20% of the group's working time).

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	light blue		light blue	dark blue			dark blue	dark blue		
Flow and Transport	light blue		dark blue	light blue	dark blue	light blue	dark blue	light blue		dark blue
Materials Modeling	light blue		light blue	light blue	light blue		dark blue			dark blue
Nano- and Optoelectronics	dark blue	dark blue	dark blue	light blue						light blue
Optimization & Control in Technology and Economy	light blue		light blue	dark blue	light blue	dark blue		dark blue	light blue	
Quantitative Biomedicine			light blue			dark blue	light blue	dark blue		

In the following, special research topics are listed that were addressed in 2018 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.

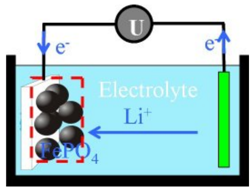


Fig. 1: *Sketch of a lithium-ion battery (LiFePO4)*

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 3 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.

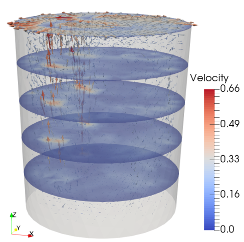


Fig. 2: *Turbulent flow through a ladle*

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

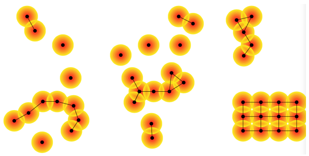


Fig. 3: *A realisation of a many-body system showing a small crystal in the lower right corner*

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 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 WG1, RG 6 and RG 7)
- Material models with stochastic coefficients (in RG 1, RG 4, RG 5, and RG 7)
- Material models and analysis of complex liquids and interface dynamics (including hydrogels and suspension flows; in RG 7 and WG1)
- Thermodynamically consistent electrochemical models of lithium-ion batteries, fuel cells, and solid oxide electrolytes (in RG 3 and RG 7)
- Stochastic and thermomechanical modeling of phase transitions (in RG 4 and RG 5)
- Hysteresis effects (electro/magneto-mechanical components, elastoplasticity, lithium batteries; in RG 1, WG1, and RG 7)
- Modeling of elastoplastic and phase-separating materials (including damage and fracture processes; in RG 1, RG 7, and WG1)
- Derivation and analysis of local and nonlocal phase field models and their sharp-interface limits (in RG 1, RG 7, and WG1)

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.

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 (high-power lasers, single-photon emitters, 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 8 and WG1)
- Modeling, analysis, and optimization of optoelectronic semiconductor devices driven by experimental data (in WG1)

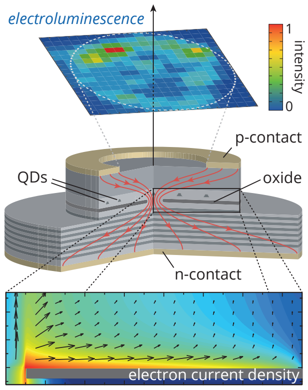


Fig. 4: *Simulated spreading of injection current density in a quantum-dot based single photon emitter with Al-oxide aperture. An improved design was proposed on that base in:* M. KANTNER, U. BANDELOW, T. KOPRUCKI, J.-H. SCHULZE, A. STRITTMATTER, H.-J. WÜNSCHE, Efficient current injection into single quantum dots through oxide-confined PN diodes, *IEEE Trans. Electron Devices,* **63***:5 (2016), pp. 2036–2042.*

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 play an important role.

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.

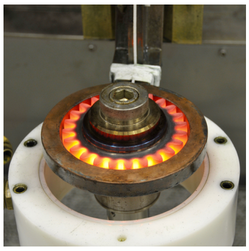


Fig. 5: *Induction heat treatment of a gear*

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 and RG 8)

- Optimal control of multifield problems in continuum mechanics and biology (in RG 3, RG 4, and RG 7)
- Design of ad-hoc telecommunication systems in realistic urban environments and evaluation of their properties with respect to connectivity, message routing, propagation of malware and capacity (in RG 5)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6)
- Optimal control of multiphase fluids and droplets (in RG 8)

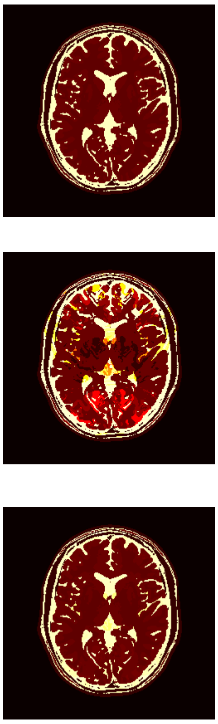


Fig. 6: *Quantitative MRI: Estimation of the T_2 relaxation times of matter leading to characterization of different types of tissue. (1) Ground truth, (2) State-of-the-art dictionary-based method (improved variant of Magnetic Resonance Fingerprinting-MRF), (3) Integrated physics-based approach where the physical processes are learned by an artificial Neural Network*

Quantitative Biomedicine

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)
- 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.

For more than five years, WIAS has been certified by passing the *audit berufundfamilie*. With the certificate, the institute documents its commitment to a sustainable family- and life-phase-conscious personnel policy. We are continuously aiming to optimize our already high standards in the corresponding arrangements. WIAS's staff has, for instance, the option to engange the services of *benefit@work*, a family service agency whose offers are optimized to meet the needs of WIAS's staff.

In every year, another member of the direction of WIAS is appointed to take the responsibility for equality affairs in the institute. In 2018, this was Uwe Bandelow, the head of Research Group 2 *Laser Dynamics*.

WIAS's equal opportunities officer Ilka Kleinod and her substitute Birgit Seeliger resigned from their tasks after four years of many activities for this cause on August 31, and now, since September 1, 2018, Jutta Lohse has been the new equal opportunities officer of WIAS.

WIAS has a team "Work and Family" consisting of the member of the WIAS direction in charge of equality affairs, the project head of the *berufundfamilie audit*, Gerd Reinhardt until August 2018 and Olaf Klein since then, the equal opportunities officer, and Laura Wartenberg.

On April 26, 2018, 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. 13 girls followed an introduction and a career counseling, joined in activities, and asked many questions, mentored by scientists from WIAS.

Besides continuous information by e-mail on equality and work and family topics, the "Work and Family" team offered the staff members a lecture by an external expert on August 30, 2018, on the "Time to breathe deeply – Breathing for more awareness, peace of mind, concentration, and mental balance", which was again well attended.

On December 17, 2018, the "Work and Family" team of WIAS organized the first Christmas party for the children of the collaborators. Six children and their parents enjoyed it very much.

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 2018, having raised a total of 3.555 million euros, from which 45[2] additional researchers (+ 9 outside WIAS; Dec. 31, 2018) were financed. In total in 2018, 26.33 percent of the total budget of WIAS and 48.6[2] percent of its scientific staff originated from grants.

[2]With scholarship holders.

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

2.5 Participation in Structured Graduation Programs

Graduate School *Berlin Mathematical School (BMS)*

Berlin's mathematicians are proud that, after its successful installation in 2006, a second funding period was granted to this graduate school in Summer 2012 for 2013–2018, for the excellent work done since its inception. Since 2019, the BMS is a part of MATH+. The BMS is jointly run by the three major Berlin universities within the framework of the German Initiative for Excellence. It attracts excellent young Ph.D. students from all over the world to the city, and many members of WIAS are contributing to its operations.

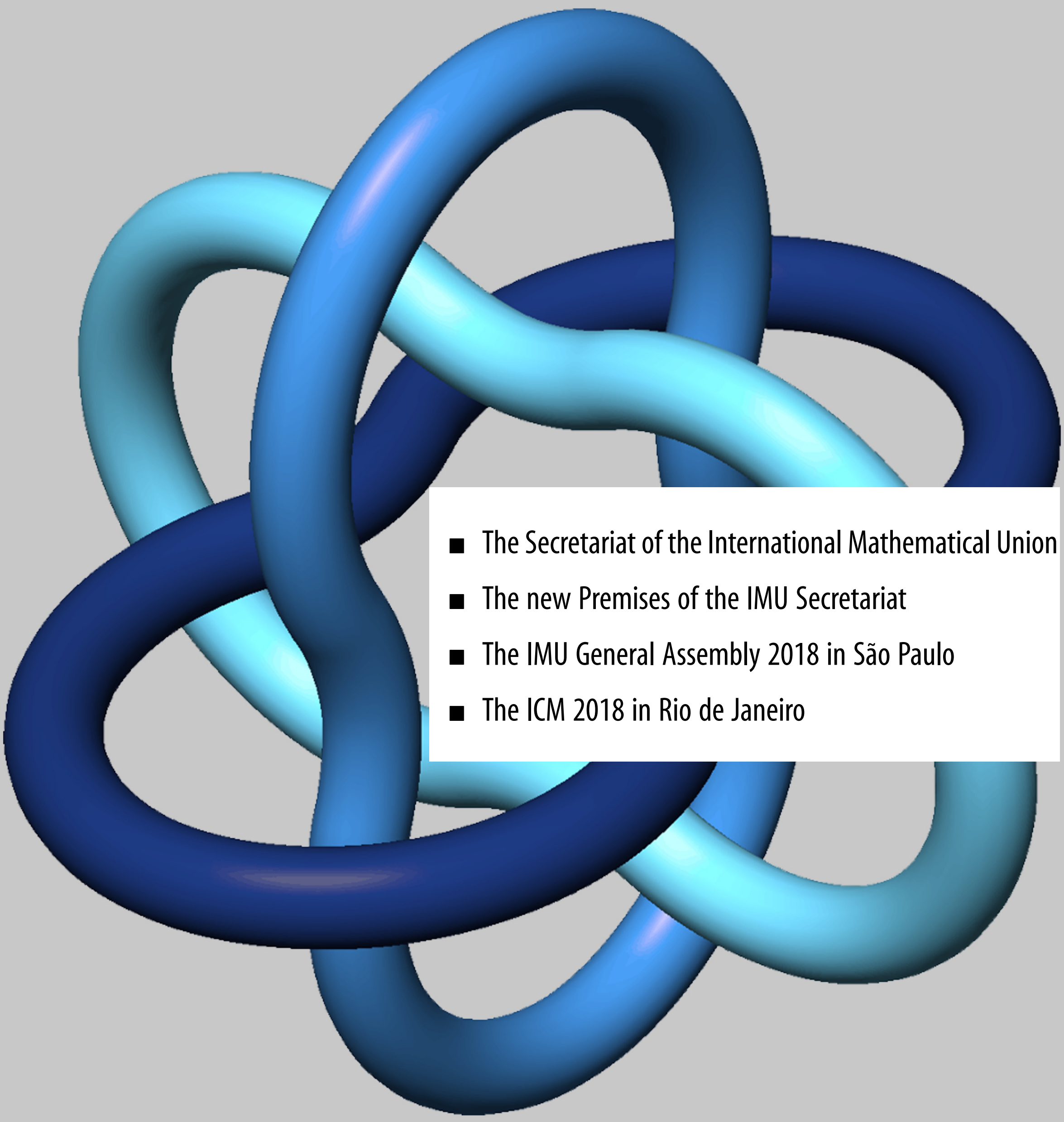
International Research Training Group (IRTG) 1792 *High Dimensional Non Stationary Time Series Analysis* of the DFG

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.

3 IMU@WIAS



- The Secretariat of the International Mathematical Union
- The new Premises of the IMU Secretariat
- The IMU General Assembly 2018 in São Paulo
- The ICM 2018 in Rio de Janeiro

3.1 The Secretariat of the 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.

The collaboration of WIAS and IMU was installed via a Memorandum of Understanding (2010) and a Cooperation Agreement (2013) that covered an initial period of ten years. After a positive evaluation of the work of the IMU Secretariat over the last eight years, the IMU General Assembly 2018 passed a resolution to enter into a new and unlimited Cooperation Agreement, which was signed directly after the end of the General Assembly.

In April 2018, the IMU Secretariat moved from its former premises on the second floor of Markgrafenstraße 32 to its new premises on the fourth floor of Hausvogteiplatz 11A.

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 General. 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 and CDC Administrative Manager*. L. Koch is responsible for supporting administratively the activities of the International Commission on Mathematical Instruction and the Commission for Developing Countries. 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.

Nicole Kärgel, *IMU Accountant*. N. Kärgel 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 was on leave.

Theresa Loske, *Project Assistant* (until January 2019). T. Loske's task was 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 General

Helge Holden is the IMU Secretary General. 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 IMU Secretary General is responsible for conducting the ordinary business of the Union and for keeping its records.

3.2 The new Premises of the IMU Secretariat

In March 2017, WIAS was informed that the renting contract for the old premises of the IMU Secretariat at Markgrafenstraße was canceled with deadline in April 2018. New rooms were found in the fourth floor of Hausvogteiplatz 11A, which was formerly used by WIAS already. After significant reconstructions, the office structure was adapted for the purposes of the IMU. As in the old premises, the office consists of the following rooms:

- an office for the IMU Manager and the IMU Secretary General,
- an office for the ICMI and CDC Administrative Manager and the Project Assistant,
- an office for the IMU Archivist and the IMU Accountant,
- an office for the IT and Technical Support of the IMU and the Head of the IMU Secretariat,
- two rooms for the IMU Archive (air-conditioned),
- a conference room for meetings of up to 16 people,
- a social room and lobby for informal meetings,
- a small kitchen and a room for printers and equipments.

Rebuilding the IMU archive in the new premises

The organization and management of the reconstruction and the planning of the relocation happened between October 2017 and March 2018. The actual move of the whole IMU Secretariat took place in April 2018. In particular, the packing, relocation, and reassembly of the materials in the IMU Archive was quite intricate. In the following months, the decoration of the IMU Secretariat was undertaken, which included the re-installation of the gallery of the IMU Prize winners and the gallery of the former IMU Presidents and the IMU Secretaries.

The gallery of former IMU Prize winners is located in front of the conference room

As a new feature, a display of the most recent prize winners and a frame with replicas of the IMU medals (Fields, Nevanlinna, Gauß, and Chern) was installed at prominent position in the foyer.

The foyer of the IMU Secretariat displays photos of the most recent prize winners and replicas of the IMU medals

3.3 The IMU General Assembly 2018 in São Paulo

The governing body of the IMU is the General Assembly, which meets every four years on the weekend before the International Congress of Mathematicians. Each member country is asked to send a number of delegates depending on their group status. Additional associate members and affiliated societies can send observers without votes. Typically, there are about 200 participants from 100 countries.

About 200 persons attended the General Assembly in São Paulo

The 18th General Assembly was held in São Paulo, Brazil, on July 29–30, 2018. The two-day agenda of the General Assembly includes reports by various bodies of the IMU, ample time for discussion of the handling of the IMU by the Executive Committee in the past four years, and finally resolutions are passed concerning the future of the IMU. Concerning the former, the General Assembly accepted the report of the IMU Treasurer Alexander Mielke and agreed to the plans for the spendings in the coming four-year period.

Concerning the future of the IMU, there was a strong debate about the location of the next ICM, and after a secret ballot Sankt Petersburg, Russia, was chosen to be the host of the ICM 2022.

Most votings at the General Assembly were done by showing hands

Also the future of the IMU Secretariat was a special topic in the agenda. At the General Assembly 2010 in Bangalore, the decision concerning the hosting of the IMU Secretariat by WIAS had a limited time horizon of ten years. Then, it was determined that the performance of the IMU Secretariat would be monitored by the IMU Office Committee, which would then report to the IMU Executive Committee and the General Assembly. Based on a report and recommendation by the Office Committee, the General Assembly voted unanimously for keeping the IMU Secretariat at WIAS and for making the cooperation agreement permanent. The exact wording of the relevant resolutions is the following:

> *1. The General Assembly of the IMU expresses its deep gratitude to Germany, and in particular to the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) for their generous support of the IMU Secretariat.*
> *2. The General Assembly of the IMU endorses that the current Stable Office for the International Mathematical Union, established as a cooperation between WIAS and the IMU be made permanent.*
> *3. The General Assembly charges the IMU President and IMU Secretary to sign an agreement with WIAS.*
> *4. The IMU EC establishes an Office Committee that reports bi-annually to the IMU EC, and the IMU EC reports about the findings to the GA.*

Directly after the closing of the General Assembly, the IMU President Shigefumi Mori, the IMU Secretary General Helge Holden, and the WIAS Director Michael Hintermüller signed a new cooperation agreement establishing an unlimited collaboration between IMU and WIAS concerning the running of the IMU Secretariat.

The new cooperation agreement between IMU and WIAS is signed in São Paulo on July 30, 2018

3.4 The ICM 2018 in Rio de Janeiro

Every four years, the IMU organizes an International Congress of Mathematicians to bring together mathematicians from all over the world, to experience mathematics as a fascinating science, and to celebrate excellent mathematicians like the winners of the *Fields Medal* for mathematicians not older than 40 years, the *Rolf Nevanlinna Prize* for outstanding contributions in mathematics for information sciences, the *Carl Friedrich Gauss Prize* for outstanding mathematical contributions with impact outside mathematics, the *Chern Medal Award* for mathematical achievements of highest level, and the *Leelavati Prize* for outstanding contributions for increasing public awareness of mathematics.

The presentation of the IMU Prize winners during the opening ceremony was embedded into cultural contributions like Samba dancing

The 28th ICM took place in Rio de Janeiro from July 31, 2018, to August 9, 2018. Most of these prizes were announced and presented in the opening ceremony, which was organized as a big festival showing the rich cultural heritage of the Americas. The interest for mathematics all over Brazil became clear by seeing the participation of almost 600 school children, that where “mathematical gold medalists” in regional mathematics competitions. Finally, the scientific program brought together prize winners, plenary speakers, invited speakers, and about 3500 regular participants.

However, already many months before, the IMU secretariat was heavily involved in the preparations of the event, e.g. in the preparations of the opening ceremony, press coverage, internet presentation, and so on. During the whole time of the congress, the IMU Secretariat presented information on the work of the IMU in its conference booth.

Many participants, and even one Fields medalist, took the chance to visit the booth of the IMU Secretariat

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 with special emphasis on

- 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

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.

Partial differential equations and regularity

This field of research provides the basic research for the analytical treatment of coupled systems of nonlinear partial differential equations arising in different application fields, e.g., in natural sciences, technology, economy and life sciences. The results of the group include, e.g., regularity theory for elliptic and parabolic operators, variational methods for evolutionary systems, generalized gradient systems, entropy methods, and generalized solution concepts.

ALEX 2018. The workshop "AnaLysis of Evolutionary and compleX systems" was held at WIAS and Humboldt-Universität zu Berlin from September 24 to 28, 2018.

Fig. 1: *The participants of the ALEX 2018 workshop*

New aspects of evolutionary PDEs were addressed with a wide range of applications in physics, biology, chemistry, and engineering. The focus was put on the following four main topics: variational methods for continuum mechanics, gradient and Hamiltonian structures, dynamical systems, and multiscale problems. Eleven keynote lectures and 27 invited talks were presented to 73 participants from eleven nations. The contributions included the modeling of smart materials, interrelation between stochastics and PDEs, multi-particle systems, transition from discrete to continuum, quantum mechanics, and reaction-diffusion systems.

Energy-reaction-diffusion systems. Recently developed energy-dissipation methods for reaction-diffusion systems could be generalized to the non-isothermal case. Here concave entropies in terms of the densities of the species and the internal energy were used, where the importance is that the equilibrium densities may depend on the internal energy. By using logarithmic Sobolev estimates and variants for lower-order entropies as well as estimates for the entropy production of nonlinear reactions, two methods were developed to estimate the relative entropy by the total entropy production, namely a somewhat restrictive convexity method, which provides explicit decay rates, and a very general, but less explicit compactness method, see [6].

Advances for the Keller–Segel model. Created already in 1970 and investigated in several hundreds of papers, the famous Keller–Segel model from mathematical biology had until 2018 one serious drawback: one did *not* know the well-posedness of the system if the underlying domain is non-smooth. This is twofold important in applications: firstly, the model reflects only a cutout within the surrounding tissue, which is chosen arbitrarily and, hence, possibly non-smooth. Secondly, and even worse: it is known from theoretical and numerical studies that existing solutions have the tendency to show concentration phenomena in a vicinity of boundary points of large curvature/angle points. This makes clear that non-smooth geometries are of particular interest as concerns qualitative properties of the solution. Resting on a fundamental theorem of Herbert Amann (Zurich) on nonlinear parabolic Volterra systems and non-trivial elliptic/parabolic regularity results of our own it was proven in [4] that indeed the Keller–Segel system admits at least a local-in-time unique solution on a wide range of geometries.

Semiconductors

In this field, the group benefits from a strong cooperation with RG 2 *Laser Dynamics* and RG 3 *Numerical Mathematics and Scientific Computing*. 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 RG 2 and Zuse Institute Berlin). Funded by the Einstein Center for Mathematics Berlin (ECMath), the Matheon subprojects D-OT7 (together with RG 6 *Stochastic Algorithms and Nonparametric Statistics*) and D-SE18 are running. Concerning the latter project, which deals with electrothermal models for organic semiconductor devices, see the scientific highlight article on page 34. Moreover, group members could acquire the three subprojects AA2-1, AA2-5, and EF3-1 (together with RG 6) in the frame of the Cluster of Excellence MATH+ starting January 2019.

Semiconductor Nanophotonics
SFB 787

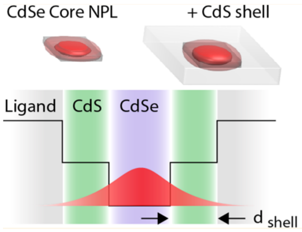


***Fig. 2:** Electron ground state in a CdSe nanoplatelet with and without CdS shell (top) and conduction band profile (bottom), see [1].*

Electronic states in semiconductor nanostructures. In close collaboration with experimental partners, computations and analysis of the electronic properties of various semiconductor nanostructures based on multiband $\mathbf{k}\cdot\mathbf{p}$ models were performed. One example are CdSe platelets formed in a ligand, see Figure 2, as produced and spectroscopically measured at the Technical University Berlin, Institute of Optics and Atomic Physics. Here, our computations of the electron and hole ground state energies and charge densities and the respective excitonic effects helped to understand the influence of a CdS layer on optical spectra of the platelets [1].

A second example is a theory-guided design study for high-quality quantum rings to observe optical Aharonov–Bohm oscillations in collaboration with the Institute for Integrative Nanosciences at the Leibniz IFW Dresden and Paul-Drude-Institut (PDI) Berlin. Axial crystal-phase heterostructures are obtained by introducing stacking faults or twin boundaries in a III-As nanowire. A radial heterostructure is formed by combining the binary alloys GaAs and AlAs in a core-shell nanowire setup. Combining these axial and radial heterostructures finally yields high-quality crystal-phase quantum rings, see Figure 3. The respective quantum rings were fabricated following the identification of promising, experimentally accessible characteristic parameters such as core doping density and active shell thickness. Magneto-photoluminescence measurements at PDI in fact revealed clear Aharonov–Bohm oscillations in these nanowires for neutral and charged excitons [2]. These nanowires open a unique way toward wavefunction engineering in 3D quantum structures for the experimental study of excitonic phase coherence phenomena.

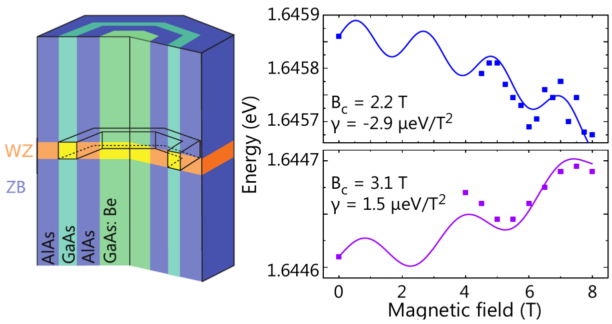


***Fig. 3:** Left: Schematic view of a GaAs/AlAs core-shell nanowire in the zincblende phase containing a single twin boundary represented as a thin wurtzite layer. Right: Energy of the Zeeman split states as a function of an applied magnetic field for two different nanowires (top, bottom) following a theory-guided design using $\mathbf{k}\cdot\mathbf{p}$-calculations [2].*

***Fig. 4:** The participants of the AMaSiS 2018 workshop*

AMaSiS 2018. In October, the group organized together with RG 3 and Eric Polizzi (University of Massachusetts) the workshop "Applied Mathematics and Simulation for Semiconductors". It addressed the modeling, mathematical analysis, and numerical schemes for the simulation of semiconductor devices as well as charge transport in electrolytes, and other physical or biological systems. The focus was on the treatment of multiple scales, and the interplay of electronic, optical, thermal, fluidic and other effects in advanced device concepts and novel material systems. The methodological emphasis was on thermodynamically consistent multiphysics semiconductor device models, on contour integrals for matrix problems in quantum mechanics and on mathematical tools for generalized Nernst–Planck–Poisson systems as well as semiconductor device models. The topics of the workshop found a broad resonance among 67 participants from ten countries and 29 institutions.

Material modeling

The research in this topic was done in cooperation with RG 5 *Interacting Random Systems* and the WG *Modeling, Analysis and Scaling Limits for Bulk-Interface Processes* and was driven by the subprojects of the Collaborative Research Centers CRC 1114 *Scaling Cascades in Complex Systems* and CRC 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*. The latter CRC has been prolongated to a third period and within project A5 “Pattern formation in coupled parabolic systems” a Ph.D. position is hosted in RG 1. In summer, also CRC 1114 successfully passed the evaluation conducted by the DFG. The group participates in three projects: B01 (together with FU and GFZ Potsdam), C02 (together with FU) and C05 (WIAS only). Due to its success in the first period, project C05 has been granted an additional Ph.D. position.

SFB 910

Multiscale problems. The project C05 “Effective models for materials and interfaces with multiple scales” provides analytical techniques for discrete or continuous material models that depend on one or several small parameters. Special emphasis is given to systems that have a variational structure such as static minimization problems or gradient-flow equation systems. Methods of static or evolutionary Γ-convergence are employed and further investigated. One aspect was the development and application of discrete homogenization techniques. Discrete homogenization could be used to show that a numerical scheme developed by Marcus Weber (ZIB) in projects A05/B05 converges to the Fokker–Planck equation, see [3]. Furthermore, together with Franziska Flegel from RG 5, the insight into the random conductance model with long range jumps was improved: it was demonstrated that under proper scaling and choice of coefficients, the model cannot only describe diffusive, but also super-diffusive processes. This insight is important for the application of discrete models to particle dynamics. Figure 5 shows the idea of the random conductance model in the simple case of nearest neighbors: at every instant in time, the random walker at point i might randomly choose a neighbor j and jump there with a probability proportional to ω_{ij}. In the long (infinite) range case, the random walk might jump to any point in $\mathbb{Z}^d$.

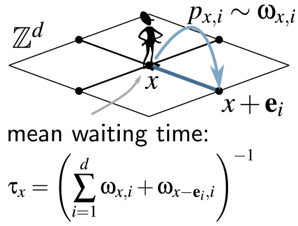


Fig. 5: *Random walk among random conductances*

Viscoplasticity. A model for rate-dependent gradient plasticity at finite strain based on the multiplicative decomposition of the strain tensor has been studied and the existence of global-in-time solutions to the related PDE system was verified. Its underlying structure as a generalized gradient system was revealed, where the driving energy functional is highly nonconvex and features the geometric nonlinearities related to finite-strain elasticity as well as the multiplicative decomposition of finite-strain plasticity. Moreover, the dissipation potential depends on the left-invariant plastic rate and thus, depends on the plastic state variable. In [5], the existence theory for a class of abstract, nonsmooth, and nonconvex gradient systems is developed, for which suitable notions of solutions, namely energy-dissipation-balance (EDB) and energy-dissipation-inequality (EDI) solutions were introduced. The toolbox of the direct method of the calculus of variations could be used to check that the specific energy and dissipation functionals for the considered viscoplastic models comply with the conditions of the general theory.

CRC 1114

Further highlights of 2018

Fig. 6: *Successful defense of Markus Mittnenzweig's Ph.D. thesis*

Dissertations. In 2018, two group members successfully defended their Ph.D. theses at the Humboldt-Universität zu Berlin, namely Pascal Gussmann on "The small-deformation limit in elasticity and elastoplasticity in the presence of cracks" (June 12, 2018) and Markus Mittnenzweig on "Entropy methods for quantum and classical evolution equations" with "summa cum laude" (November 26, 2018).

ISIMM Prize. The junior prize of the International Society for the Interaction of Mechanics and Mathematics (ISIMM) 2018 was awarded to Matthias Liero. The recipient of the prize is selected among the researchers who made significant contributions linking Mathematics and Mechanics. Matthias Liero's research is focused on the mathematical analysis of partial differential equations, e.g., describing the electrothermal interplay in organic light-emitting diodes.

Fig. 7: *Bicycle tour 2018*

WIAS excursion 2018. This year, RG 1 organized the annual excursion of the institute on September 6, 2018. RG 1 laid out four different tours, all of them approaching Königs Wusterhausen. There was a hiking tour from Bestensee to Königs Wusterhausen (about 12 km), a cycling tour from Grünau via Schmöckwitz, Wernsdorf, Ziegenhals, Niederlehme to Königs Wusterhausen (about 24 km), a guided tour at the castle Schloss Königs Wusterhausen, and a guided tour at the Radio Technology Museum Königs Wusterhausen on mount Funkerberg. Finally, all participants met for lunch to share the various impressions and to connect amiably beyond established working relations.

References

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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 2018 within 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). Further funding was received by the DFG individual funding program AM 239/1-1. RG 2 also received funding from the EU Eurostars project E!10524 “High Power Composites of Edge Emitting Semiconductor Lasers” (HIP-Lasers) in close collaboration with Universitat Politécnica de Catalunya (Barcelona), WIAS RG 4, the companies Monocrom (Vilanova), Femtika (Vilnius), and Raab-Photonik GmbH (Potsdam). Further funding was received by subcontracts from Ferdinand Braun Institute for High-Frequency Technology (FBH) within the projects HoTLas (high-performance efficient and brilliant broad-area diode lasers for high ambient temperatures) and PLUS (pulse lasers and scanners for LiDAR applications – automotive, consumer, robotics), both belonging to the framework of the BMBF funding measure “Efficient high-performance laser beam sources” (EffiLAS), which were carried out in close collaboration with FBH, WIAS RGs 1 & 3 as well as the companies Jenoptic Diode Lab GmbH (Berlin) and Coherent | DILAS (Mainz).

Dynamics of semiconductor lasers

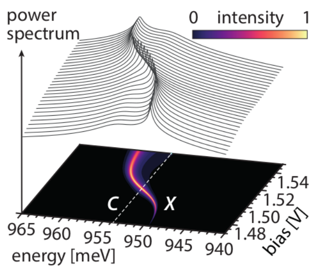

Fig. 1: *Spectral shift of a QD exciton (X) across the optical cavity mode (C) in a single-photon emitting diode*

Electrically driven quantum light sources (e.g., single-photon emitters, sources of entangled photon pairs) based on semiconductor quantum dots (QDs), are key elements for applications in future quantum technologies. The mathematical modeling of quantum light emitting diodes requires novel approaches that combine classical device physics with cavity quantum electrodynamics. Within the CRC 787 *Semiconductor Nanophotonics*, the previously developed hybrid-quantum classical modeling approach, which self-consistently couples the drift-diffusion system with a Lindblad-type quantum master equation, was extended by a Schrödinger–Poisson system. The model describes the quantum optical features (non-classical correlation functions of the optical field, emission spectrum, line broadening and photon generation rate) of the coupled QD-photon system along with the spatially resolved carrier injection into the QD in a unified framework. The model gives access to the line shifts of the QD excitons due to the quantum confined Stark effect within the diode’s self consistently calculated interal electric field, see Figure 1. The research will be continued within the new Excellence Cluster Math+ under grant AA2–3 "Quantum-classical simulation of quantum dot nanolasers".

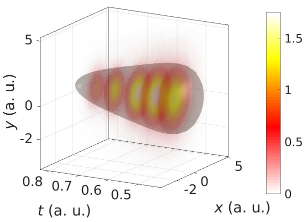

***Fig. 2:** Spatio-temporal profile of the light bullet (LB) intensity*

Low-noise optical frequency combs generated by ultra-short pulse mode-locked lasers and optical microcavities, revolutionized fields of science and technologies such as high-precision spectroscopy, metrology, and photonic analog-to-digital conversion. RG 2 developed the asymptotic theory of the interaction of temporal cavity solitons in the generalized Lugiato–Lefever model describing coherently driven all-fiber cavities and microresonator-based optical frequency comb generators [1]. It was shown that Cherenkov radiation induced by third-order dispersion breaks the symmetry of the cavity soliton interaction and greatly enhances their interaction thus facilitating the experimental observation of the cavity soliton bound states. Reduced equations governing the slow time evolution of the positions of two interacting cavity solitons were derived and analyzed. The results of the analysis are applicable to a broad class of bistable optical systems with external driving beam.

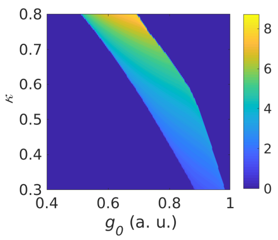

***Fig. 3:** Domain of existence of stable LBs obtained by varying injection current g_0 and loss parameters κ*

Since the seminal work by Y. Silberberg, who introduced the term "light bullets" to describe pulses of electromagnetic energy, localized both in space and time and preserving their shape in the course of propagation, experimental observation of such localized states remains one of the challenging problems in nonlinear optics. In [2], a nonlocal delay-differential model was proposed to study the formation of light bullets in wide-aperture passively mode-locked semiconductor lasers. Using this model, which is valid well beyond the mean-field approximation, the existence of light bullets in a laser with relatively large gain and losses per cavity round trip was predicted theoretically; see Figure 2. The increase of the absolute value of the absorber reverse voltage can lead to an increase of the stability range of light bullets, and, in particular, to a compensation of the destabilizing effect of large linear losses; see Figure 3. Thus, the results obtained provide further guidelines for future experimental detection of light bullets in mode-locked semiconductor lasers.

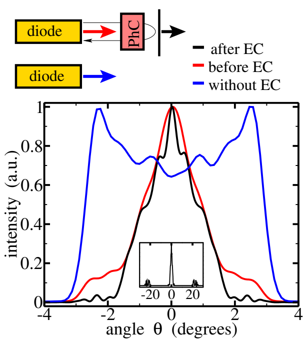

***Fig. 4:** Simulated emission pattern of a BA laser with and without optical feedback from external chirped photonic crystal filter*

Nonlinear dynamics in high-power broad-area (BA) semiconductor lasers were studied with further development of the related software kit BALaser. In the frame of the Eurostars HIP-Lasers project, optical feedback from various types of external cavities was efficiently modeled, including spatial (angular) and frequency filtering elements, which are specially designed chirped photonic crystals and birefringent crystals, respectively. The impact of angularly filtered optical feedback to the quality of the emitted beam was analyzed, see Figure 4 [3], as well as the efficiency of spectral filtering and beam combining provided by external cavities. In the frame of EffiLAS, RG 2 studied the impact of inhomogeneous current spreading [4] and Joule heating to the laser emission quality by selfconsistently coupling of the dynamic electro-optical solver BALaser to the static pdelib-based current-spreading and heat-flow solvers developed in RG 3, see Figure 5.

The dynamics in various narrow-waveguide (single-transverse-mode) lasers was simulated and analyzed with the WIAS software LDSL-tool. State switching dynamics in a micro-ring semiconductor laser with several integrated filtered optical feedback branches, see Figure 6, was studied in cooperation with the colleagues from Vrije Universiteit Brussel and TU Moldova.

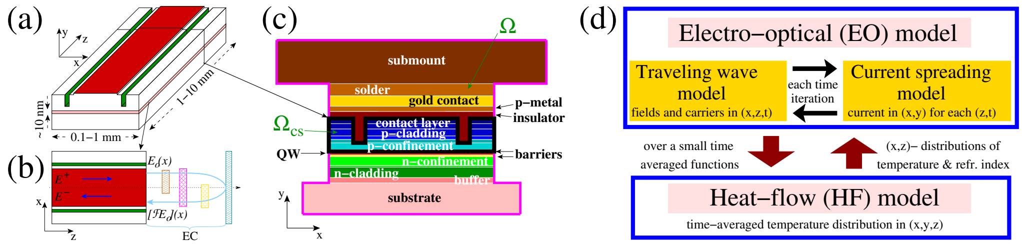

Fig. 5: *(a) BA laser scheme, its projection to the active zone (b), and transverse cross-section (c), where heat-transport and current-spreading is calculated. (d): Scheme of extended BALaser simulator.*

Dynamics and stability of the steady states in multisection distributed-Bragg-grating lasers was investigated together with the collaborators from FBH Berlin and TU Moldova. Furthermore, RG 2 studied the characteristics of chaotic dynamics in semiconductor lasers with optical feedback during a research visit of Mindaugas Radziunas to Macquarie University in Sydney, which was funded by the Macquarie University Faculty of Science and Engineering Visiting Researcher Fellowship.

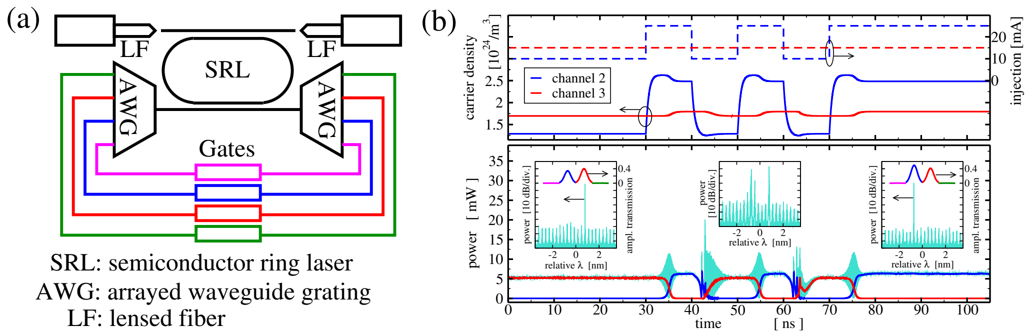

Fig. 6: *(a): Scheme of a semiconductor ring laser with filtered optical feedback. (b): Simulated switching between two states supported by different channels. Top: injected currents and carrier densities. Bottom: total emission power (cyan) and its portions along two activated channels. Inserts: optical spectra and channel transmissions.*

Pulses in nonlinear optical media

An explicit infinite hierarchy of Sasa–Satsuma-type evolution equations was presented. The corresponding Lax pairs were given, thus proving the integrability of all involved equations. The whole hierarchy is combined into a single equation with free parameters, i.e., the model is ready for adaptation to the practical needs. Examples of exact solutions of the general equation are given [6].

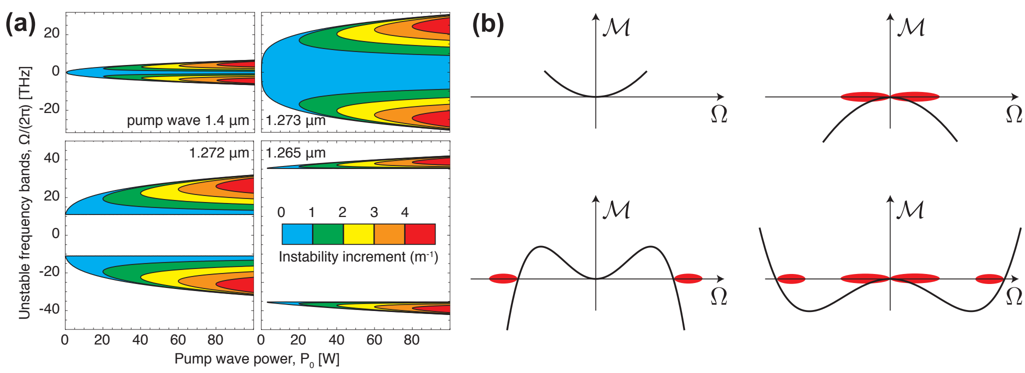

Fig. 7: *(a) MI can be replaced by the Turing-like four-wave mixing instability with the change of the carrier wavelength; (b) instabilities (in, e.g., a focusing fiber) appear if and only if a small negative wave vector mismatch* $\mathcal{M}$ *is present.* See SH. AMIRANASHVILI, E. TOBISH, Extended criterion for the modulation instability, *to appear in New Journal of Physics (WIAS Preprint no. 2512, 2018)).*

Following the classical Lighthill criterion, a continuous wave is destroyed by modulations if nonlinearity and dispersion make opposite contributions to the wave frequency. Studies of the modulation instability (MI) in optical fibers revealed four wave mixing instabilities that are not covered by the Lighthill criterion, see Figure 7. RG 2 proposed an extended criterion, which applies to all four-wave interactions, covers arbitrary dispersion, and depends neither on the propagation equation nor on the slowly varying envelope approximation.

Theory of dynamical systems

Fig. 8: *SFB 910 has been prolongated for the years 2019–2022*

The research in the field of dynamical systems provides the mathematical background for the applied research on semiconductor lasers and optical fibers and is focused on the topics of self-organized patterns and dynamics in delay-differential equations and coupled oscillator systems. A major success in 2018 was the positive evaluation of the DFG Collaborative Research Center 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*, where the subproject A3 "Self-organization and control in coupled networks and time-delayed systems" can now be continued during the fundig period 2019–2022.

A further highlight was the WIAS Workshop "Dynamics of Coupled Oscillator Systems" organized together with Serhiy Yanchuk (TU Berlin) offering a platform for the discussion of recent results in the field of coupled oscillator systems including aspects from dynamical systems theory, statistical physics, as well as applications in various fields of science.

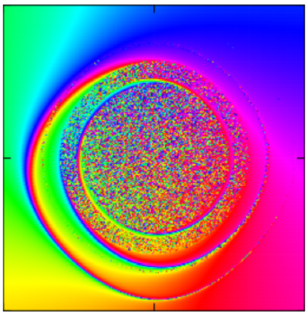

Fig. 9: *Self organized coherence-incoherence pattern in a two-dimensional array of coupled phase oscillators*

In the field of coupled oscillator systems, a new class of self-organized coherence-incoherence patterns in two-dimensional lattices of coupled oscillators was investigated. In [5], the stability and bifurcations of a spiral pattern (see Figure 9) was analyzed. Employing the linearization of the Ott–Antonsen equation that is valid in the continuum limit, a detailed two-parameter stability analysis was performed, identifying fold, Hopf and parity-breaking bifurcations as the main mechanisms whereby spiral patterns can lose stability. Beyond these bifurcations, RG 2 finds new spatio-temporal patterns, in particular also quasiperiodic and drifting patterns of various symmetry types.

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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 research topics of the group will be described briefly. Further topics include tetrahedral mesh generation, physically consistent discretizations for scalar convection-diffusion equations, numerical methods for population balance systems with applications in chemical engineering (in collaboration with RG 5), see the Scientific Highlights article on page 21, and the simulation and control of flows modeling ladle stirring (in collaboration with RG 4); see the article on page 27.

Pressure-robust mixed methods for the incompressible Navier–Stokes equations

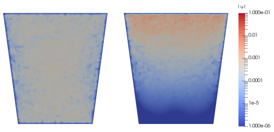

***Fig. 1:** Hydrostatic example with $f(x,y) = \nabla(9.81 y^\gamma)$ for $\gamma = 1$ (left) and $\gamma = 6$ (right), $|\mathbf{u}|$ for the classical Bernardi–Raugel FEM*

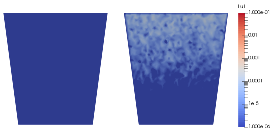

***Fig. 2:** Hydrostatic example with $f(x,y) = \nabla(9.81 y^\gamma)$ for $\gamma = 1$ (left) and $\gamma = 6$ (right), $|\mathbf{u}|$ for the classical Taylor–Hood FEM*

***Fig. 3:** Hydrostatic example with $f(x,y) = \nabla(9.81 y^\gamma)$ for $\gamma = 1$ (left) and $\gamma = 6$ (right), $|\mathbf{u}|$ for a modified pressure-robust Bernardi–Raugel FEM [5]*

In 2018, long-term WIAS fundamental research on novel *pressure-robust* space discretizations [5] for the incompressible Navier–Stokes equations

$$\partial_t \mathbf{u} - \frac{1}{\mathrm{Re}} \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \mathbf{f}, \qquad \nabla \cdot \mathbf{u} = 0 \tag{1}$$

has made important progress, which is described briefly below.

The novel notion of *pressure-robustness* was connected to *common mathematical language*: a *semi norm* and corresponding equivalence classes of forces matter for the development of the velocity field $\mathbf{u}$, see [6]. Two forces $\mathbf{f}_1 \simeq \mathbf{f}_2$ are equivalent (assuming, e.g., Dirichlet boundary conditions), if and only if they differ only by a gradient field, i.e.,

$$\mathbf{f}_1 \simeq \mathbf{f}_2 \quad \Leftrightarrow \quad \exists \nabla\phi : \mathbf{f}_1 - \mathbf{f}_2 = \nabla\phi, \quad \Leftrightarrow \quad \text{Helmholtz projectors } \mathbb{P}(\mathbf{f}_1) = \mathbb{P}(\mathbf{f}_2) \text{ are equal,}$$

and lead in (1) with $\mathbf{f} \in \{\mathbf{f}_1, \mathbf{f}_2\}$ to the same velocity field $\mathbf{u}$. The difference $\nabla\phi$ is compensated by the pressure gradient ∇p. *Hydrostatics* is a special case of pressure-robustness: any gradient field forcing $\mathbf{f} := \nabla\phi$, leads to *no flow* $\mathbf{u} \equiv \mathbf{0}$. The forcing is completely balanced by a pressure gradient $\nabla p = \nabla\phi$. A pressure-robust scheme delivers the same discrete velocity for every force from the *same equivalence class*, see Figures 1–3. The significance of pressure-robustness was not recognized in the numerical analysis community since the early 1970s, which may explain why some obvious advantages of finite element schemes did not pay off so much in practical computations as it was expected.

The significance of *pressure-robustness* for a large class of *high Reynolds number* flows is demonstrated in [6]. High Reynolds number flows are challenging problems that are characterized by a dominant nonlinear convection term $(\mathbf{u} \cdot \nabla)\mathbf{u}$. However, the notion of *pressure-robustness* reveals that there definitely exists a large class of high Reynolds number flows, which are less difficult than usually thought. Indeed, for all time-dependent *generalized Beltrami flows*, the nonlinear convection term is a gradient field, i.e., $(\mathbf{u} \cdot \nabla)\mathbf{u} \simeq \mathbf{0}$.

The first pressure-robust variant of an explicit residual-based a-posteriori velocity error estimator for the incompressible Stokes equations was designed and investigated in [7], which is the perfect match for efficient adaptive mesh refinement for pressure-robust schemes.

Further, it was shown that the real gain of pressure-robust space discretizations is the possibility to use discretizations with a (formally) small *approximation order without compromising the accuracy* of the results, see [6], leading finally to *very efficient* algorithms. The lack of pressure-robustness can be compensated by increasing the approximation order, compare Figures 1 and 2, by paying the price of a more expensive discretization.

Robust equal-order finite element methods for porous media flows

The Brinkman problem was originally proposed as an alternative model for describing flows in a porous medium, see Figure 4 for examples, by considering Darcy's law with an additional resistance term proportional to the fluid's viscous stresses. The introduction of this additional term has the purpose of better capturing the flow dynamics within high permeability regions, i.e., where the fluid's viscous stresses are comparable to porous resistance. Let $\Omega \subset \mathbb{R}^n$ be the domain of interest. The Brinkman problem can be written as

$$-\nabla \cdot (\mu_{\text{eff}} \nabla \mathbf{u}) + \nabla p + \sigma \mathbf{u} = \mathbf{f} \quad \text{in } \Omega, \quad \nabla \cdot \mathbf{u} = g \quad \text{in } \Omega, \tag{2}$$

where $\mathbf{u}$ and p denote fluid velocity and pressure, respectively, while $\mathbf{f}$ and g stand for volume forces and mass sources or sinks. Depending on the values of the physical parameters μ_{eff} (effective viscosity) and σ (inverse of permeability), system (2) describes a whole range of problems between the Stokes ($\sigma = 0$) and the Darcy ($\mu_{\text{eff}} = 0$) models. However, this transition does not depend continuously on the physical parameters. In particular, the standard boundary condition for $\mu_{\text{eff}} > 0$ is an essential boundary condition for the velocity, whereas for $\mu_{\text{eff}} = 0$, it has to be replaced by a condition for the normal velocity. Likewise, when focusing on the weak counterpart of (2), one has to consider different natural functional settings for the Stokes/Brinkman ($\mu_{\text{eff}} > 0$) and Darcy ($\mu_{\text{eff}} = 0$) problems. These aspects affect also the strategies for the discretization of (2) in the context of finite element methods.

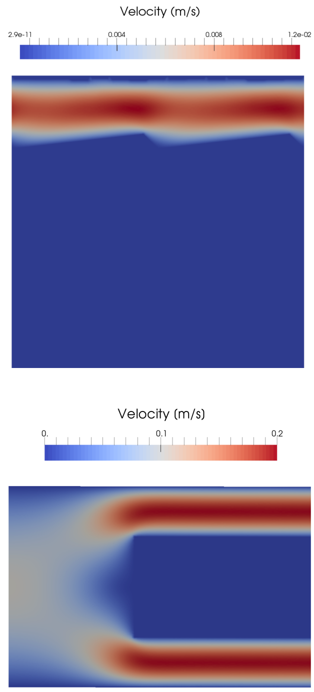

Fig. 4: *Magnitude of the velocity for fluid flows through heterogeneous porous media: top: model of a riverbed, bottom: domain with obstacles of different permeability*

In order to tackle the issue of needing different boundary conditions depending on the (Stokes or Darcy) regime, we focus on the weak imposition of essential boundary conditions with a Nitsche method. In the original version of the method, the boundary conditions are imposed via a penalty term depending on a penalty parameter and on the discretization. We considered the non-symmetric penalty-free Nitsche method, assessing the stability and the accuracy of the approach even without the presence of a penalty parameter. In this case, the method can be interpreted as a Lagrange multiplier method, where for the Brinkman problem the normal fluxes at the boundary and the pressure play the role of Lagrange multipliers. In order to achieve a unified discretization for the whole range of physical parameters, we utilized a stabilized finite element formulation based on linear equal-order finite element spaces. In [1], stability and optimal convergence in a natural (energy) norm were proved for the penalty-free Nitsche method combined with a Galerkin Least Squares (GLS) and a grad-div stabilization. To this aim, it was shown that the natural fluxes allow for controlling the norm of the velocity on the Nitsche boundaries and that the finite element spaces satisfy an inf-sup condition. Moreover, it was proved that the inf-sup constant does not depend on physical parameters, but only on the regularity properties of the mesh and on the stabilization parameters. These results extend available estimates using a similar setting (stabilized finite elements) but a nonzero Nitsche penalty parameter to the case without penalty term and the inclusion of the limit cases $\sigma = 0$ and $\mu_{\text{eff}} = 0$. In order to obtain a robust method, we introduced an additional stabilization term at corner nodes of the domain boundary (in two dimensions) yielding unconditional stability in the Darcy regime. The extension of the analysis to three dimensions and the possibility of avoiding this additional regularization term are currently under investigation.

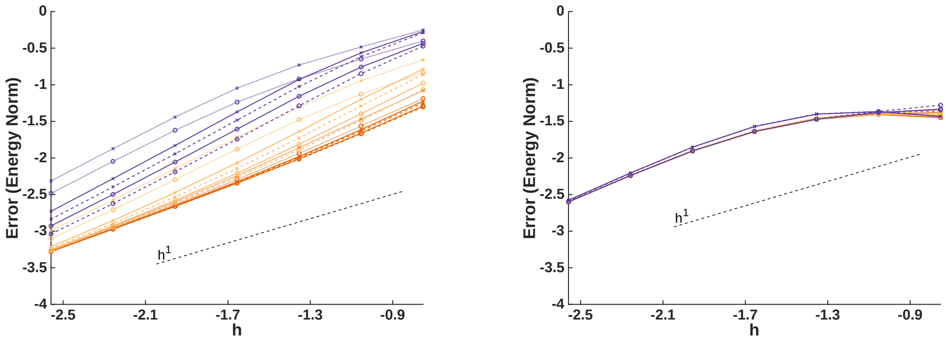

Fig. 5: *Brinkman flow in a rectangular pipe. Error in the (mesh-dependent) energy norm against the mesh size for the cases $\mu_{\text{eff}} = \sigma = 1$ (left) and $\mu_{\text{eff}} = 0.001$, $\sigma = 10$ (double logarithmic plot). Different colors, line styles, and markers refer to different choices of stabilization parameters. The dashed line shows the slope equal to one, predicted by the numerical analysis*

A main motivation behind this work lies in the simulation of flows in highly heterogeneous porous media, considering applications from geophysics and biomedicine. In particular, the use of the proposed finite element formulation in the context of the simulation and optimization of geothermal energy production is currently a subject of an interdisciplinary collaboration with the Leibniz Institute for Applied Geophysics (LIAG, Hanover). Further applications include the simulation of flows in biological tissue, also in connection with recently proposed multiscale methods for efficient simulation of vascular structures [4].

Drift-diffusion processes in semiconductors and electrochemistry

Charge transport in a self-consistent electric field is a fundamental process present in many physical systems. Among them are semiconductor devices and electrolytes in electrochemical and biological cells. Forces acting on charged species arise from gradients of species chemical potentials (causing diffusion), from gradients of the electric potential (causing drift), and from gradients of chemical potentials of competing species. In a self-consistent manner, the distribution of charged species influences the electric field. In cooperation with RG 1, RG 2, and RG 7, the group continues the development of numerical methods and simulation tools that describe such processes in a physically and thermodynamically accurate manner, contributing to the long-standing tradition of research on drift-diffusion problems at WIAS.

The mathematical description of degenerate semiconductors results in a nonlinear enhancement of the diffusion coefficient which needs to be treated in a thermodynamically consistent way during the space discretization process. Our discretization method of choice is a finite volume method that requires the description of species' fluxes depending on electric potentials and species' chemical potentials in neighboring control volumes. In the literature, it was proposed to describe these fluxes by a nonlinear two-point boundary value problem. Their calculation results in the solution of an integral equation. In [8], it was proposed to solve this equation by an approximation of the integral via quadrature rules, resulting in a highly accurate scheme for degenerate semiconductors that is able to compete with other modifications of the Scharfetter–Gummel scheme.

Another modification of the Scharfetter–Gummel scheme is used in the numerical approximation of electrolyte models with finite ion size constraints developed in RG 7. An electrolyte flow model, based on a coupling procedure with a pressure-robust mixed finite element method [5] for fluid flows, was verified based on a number of relevant examples [2, 3] within the MATHEON project CH11 "Sensing with nanopores" (now MATH+ Transition Project CH11, Co-PI: Clemens Guhlke, RG 7).

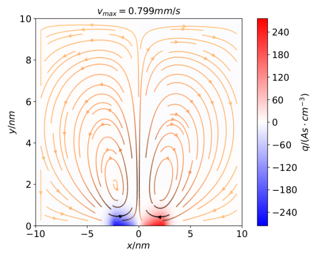

Fig. 6: *Induced charge electro-osmotic flow in the vicinity of an electrode with floating potential [3]*

Three successful third party funding applications have been submitted in cooperation with RG 7. The projects started in late 2018 or early 2019. They focus on multi-material electrocatalysis, continuum-based modeling for the development of secondary Mg/Ca–Air Batteries, and electrochemical double layers in solid oxide cells.

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4.4 Research Group 4 "Nonlinear Optimization and Inverse Problems"

The research group investigates optimization and inverse problems occurring in current engineering and economic applications. A specific focus of research in optimization and optimal control is the investigation of special structures resulting from the presence of uncertain and non-smooth data. 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.

The group successfully applied for the second phase (2018–2022) of the DFG Transregio (TRR) 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks*. Moreover, the existing participation in the Gaspard Monge Programme for Optimization (PGMO) funded by the Fondation Mathématique Jacques Hadamard (FMJH) could be renewed for another two years. The results of our research within these projects have been presented among others at the leading congress on Mathematical Optimization (ISMP 2018) in Bordeaux and at the Oberwolfach Workshop 1834 on "New Directions in Stochastic Optimization".

In the following, selected scientific achievements of the research group in 2018 are detailed.

Stochastic and nonsmooth optimization

The group continued its intensive research on stochastic and nonsmooth optimization. Within TRR 154, the focus was on continuing the theoretical analysis and application to gas networks of the recently introduced class of optimization problems with probust (probabilistic/robust) constraints. Extending earlier work in finite dimensions, gradient formulae for the resulting probability function could be established in a Banach space context. Here, the cooperation with colleagues from our partner institute CMM in Santiago de Chile turned out to be very beneficial. This cooperation led to a joint publication and supervision of a Ph.D. thesis at CMM. The mentioned analysis paves the way for applying probabilistic constraints not just in the specific gas network environment, but generally for PDE-constrained optimization with probabilistic state constraints uniformly over some domain. A first major step in this direction was undertaken in [4]. At the same time, the algorithmic approaches have been advanced and applied, for instance, in a comparative study with an application to gas network optimization [1].
For optimization problems with linear chance constraints under Gaussian distributions, a specialized solution approach based on the approximation of the multivariate Gaussian distribution function and its gradients has been pursued. The emphasis was on deriving confidence intervals for the optimal value.
The supervision of a master thesis devoted to bilevel models of gas market equilibria served as a starting point for more systematic investigations planned in the second phase of TRR 154. Moreover, in a supervised Ph.D. thesis (to be defended in 2019), substantial progress could be obtained in the analysis of dynamic probabilistic constraints. Several semi-continuity properties could be

derived in a general multistage model. Moreover, for certain two-stage models, the optimal second-stage policy could be identified in fully explicit form.

Inverse problems for stochastic data and reconstruction of stochastic surfaces

For the indirect measurement of surfaces generated by reactive-ion etching, the geometry is to be reconstructed efficiently from reflection spectra. As an example, a new process for the fabrication of periodic structures (cf. Figure 1 and Figure 2) has been developed at IHP/Frankfurt, and a gradient algorithm based on sparse grids has been adapted to the reconstruction from data provided by a new measurement device of LayTec Co. In [5], it has been demonstrated that device and algorithm can track the surface in order to control the process.

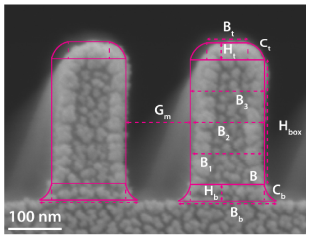

Fig. 1: *Crosssectional SEM picture of line-space surface structure after 100 s of etching process*

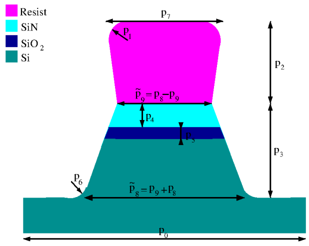

Fig. 2: *Geometry parameters for computational model of line-space structure*

Together with Guanghui Hu (Beijing), the scattering by local perturbations to periodic surface structures has been investigated. For acoustic waves and sound-soft surfaces the scattered field is shown to be the sum of the field for the non-perturbed surface and a wave caused by perturbation. An adaptive Galerkin FEM for random PDEs with low-rank tensor representations for log-normal random fields was developed [2]. In collaboration with Michael Multerer (Lugano), the approach was employed for a random domain problem with affine perturbation vector field. Moreover, a statistical learning approach for high-dimensional parametric problems based on tensor reconstruction was derived.
As a generalization to probabilistic modeling, an Artificial Neuronal Network (ANN) approach for the propagation of polymorphic uncertainties within linear elastic problems was devised. Moreover, for linear PDEs with local possibly non-smooth parametric dependency, a hybrid domain decomposition techniques based on adapted generalized multi-element polynomial chaos was developed in [3], see Figure 3.

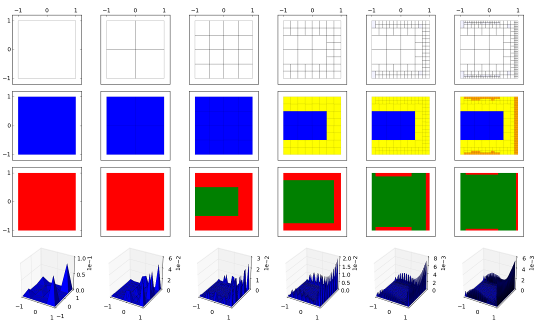

Fig. 3: *Problem-adapted domains and surrogate trust-regions for hybrid FETI domain decomposition*

Optimal control of multifield and multiscale problems

One focus of this year's research was on anisotropic fluids, so-called *liquid crystals*. These materials reveal remarkable physical properties, due to a directional ordering in the material. The rod-like molecules, which build (or are dispersed in) these fluids are aligned in a similar direction (see Figure 4).

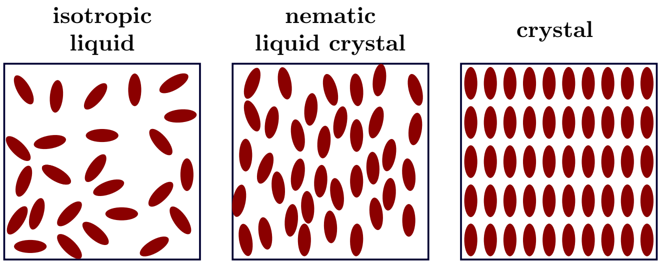

***Fig. 4:** Anisotropic structure of nematic liquid crystal in comparison to isotropic liquids and crystals*

The ordering and its direction heavily influence the properties of the material such as light-scattering or rheology. This gives rise to many applications, where liquid crystal displays are only the most prominent ones. Mathematically, anisotropic fluids are not yet well understood, since their modeling involves highly nonlinear coupling terms, and the evolution is driven by a nonconvex energy functional on a nonorientable manifold. To cope with these difficulties and to develop an existence theory for the full Ericksen–Leslie model, the concept of dissipative solutions was introduced in [6]. In [7], an optimal control problem for the alignment of the molecules by means of an static electro-magnetic field is investigated. This mechanism is at the heart of many applications (like liquid crystal displays) and, hopefully, this new results will allow to develop numerical simulations and gain further insight to the optimal control of these nonlinear materials.

On September 24–25, 2018, the status meeting for the EID project MIMESIS coordinated by the research group took place at the industrial partner SSAB in Raahe, Finland. SSAB and the other industrial partners EFD Induction (Skien, Norway) and Outokumpu (Tornio, Finland) as well as the scientific partners WIAS and University of Oulu met to reflect on the achievements of the MIMESIS project and discuss its goals for the last year of the project. All Ph.D. students presented recent progress in their field of research on the interface of mathematics and material science. It was agreed that in 2019 a final workshop meeting will be held in Skien at EFD Induction.

The group's projects within MIMESIS are all centered around manufacturing processes which include an induction heating component, ranging from modeling, simulation and optimal control of high frequency induction welding over single- and multi-frequency induction hardening of helical and bevel gears to inductive pre- and post heating for the thermal cutting of steel plates. The heating is caused by eddy currents induced by a varying magnetic flux. The oscillations of the magnetic field are rather fast in comparison to the distribution of heat in the work piece. To handle these two different time scales numerically, the influence of the magnetic field is usually averaged over one frequency sweep. This was analytically analyzed by deriving an estimate for the error introduced by this averaging technique on the emerging solution (see [8]).

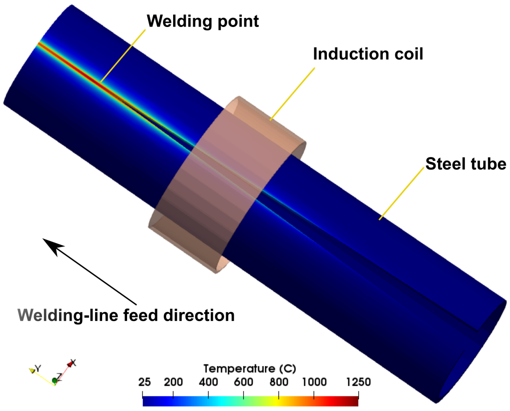

Fig. 5: *Temperature profile of tube edges and heat affected zone during HF induction welding*

For the tube welding project a novel approach to compute velocities and a stabilization scheme allowed for the first complete electro-thermal simulation in 3D for the quasi-stationary case (see Figure 5). New results regarding the thermal cutting of steel are shown in the highlights section on page 27.

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4.5 Research Group 5 "Interacting Random Systems"

In 2018, the RG 5 continued its scientific work on various types of interacting stochastic systems, mostly of particle type, with various applications in, and motivations from, telecommunication, chemical engineering, and physics.

The group's activities in stochastic geometry for telecommunications took broad space in 2018: in research, industrial contacts, and teaching. In fact, two new contracts with our prominent partner Orange S.A. (Paris) on applied questions in telecommunication (related to new 5G technologies) were commenced, two Ph.D. projects were running in this field within RG 5, one lecture and one students' seminar at Technische Universität Berlin were given by two members of RG 5, and corresponding lecture notes were written (which will be extended to book form in 2019). This field is also the topic of the group's project in the newly established *Berlin Research Center MATH+*, starting at the beginning of 2019. This project will be briefly introduced below. Other new third-party funds in this field (and beyond) were awarded by the Deutscher Akademischer Austauschdienst *DAAD* for four years, starting in Summer 2018. Within this project, a new Ph.D. student from Ghana took up his work at RG 5.

Another field of strong activity within RG 5 is the field of interacting particle systems, which are considered from various angles. In particular, the viewpoint of large-deviations analysis and connections between the corresponding rate function and deeper analytic properties of the particle system play a big role in the group's considerations. Various types of particle systems and interactions are under consideration, like chemical reactions on one hand and ferromagnetic systems on another, and effects like fluctuations and dissipation, respectively, are studied. See below for brief reviews of two of the group's activities.

Apart from these main topics, many efforts are also spent on the study of models for random heat flow through highly irregular random spatial potentials from the viewpoint of stochastic partial differential equations with strong irregularities, see the corresponding highlight article on the achievements of the DFG Research Unit *FOR 2402: Rough Paths, Stochastic Partial Differential Equations and Related Topics* on page 10. Further topics that kept RG 5 busy in 2018 are self-repellent random walks in a random potential, the heat equation with random potential on (random) discrete structures like the high-dimensional hypercube or random graphs, and random Gibbs measures and large spin systems.

One of the Ph.D. projects within RG 5 came to a particularly good end in Summer 2018, when Franziska Flegel achieved the highest distinction in her defense of her work on "Spectral properties of the random conductance Laplacian" at Technische Universität Berlin.

Two scientific conferences were co-organized in 2018 by the head of RG 5, one in the Mathematisches Forschungsinstitut Oberwolfach (MFO) on the "Interplay of Analysis and Stochastics in Complex Physical Systems", and one at Technische Universität Berlin on "Random Media and Stochastic Interface Models". He also organized one of Berlin's major public events in popularizing mathematics, the *23rd Tag der Mathematik* on April 21 at Technische Universität Berlin. In this team competition, altogether 1 000 pupils participated.

In teaching, the head of RG 5, supported by group members and a Ph.D. student, 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 RG 5.

Please find below a closer description of some of the group's achievements in 2018.

Malware propagation in ad-hoc telecommunication networks

The mathematical analysis of random propagation of infections in a network goes back to the works of Reed and Frost in the early 30s. There, the network was the complete graph, where every network component interacts with every other component in the same way, a so-called *mean-field model* (see also below).

Ever since, such models enjoyed a huge interest both from the probabilistic community as well as from applications. In particular, the 80s saw a rise in scientific publications (e.g., by Liggett, Griffeath, Durrett, and Hammersley) extending the models to include a non-random spatial component. More precisely, their focus was on Markovian models, for example, on the d-dimensional lattice.

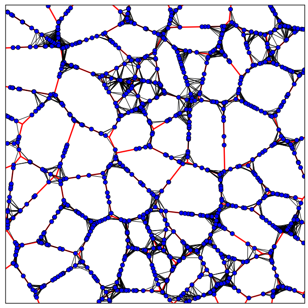

Fig. 1: *Ad-hoc network of users on a street system*

However, in order to model mobile ad-hoc telecommunication networks, a more realistic and less regular spatial distribution of users is required.

It was shown that the edges of Voronoi cells formed by a homogeneous Poisson point process share a resemblance with street systems of European cites. We now distribute users on the streets as depicted in Figure 1 and connect them if they are close enough that their cell phones can connect. The network formed by such connections is called an *ad-hoc network*. While the lack of infrastructure makes such networks cost-efficient, they also bear a security risk, as phones are allowed to directly communicate with each other. Together with our collaboration partner Orange S.A. (Paris), we explore the risk of such a spatially distributed epidemic. One such model is the so-called *white-knight model*.

In ongoing contracts with Orange, we build models to analyze the size and shape of serving zones [3] and analyze the efficiency of possible countermeasures.

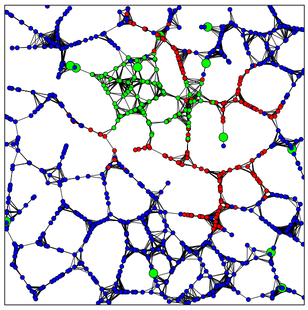

Fig. 2: *Possible state of the white-knight model: susceptible (blue), infected (red), and users with goodware (green)*

We assume that for every malware a positive counterpart is developed in form of so-called *goodware* that is able to detect, clean, and protect the device from future infections. Therefore, devices can be in three states: They can be infected, susceptible to an infection, or they can have the proper goodware installed and are therefore safe. Furthermore, the goodware has one additional feature: it is able to detect incoming infection attempts and identify the attacker. Once the attacker is identified, as a direct response to the imminent security thread, the goodware is allowed to retaliate and install itself on the compromised system, cleaning the device and protecting it from that point onwards. In the initial state of the system, only a portion of the users have the goodware installed. They are called *white knights* as they provide protection to their neighbors. Now the infection spreads through the susceptible devices and the goodware chases after it, see Figure 2.

Like other epidemic models, we can observe a so-called *phase transition*. In our case, with a slight increase in the transmission rate of the infection, we are able to see a fundamentally different behavior of the system: Below the critical value, we see only local outbreaks that are cured exponentially fast, above the critical value a global outbreak is possible.

We were able to prove phase transition in our model and compute upper and lower bounds for the critical value. With the help of simulations, we further narrowed down the actual critical value.

Mean-field interacting particle systems

Mean-field interacting particles were introduced by Kac with the aim of microscopically justifying the spatially homogeneous Boltzmann equation. Since then, they have been extensively studied due to their flexibility and their connections with nonlinear processes and PDEs.

This type of models consists in a microscopic and a macroscopic description of a phenomenon, in a way that the nonlinearity observed in the macroscopic behavior is explained by an interaction term at the microscopic level.

Nonlinear processes arising as hydrodynamic limits of mean-field interacting particle systems, also called *McKean–Vlasov processes*, are non-trivial stochastic processes. The study of the convergence and of their features involves various techniques that are usually not needed for classical Markov processes. For instance, stopping times and compactness methods are not useful in the proof of well-posedness of the correspondent nonlinear SDE, and the development of different approaches is needed.

In [1], a general system of interacting SDEs was introduced, where diffusion and jump terms coexist and the key interaction is given by the so-called *simultaneous jumps*. This is a system of N jump diffusions in $\mathbb{R}^d$, for $d \geq 1$, that interact with each other via classical mean-field interactions. This system is endowed with an additional interacting mechanism, inspired by neuroscience problems: Each particle performs a jump, called a *main jump*, with a certain rate and it simultaneously induces in all the other particles a *collateral jump*, whose amplitude is of the order $O(\frac{1}{N})$. The model is interesting for the dissimilarity in the treatment of the jump terms, since it was proved that, in the limit for $N \to \infty$, the main jump component is preserved, while the collateral jump, although simultaneous, collapses into an additional nonlinear drift term. Moreover, pathwise propagation of chaos for interacting diffusions with jumps was less widespread in literature than the continuous case, probably because of the discontinuities in the paths and the impossibility to use a compactness approach as in the proof of well-posedness for classical SDE with jumps.

The paper [1] focuses on well-posedness of the corresponding nonlinear limit process and on the proof of pathwise propagation of chaos by means of a coupling method. Under quite general assumptions, it proves results for a wide class of processes, including in the same framework nonlinear processes with unbounded jump rates and with diffusive terms, which rarely appeared in the previous mean-field literature.

Besides the interesting technical features arising in the proof of convergence, nonlinear processes display a much richer long-time behavior than their correspondent particle systems. In particular, they may show stable oscillatory laws or multiple stationary measures. The paper [2] focuses on a system coming from a generalized Curie–Weiss model that evolves in time according to a suitably modified dynamics, with an interaction term that undergoes a dissipative evolution. This was proved to be one of the ways in which the reversibility of the model may be broken, giving rise to self-sustained periodic behaviors in the nonlinear limit.

Moreover, by suitably modifying the interaction function of the model, it was possible to recreate an interacting particle system that shows as many stable limit cycles as wanted. This confirms that the addition of a dissipation term in the time evolution of the interaction favors the presence of self-sustained periodic behavior for particle systems without any tendency to behave periodically. The paper [2] gives a model that is extremely flexible and it is able to adapt to multiple modeling situations.

Large deviations of reaction fluxes

More information about random fluctuations around the above-described hydrodynamic limits are described by so-called *large-deviation principles*, which give variational descriptions of the exponential decay rate of probabilities in the limit $N \to \infty$ of a large number of particles. In a previous work, we were able to show that large deviations of reversible random particle systems can always be rewritten as an energy balance between free energy loss and dissipation.

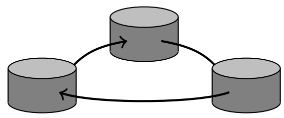

Fig. 3: *A simple example where mass is transported in a cycle, leaving the mass distribution invariant*

Such energy balances characterize the corresponding macroscopic dynamics as a thermodynamically meaningful gradient flow, in the sense that the dynamics are driven towards the equilibrium by a free energy functional that decreases along solutions. However, one of the biggest challenges of non-equilibrium thermodynamics today is to understand the evolution of systems that are driven by external forces or inflow and outflow of mass, which roughly corresponds to irreversible particle systems on a microscopic level. Indeed, the irreversibility is likely to cause a gap in the energy-dissipation balance, so that the macroscopic dynamics can no longer be described by a gradient flow.

What makes these irreversible systems so challenging is the possible occurrence of “divergence-free” mass fluxes through the system that do not alter the mass distribution, see Figure 3. Hence, the study of mass distribution functions typically yields an incomplete picture unless one also takes fluxes into account.

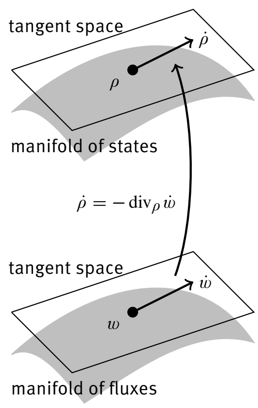

Fig. 4: *Fluxes and states related by a continuity equation*

Most studies of flux large deviations in the literature concern systems for which the microscopic fluctuations are approximately white, in the sense that the dynamic large-deviation rate are quadratic action functionals. For typical particle systems that model chemical reactions however, the rate functional will be “entropic” rather than quadratic.

In our recent work [4], we were able to prove the dynamic large-deviation principle for “reaction fluxes”. A reaction flux is the chemical equivalent of fluxes occurring in mass transport systems, measuring the number of reactions taking place at each time. As a mathematical by-product, the concentration large deviations follow directly from the reaction flux large deviations.

With the reaction flux large deviations at hand, one can study whether for irreversible processes the energy balance can be restored by taking fluxes into account. This turns out to be impossible. In [5], we showed in great generality that for systems where fluxes and states are related through a linear continuity equation (see Figure 4), the large deviation energy balance for fluxes is equivalent to the energy balance for states.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

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

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

Members of the research group participated in the DFG Collaborative Research Center SFB 1294 *Data Assimilation*, DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, and DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*, 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", a collaboration with Deloitte, and other projects.

Scientific highlights achieved by the research group in 2018 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 barycenter. Research within this subarea covered both theoretical and applied statistical problems.

Highlights 2018:

- Thomas Koprucki (RG 1) and Karsten Tabelow (RG 6) receive funding for the MATH+ project EF3-1 "Model-based geometry reconstruction from TEM" running from 01/2019–12/2021.
- The new MATH+ project EF3-3 "Optimal transport for imaging" (PIs: Pavel Dvurechensky (RG 6), Michael Hintermüller (RG 8), and Vladimir Spokoiny (RG 6)) was approved for funding.
- Darina Dvinskikh and Pavel Dvurechensky (both RG 6) presented their work "Decentralize and randomize: Faster algorithm for Wasserstein barycenters" (jointly with Alexander Gasnikov, César A. Uribe, and Angelia Nedic) at the 31st Conference on Neural Information Processing Systems in Montreal, Canada. The paper was accepted as a spotlight presentation, i.e., it was in the top 4% out of 4856 submissions.

In 2018, the members of the group made some significant contributions to statistical literature.

The bootstrap-based approach from [1] to estimation of the spectral projector of a large random matrix is extended in [2], where a new Bayes procedure with Wishart priors is used for uncertainty quantification in finding a spectral projector.

We offered a complete solution to the so-called *large ball probability* problem which 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 SFB 1294.

There were also several contributions to the Optimal Transport literature. We provide a new complexity analysis for the ubiquitous Sinkhorn's algorithm for solving the optimal transport problem and a new accelerated-gradient-based algorithm for this problem together with its complexity analysis. Paper [3] considers calculation of Wasserstein barycenter of a distributed set of probability measures, stored in a network of agents, e.g., large datasets stored distributedly in a number of computers or a network of sensors, measuring and storing some signals. A novel accelerated primal-dual stochastic gradient descent method is developed for a general class of optimization problems and applied to the Wasserstein barycenter problem.

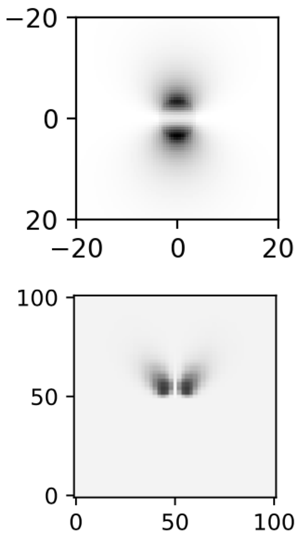

Fig. 1: *Calculated strain field for Upper: a spherical QD; lower: a pyramidal QD*

Modeling and simulation of TEM imaging of quantum dots. Within the ECMath project OT7, we worked, together with RG 1, on the simulation of transmission electron microscopy (TEM) images from quantum dots (QD). In collaboration with Technical University Berlin, Institute of Optics and Atomic Physics and RG 3, we developed a mathematical model describing the imaging of semiconductor QDs by TEM. For the numerical simulation of TEM images we coupled an elasticity solver to obtain the strain profile, which enters a solver for the Darwin–Howie–Whelan equations, describing propagation of the electron wave through the sample. We demonstrated, by numerical simulations, nonlocal effects in the imaging process due to strain. We have shown that the images strongly resemble the displacement field caused by the mechanical strain between the quantum dot and bulk material, see Figure 1. The developed software now enables the creation of a database of simulated TEM images for different configurations of QDs which we will use in the envisaged model-based reconstruction approach MBGR. We successfully applied for a follow-up project EF3-1 within the excellence cluster MATH+.

Neuroscientific applications of statistical methods. Together with colleagues from a large European consortium of neuroscientists, we further developed the new comprehensive toolbox `hMRI` (`http://hmri.info`) for multi-parameter mapping MRI data. This will be the basis for making new statistical tools developed within the RG 6 available for a broad scientific community in the neurosciences. In this connection, we developed a major improvement of the structural adaptive smoothing procedure and compared it, together with RG 8, with a large number of other image denoising method large total (generalized) variation.

A manuscript on dynamic functional connectivity (dFC) by Jun Young Park (University of Minnesota (UMN), Biostatistics), Jörg Polzehl (RG 6), Snigdhansu Chatterjee (UMN, Statistics), André Brechmann (LIN Magdeburg), and Mark Fiecas (UMN, Biostatistics) is currently under review. The paper proposes a method to simultaneously estimate time-varying activation effects and a time-varying dFC between regions in task-based functional MRI.

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 modeling in financial and energy markets, for instance volatility modeling, calibration, and the modeling of complex-structured products in energy and volatility markets, for example.

Highlights 2018:

- The Research Unit 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics* was positively evaluated to be funded for another period. The research group contributes with the project "Numerical analysis of rough PDEs" (PIs: Christian Bayer, John G.M. Schoenmakers (both RG 6)).
- The new MATH+ project AA4-2 "Optimal control in energy markets using rough analysis and deep networks" (PIs: Peter Friz, Christian Bayer, John G.M. Schoenmakers, Vladimir Spokoiny; all RG 6) was approved with one PostDoc position at WIAS and one Ph.D. position at TU Berlin.
- The new MATH+ project EF1-5 "On robustness of deep neural networks" (PIs: Christian Bayer and Peter Friz; both RG 6) was approved with one PostDoc position jointly at WIAS and TU Berlin.
- The book "Avanced Simulation-Based Methods for Optimal Stopping and Control" by John G.M. Schoenmakers (RG 6) and Denis Belomestny from Universität Duisburg-Essen has been published with Palgrave-Macmillan (2018).

American options are solved by either explicitly or implicitly determining so-called *exercise regions*, which consist of points in time and space at which the option is exercised. In our group, a new method was developed based on exercise rates of randomized exercise strategies (see preprint arXiv:1809.07300). The supremum of the corresponding stochastic optimization problems provides the correct option price under general conditions. To find this supremum numerically, the space of exercise rates is parameterized and the resulting coefficients are optimized using off-the-shelf optimization routines. This procedure exploits the fact that the expected payoff is differentiable with respect to perturbations of the exercise rate. Starting optimization in a neutral strategy with constant exercise rate allows finding globally optimal rates in a gradual manner. Preliminary theoretical analysis and numerical experiments on one- and multi-dimensional put options in the Black–Scholes model underline the efficiency of our method both with respect to the number of time-discretization steps and the required number of degrees of freedom in the parameterization of exercise rates.

In the area of regression-based methods for optimal stopping and control, a new approach towards solving numerically optimal stopping problems via boosted regression-based Monte Carlo algorithms was developed. The main idea of the method is to boost standard linear regression algorithms in each backward induction step by adding new basis functions based on previously estimated continuation values, and as such this method has a flavor of "deep learning". As a result, a regression-based Monte Carlo approach is developed for building sparse regression models at each backward step of the dynamic programming algorithm. This enables estimating the value function with virtually the same cost as the standard regression algorithms based on low degree polynomials, but with higher precision. As such this approach has much potential for reducing the complexity of regression-based methods for dynamic programs connected with more general 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), population dynamics, neuroscience, and financial mathematics. The analysis of effective projection-based particle methods resulted in the article [5]. The next focus was (and still is) 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. These novel estimators were successfully effectuated in a numerical framework for optimal stopping of McKean–Vlasov processes. The study of more general common noise mean-field processes, i.e., McKean–Vlasov processes with a common stochastic driver, has been started. Solving optimal stopping and control problems for such kind of processes has many applications in economics, for example, and is considered a challenge from a mathematical point of view.

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 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, which can also be used to improve classical regression techniques for computing American option prices in mathematical finance, see WIAS preprints no. 2506 and 2532.

The research on the rough volatility model continued successfully in 2018. Precise asymptotic expansions of call prices for general stochastic volatility models have been studied. Such expansions hold in the large deviations regime and apply, in particular, to rough volatility models. These results are based on the Laplace method on the space of models, and use as a main tool the theory of regularity structures. With the aim of reproducing empirical implied volatility surfaces, certain stochastic local volatility models have been investigated. These models produce extreme implied skews, similar to the ones associated with rough volatility with Hurst parameter going to 0.

Work on deterministic sparse quadrature methods for stochastic rough systems has continued based on [4]. In particular, these methods are highly efficient for rough volatility models when combined with proper hierarchical constructions of the underlying noise and Richardson extrapolation for the time discretization.

Many phenomena in real life can be described by partial differential equations. To find an accurate model, nonlinearities and uncertainties have to be taken into account along with a high-order spatial discretization, leading to large-scale nonlinear/stochastic dynamical systems. As a result, it is hard to use these models in engineering studies such as control and optimization. To mitigate this issue, model order reduction (MOR) techniques are often used to reduce the order of large-scale nonlinear/stochastic systems and, hence, reduce the computational complexity.

In [6], a large-scale stochastic system with bilinear drift and linear diffusion term is investigated which can be interpreted as a semi-discretized stochastic partial differential equation. These bilinear systems can be seen as bridge between linear and nonlinear systems, because many nonlinear systems can be represented by bilinear systems using a so-called *Carleman linearization*. We study a particular MOR technique called *balanced truncation (BT)* to reduce the order of the high-order stochastic bilinear system. We introduce suitable Gramians to the system and prove energy estimates that can be used to identify states which contribute only very little to the system dynamics. When BT is applied, the reduced system is obtained by removing these states from the original system. The main contribution of this paper is an L^2-error bound for BT for stochastic bilinear systems. This result is new even for deterministic bilinear equations. In order to achieve it, we develop a new technique which is not available in the literature so far.

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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 are the thermodynamically consistent modeling, systematic asymptotic methods, in particular, singularly perturbed problems, rigorous analysis of the derived models, and analysis of hysteresis properties. Application areas focussed on electrochemical processes, fundamental processes of micro- and nano-structuring of interfaces, dynamics of complex liquids, electro-magneto-mechanical components.

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

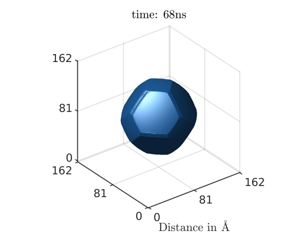

Fig. 1: *Simulation of a 3D Si grain in an undercooled melt. Intialized as a sphere, it developed the typical {100} and {111} facets.*

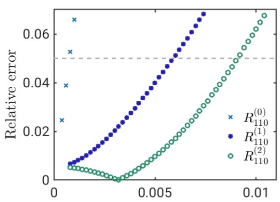

Fig. 2: *Relative error between MD velocity and that from the simulation using the asymptotical mobility of three different orders*

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

The atomistically informed phase field model that has been developed during a project (headed by Barbara Wagner) within the Helmholtz Virtual Institute *Microstructure Control for Thin Film Solar Cells* has been further extended to allow for the quantitative comparison with experiments, in particular, regarding the exact shape of the solid-liquid interface of silicon grains, which is essential to understand and control the LPC process. The main focus concerned the delicate matched asymptotic analysis that was carried out to higher order to obtain the necessary correction of the anisotropic mobility of the phase field model in one, two, and three dimensions. One can observe in Figure 2, that with each higher order, the variable ε and, hence, the interface thickness can use more realistic values without loss of exactness of the numerical simulation.

Furthermore, an optimization of the surface energies leads to a higher efficiency of the numerical algorithm. At the same time, the choice of these energies is consistent with experiments and with MD simulations regarding the critical radius of a nucleus in an undercooled melt.

Mathematical models and theory of electrochemical processes

Project grant in Berlin Mathematics Research Center MATH+ (DFG funded). Within the Berlin Mathematics Research Center MATH+, RG 7 (Manuel Landstorfer) submitted together with RG 3 (Jürgen Fuhrmann) a joint proposal "Modeling and Simulation of multi-material electrocatalysis" (MultECat). The project goal are continuum models for electrocatalysis at the $nm - \mu m$ scale coupling reactions on catalytic interfaces, reactant transport in electrolytes and charge transport in catalyst substrates. Numerical simulations will support the interpretation of electrochemical measurements and allow for a scientific exchange with the Berlin-based research network *UniSysCat* (Unifying Systems in Catalysis). The proposal was evaluated positively in November 2018 and starts in early 2019 as MATH+ project AA2-6 within the application area *Materials, Light, Devices*.

More in detail, the project aims to extend the WIAS model and simulation framework for electrochemical interfaces towards multi-material electrodes (see Figure 3), which are used in modern electrocatalysis, and especially in UniSysCat. In such multi-material electrodes, nano-particles of different materials are deposited on a single electrode with the goal to optimize a certain electrocatalytic reaction. Main aspects of the model development in MultECat are (i) a general modeling of electrode surfaces composed of different materials; (ii) a formulation of the balance equations reflecting this multi-material situation; (iii) a general scheme capable of describing reactions occurring on each phase; (iv) a careful re-derivation of the measurable current accounting for the different surface phases, and (v) functional representations of the surface chemical potentials on each phase. This approach allows to model multi-material electrodes and, in particular, the experimental techniques used today to investigate such catalysts, i.e., current – voltage measurements (CV), Differential Electrochemical Mass Spectroscopy (DEMS), and Scanning Tunneling Microscopy (STM). Numerical simulations of these electrochemical measurement techniques allow for a systematic validation of the modeling procedure. The ultimate goal is a model-based interpretation of CV and STM in order to provide a deeper insight into the complex interactions between the various physico-chemical processes occurring in modern electrocatalysis.

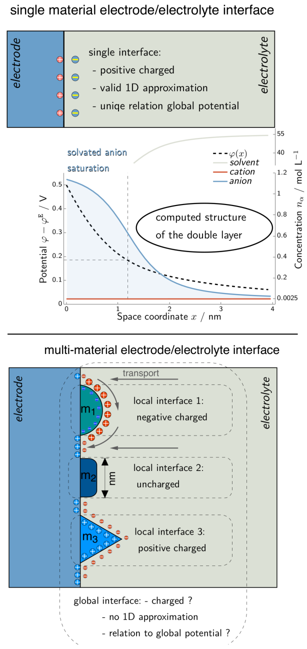

***Fig. 3:** Top: Sketch and numerical simulation of the electrochemical double layer at the planar interface between a single crystal electrode and some electrolyte. Bottom: Sketch of a multi-material electrode where different local interface structures can be present.*

Project start of MALLi [2] (BMBF funded). The BMBF compound project MALLi [2] [1], with RG 7 (Manuel Landstorfer) as project coordinator, and Mario Ohlberger (WWU Münster), Volker Schmidt (U Ulm), Sven Simon and Kai Birke (both U Stuttgart) as scientific partners as well as VARTA Microbattery, Daimler AG, and Continental Services Engineering as industrial partners, successfully started in early 2018.

The project aims to improve the lifetime estimation of lithium-ion batteries from electric vehicles for their continued use as stationary energy storage device. This is addressed with a mathematical model that accounts for diffusion and conductivity in the electrolyte phase, lithium concentration in the active particles, intercalation reactions at the electrode-electrolyte interface, as well as porous structure of the electrodes. Within RG 7, such a model was derived on the basis of non-equilibrium thermodynamics and the WIAS framework for electrochemical interfaces ([3], [4]). This system of PDEs is numerically solved to compute the discharge behavior of a battery cell. Figure 4 displays, for example, the computed cell voltage E as a function of the cell capacity Q for various discharge rates C_h ([4]). For non-phase separating materials and periodic micro-structures of the intercalation electrodes, a spatial homogenization is carried out which leads to a system of non-linearly coupled PDEs for a homogenized battery cell. This model is the foundation for a comparison to experimental data provided by the project partners.

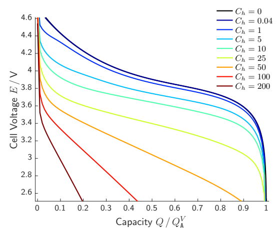

***Fig. 4:** Computed cell voltage E as function of the capacity Q/Q_A^V for various discharge rates C of a lithium NMC intercalation cell. The discharge curve accounts for solid state diffusion and electrical conductivity in the intercalation phase, Li+ and PF6- diffusion in the electrolyte, and charge transfer at the electrode/electrolyte interface.*

Sensing with nanopores. The ECMath project CH11 "Sensing with nanopores", headed by Jürgen Fuhrmann (RG 3) and Clemens Guhlke (RG 7), aims at gaining deeper insight into the electrochemical and fluidic processes that determine macroscopic behavior of nanopores. Improved Nernst–Planck models are coupled to the fluid flow and are analyzed. In order to provide physically meaningful numerical models of the double layer structure, novel numerical discretization schemes, like pressure-robust methods for fluid flow, and property preserving finite volume schemes for the

[1] Model-based assessment of the life span of aged Li batteries for second-life use for stationary energy storage.

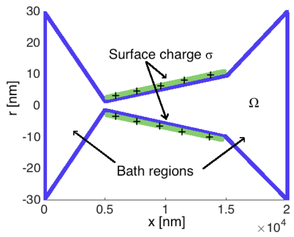

Fig. 5: *Simulation domain for a conical nanopore with positively charged walls between two electrolyte bath regions*

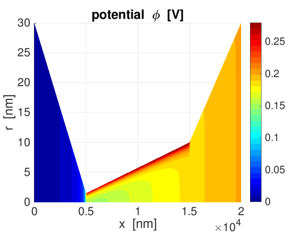

Fig. 6: *2D reconstruction of the asymptotic 1D solution for the electrostatic potential inside the nanopore. The potential shows steep boundary layers at the charged wall that overlap at the narrow opening of the pore.*

Poisson–Nernst–Planck system are applied. Electrochemical models are nonlinear coupled multiscale models, and a generalization of the standard Poisson–Nernst–Planck model is far from being obvious. The results in [1] suggest that ion solvation has a considerable impact on the characteristic transport properties of nanopores. By asymptotic analysis, approximate models for the high aspect ratio nanopores under consideration are derived. The structure of equilibrium solutions of the improved Poisson–Nernst–Planck model allows to reduce the numerical method to the solution of a one-dimensional problem, instead of the complete spatially fully resolved 3D problem; see Figures 5 and 6. These dimension-reduced models have the potential to significantly reduce computation times, and thereby to allow the study of complex geometries and to optimize the surface charge distribution.

Multiphase flow problems in complex liquids

Concentrated suspensions. Within the new Berlin Mathematics Research Center MATH+ joint project "Modeling and analysis of suspension flows", headed by Volker Mehrmann (TU Berlin), Dirk Peschka (WG1), Matthias Rosenau (GFZ Potsdam), Marita Thomas (WG1), and Barbara Wagner (RG 7), new mathematical models for suspension flows are being developed, building on models by [5]. Mathematical analysis and structure-preserving discretizations are used to identify material laws and validate the suspension models.

Mutiphase flows in quantitative biomedicine. A newly formed network for Quantitative Regenerative Medicine, that has been initiated by Sarah Waters, Andreas Münch (both U Oxford), Georg Duda (Charité), and Barbara Wagner (WIAS) has received funding for a seed grant via the Oxford–Berlin Partnership. The aim is to build interdisciplinary research teams and to obtain funding for joint research to unravel underlying mechanisms of healing cascades and enable the predictive quality of pre- and early clinical analyses for the up-scaling of treatments to diverse patient populations. One of a number of problems is the controlled tissue regeneration, guided by responsive scaffolds, such as hydrogels [6], to optimize cell proliferation.

Analysis of PDE models describing the transport of mass and momentum in isothermal liquid mixtures

As a principal investigator (temporary positions for principal investigators, DFG), Pierre-Étienne Druet developed new techniques to handle the analysis of PDE models describing the transport of mass and momentum in isothermal liquid mixtures subject to a generalized incompressibility constraint. The correct generalization of the condition, that is well known in the context of single component fluids, was derived. Analytical results for multicomponent fluids under such constraints are nonexistent in the literature. The main new results obtained in the DFG project concern: The weak solution analysis of mass-transfer equations for N species with full Navier–Stokes equations for the barycentric velocity under the new incompressibility constraint; the local-in-time well-posedness analysis in classes of strong solutions; the vanishing diffusion limit for Darcy flows.

These results, partly in collaboration with Dieter Bothe (TU Darmstadt) and Ansgar Jüngel (TU Vienna) are currently compiled and submitted. An earlier result on the regularity of second derivatives in elliptic transmission problems near an interior multiple line of contact has been published [2].

Hysteresis, electromagnetic-mechanical components, and uncertainty quantification

Experimental data for Terfenol-D, provided by Daniele Davino (Benevento, Italy), were used to compute 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 [7].

Moreover, for a fixed final time $T > 0$, a fixed initial state and a fixed continuous and piecewise monotone input function on $[0, T]$ the mapping from the yield limit to the output function on $[0, T]$ of the corresponding play operator was considered as a mapping from $(0, \infty)$ to $L^p(0, T)$ with any $p \in [1, \infty)$. It was shown that this mapping is Hadamard-differentiable and an explicit formula for the derivative was derived.

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

The research group's focus is the analysis, modeling, and optimization associated to partial differential equations (PDEs) with nonsmooth structure and nonsmooth energies in infinite-dimensional spaces, together with the development of solution algorithms and their computational realization. Particular fields of interest involve nonsmooth energy functionals and/or state systems in image processing and fluid dynamics, generalized Nash equilibrium problems, and quasi-variational inequalities.

Concerning the main application areas of WIAS, RG 8 contributes to *Quantitative Biomedicine*, *Optimization and Control in Technology and Economy*, *Flow and Transport*, as well as aspects of *Materials Modeling*. Specific topics of application are quantitative magnetic resonance imaging (qMRI), uncertainty quantification in the transport of natural gas, and equilibrium problems arising in competition in markets modeling.

RG 8 started its research activities in 2016, and through 2018 has continued to mature and integrate within WIAS. One new member has started in the reported period: Olivier Huber (postdoc within the DFG SFB-TRR154 subproject at Humboldt-Universität zu Berlin).

General relevance of the scientific topics considered by the RG

The research of RG 8 is associated with problems related to partial differential operators together with non-differential structures. The study of such problems is motivated by topics in applied sciences where nonsmoothness arises, e.g., directly via the problem formulation or the constitutive laws, as constraints, as the consequence of competition models, or it appears in optimization / identification frameworks due to the lack of differentiability of an associated map of interest.

One of the main goals of the research agenda of RG 8 consists in properly capturing nonsmooth phenomena in mathematical models and related optimization problems. For instance, the determination of appropriate boundary conditions for thermal fluids on domains with open boundaries is an example where a nonsmooth model is able to capture counter-intuitive behaviors of flow and temperature near boundaries. On the other hand, in non-cooperative games, an appropriate concept that accounts for shared constraints is given by generalized Nash equilibrium. Here, nonsmoothness arises in the study of their first-order optimality conditions.

Additionally, in the report period RG 8 considered nonsmooth inverse and parameter identification problems which are known for their ill-posed nature. For instance, the identification of an uncertain friction coefficient in an Euler system of equations for modeling gas flow through a pipe was considered. In order to solve the identification problem, a Bayesian approach was adopted. Furthermore, in image processing significant advances in magnetic resonance fingerprinting were achieved. In this setting, the pre-computation of a dictionary via Bloch equations (arising from a mathematical description of the underlying physics) was replaced by integrating the physics model right into the reconstruction process leading to a constraint in form of a nonlinear operator equation. Finally, another topic in image reconstruction which was treated in 2018 is associated with structural priors for multi-modal data.

Selected research results

Uncertainty quantification (UQ) for gas networks. The change of direction in energy policy is one of the focus areas of political decision-making and public opinion in the energy sector. The phaseout of nuclear and fossil energy supplies will only be possible by exploring new sustainable resources and facilitating their optimal distribution. It is understood that gas plays a role as an intermediate energy resource during this transition. In this vein, RG 8 participates in the DFG Collaborative Research Center SFB/TRR 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks*.

The transport of natural gas is typically achieved through a complex network of pipelines emanating at production sites or storage facilities and ending at customer locations. Mathematically, the gas transport in pipes is described by the isothermal semilinear Euler equations, a system of hyperbolic PDEs. In order to consider optimization questions involving the Euler system, the estimation of the friction coefficient, which is in general uncertain, is required.

The inverse problem of identifying the friction coefficient adopting a Bayesian approach in infinite dimensions has been considered; see [1]. Here, the goal is to identify the distribution of the quantity of interest based on a finite number of noisy measurements of the pressure at the boundaries of the domain. Numerical results in this direction are shown in Figure 1. This project also led to the release of a software package for Bayesian inverse problems of gas pipes, publicly available at: `https://github.com/fg8/UQ`

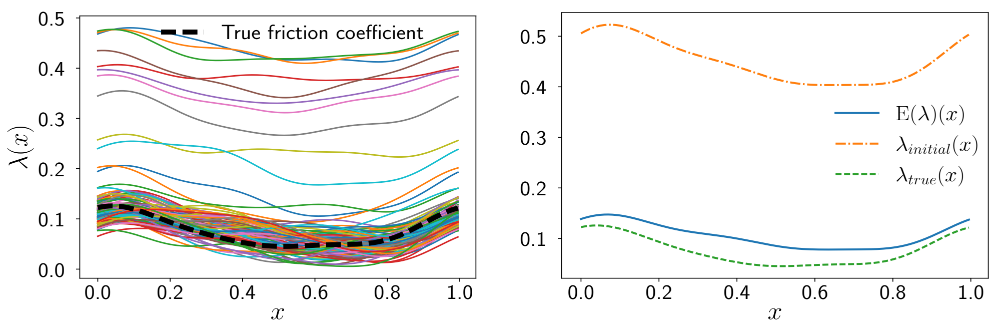
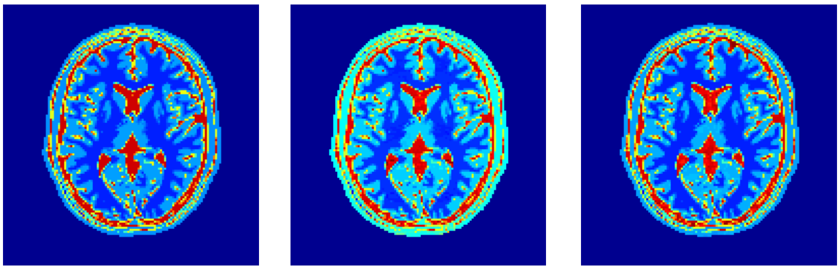


Fig. 1: *True and Markov Chain Monte Carlo samples of the friction coefficient (left) and the pointwise mean friction function (right)*

Image processing. The group has continued and expanded its activities on image processing with highlight being the recently completed ECMath CH12 project on "Advanced magnetic resonance imaging: Fingerprinting and geometric quantification". In [3], an introduction and analysis of a mathematical framework for Magnetic Resonance Fingerprinting (MRF) was developed and extended. MRF belongs to the realm of quantitative MRI (qMRI) and has been recently introduced as a highly promising scheme which allows for the simultaneous quantification of the tissue parameters, e.g., the magnetization relaxation times T_1 and T_2, using a single acquisition process. It requires the pre-computation of a dictionary that reflects the underlying physical laws of MRI (Bloch equations), whose elements (fingerprints) are matched to magnetization maps inferred by the data. In our work [3], an analysis of MRF and its extensions in an inverse problems setting was performed. Additionally, a novel physically oriented method for qMRI, where a single step, dictionary-free model for estimating the values of the tissue parameters, was proposed, analyzed, and implemented. The proposed model relies on a nonlinear operator equation instead of conventional two-step models (comprised of (i) reconstruction of the magnetization and (ii) matching to dictionary). In a compact form, this operator equation reads

$$P\mathcal{F}(\rho T_{x,y} M(\theta)) = D, \tag{1}$$

where D is the detected MRI signal, $\theta = (T_1, T_2)$, $T_{x,y}M(\theta)$ is the solution of the Bloch equations corresponding to θ, and $P\mathcal{F}$ represents a subsampling of Fourier coefficients. Differentiability properties for the operator $P\mathcal{F}(\rho T_{x,y} M(\cdot))$ in equation (1) were proved, and a Levenberg–Marquardt method was proposed for its solution. Stability under noise and subsampling was shown and verified via numerical examples. In contrast to state-of-the-art MRF-type algorithms, the performance of our proposed method is not restricted by the fineness of a dictionary, and it is superior in terms of accuracy, memory, and computational time; see Figure 2.



T_1 map: ground truth T_1 map: MRF-based T_1 map: proposed model

Fig. 2: *Improved reconstruction of the T_1 map using our proposed physics-based model*

Further research projects related to image processing were completed during 2018. A cooperation with WIAS Research Group 6 *Stochastic Algorithms and Nonparametric Statistics* on a new image denoising method, called *patch-wise adaptive smoothing (PAWS)* [4] was established.

Building partially on the group's experience in adaptive regularization and dualization, in [5] variational problems incorporating structural priors were investigated. It was shown that, while in general, an explicit form of the dual problem may not be within reach, an equivalent saddle-point formulation can be used for the efficient numerical solution. Concerning applications, PET-MR[2] data were used where MR data helped to generate a structural weight for a TV-type prior for reconstruction from PET data.

[2] PET: Positron Emission Tomography; MR: Magnetic Resonance.

Thermal fluid problems with do-nothing boundary flow. The investigation of optimal sensor placement and filtering for fluid problems where thermal buoyancy plays a significant role is within the scope of the ECMath project SE19 “Optimal network sensor placement for energy efficiency”. Here, the estimation of fluid velocity $\mathbf{v}$ and temperature distribution u is required, and they are modeled by the Boussinesq system

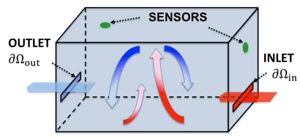


Fig. 3: *Thermal buoyancy in a domain with heated inflow*

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} - \frac{1}{\mathrm{Re}}\Delta\mathbf{v} + \nabla p = \frac{\mathrm{Gr}}{\mathrm{Re}^2}\, u\,\mathbf{e} + \mathbf{f}_1;$$
$$\frac{\partial u}{\partial t} + \mathbf{v}\cdot\nabla u - \frac{1}{\mathrm{Re}\,\mathrm{Pr}}\Delta u = f_2.$$

Appropriate boundary conditions that model the free flow of the thermal fluid outside the domain are still a matter of debate. Recently, in [2] via an energy balance argument, the nonsmooth boundary condition for the temperature $\frac{1}{\mathrm{Re}\,\mathrm{Pr}}\frac{\partial u}{\partial \mathbf{n}} - u\beta(\mathbf{v}\cdot\mathbf{n})\mathbf{v}\cdot\mathbf{n} = 0$ at the outlet with β nonsmooth was proven suitable for the studied setting. Additionally, well-posedness results for variational inequality versions of the Boussinesq system and approximation results were given.

Generalized Nash equilibrium problems. In our Project 10 “Generalized Nash equilibrium problems with partial differential operators: Theory, algorithms, and risk aversion” within the DFG Priority Program SPP 1962, we considered Nash equilibrium problems with nonlinear PDE constraints subjected to control and state constraints. First-order systems in terms of Karush–Kuhn–Tucker conditions for Nash and variational equilibria as well as of their penalized counterparts were derived. The convergence behavior of solutions and multipliers were studied on an abstract level. By this, the previous work for linear equation systems by group members has been generalized to the case of nonlinear PDE restrictions.

The existence of an equilibrium is equivalent to a fixed point problem of a set-valued operator and hence a challenging task. In the literature, most results need a certain topological structure of the operators’ values, which translates in our situation to a characterization of the solution set of an optimization problem. Hence, structural assumptions were made on the involved PDE as well as the players’ objectives to guarantee the convexity of the underlying optimization problems. Examples for this type of preorder-induced convexity notion can be found for elliptic or parabolic equations as well as for variational inequalities. Future work involves leveraging this setup for the derivation of first-order systems in the presence of a nonsmooth PDE or VI constraints.

Further highlights in 2018

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. The annual meeting was held on October 1–3, 2018, featuring three keynote lectures by renowned international experts in addition to talks reporting on the scientific progress of the subprojects of the SPP. Connected to the latter, the SPP 1962 Young Researchers’ Book Camp on Non-smooth Optimization took place on October 4–5, 2018, at WIAS.

The group actively participated in the last SIAM Conference on Imaging Science, June 5–8, 2018, Bologna, Italy, by organizing a minisymposium on "Learning and Adaptive Approaches in Image Processing" and three talks by Michael Hintermüller, Kostas Papafitsoros and Guozhi Dong.

The group also participated in the 23rd International Symposium on Mathematical Programming, ISMP 2018, where Michael Hintermüller was an invited speaker, with Carlos Rautenberg and Jo Brüggemann also contributing with two talks.

In September 2018, the DFG decided to provide funding for MATH+, the Berlin Mathematics Research Center, an interdisciplinary Cluster of Excellence and cross-institutional venture of FU Berlin, HU Berlin, TU Berlin, WIAS, and Zuse Institute Berlin (ZIB). Michael Hintermüller is a founding member (PI), a vice-speaker of the center, and a Scientist-In-Charge of the MATH+ Emerging Field *Model-Based Imaging*. Within MATH+, RG 8 successfully applied for projects which started in early 2019. These projects are: AA4-3 "Equilibria for energy markets with transport", EF3-3 "Optimal transport for imaging", EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization". Additionally, funds were also acquired for the Transition Projects "Optimization and control of electrowetting on dielectric for digital microfluidics in emerging technologies" and "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization", that serve as extensions to successful currently running projects.

Since April 2018, Michael Hintermüller and Karl Knall (Math.Tec) are heading the subproject "Optimal shape design of air ducts in combustion engines", within the *Reduced Order Modelling, Simulation and Optimization of Coupled Systems* (ROMSOC) project. The latter is a European Industrial Doctorate (EID) project and part of the Marie Skłodowska-Curie Actions (MSCA) that support the careers of scientists and encourage their transnational, intersectoral, and interdisciplinary mobility.

The latest edition of the International Conference on "Mathematics and Image Analysis" (MIA 2018) was organized on January 15–17, 2018, in Berlin, and supported by ECMath and DFG. The conference consisted of invited plenary talks, a poster session for young researchers, as well as a newly established Ph.D. prize in mathematical imaging. The conference will be subsequently organized in Paris and Berlin in an alternating fashion.

Michael Hintermüller co-organized the "International Workshop on PDE-Constrained Optimization, Optimal Controls and Applications" on December 10–14, 2018. The workshop took place in the recently opened Tsinghua Sanya International Mathematics Forum (TSIMF) in Sanya City, Hainan Province, China.

During the reported period, organizational activities for ICCOPT 2019 took place. The "Sixth International Conference on Continuous Optimization" will be held in August 2019, and will be hosted by WIAS. Michael Hintermüller is the Chair of both the Organizing and the Program Committees, and several RG 8 members are in the Local Organizers Committee.

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

Fig. 1: *Weierstrass Group in 2018, from left to right: Andrea Zafferi, Sven Tornquist, Olga Moiseewa, Marita Thomas, Andrea Eismann, Dirk Peschka*

The group was installed at WIAS in April 2017 as an 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.

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) multiphase flows with free boundaries. 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 2018 for these three topics:

Dissipative processes in elastic solids. In July 2018, Sven Tornquist started Ph.D. within the newly granted project "Reliability of efficient approximation schemes for material discontinuities described by functions of bounded variation" within the DFG-funded Priority Program 1748 *Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretisation Methods, Mechanical and Mathematical Analysis*. The project focuses on the analytical study of the convergence of time- and space-discrete schemes for damage and fracture models with different types of coupled dynamics.

The Weierstrass group also contributed to the organization of the scientific workshop "ALEX 2018: AnaLysis for Evolutionary and compleX systems" that was held at WIAS on September 24–28, 2018, to the honor of Alexander Mielke's 60th birthday; see page 123 for more details.

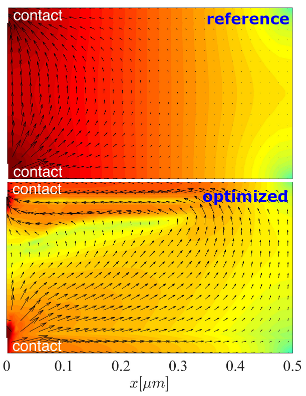

Fig. 2: *Electric current with (top) reference design and (bottom) guided current with optimized doping*

Optoelectronic processes in mechanically strained semiconductor devices. Within the ECMath-funded MATHEON Subproject OT8 "Modeling, analysis, and optimization of optoelectronic semiconductor devices driven by experimental data", a 2D simulation tool for the doping optimization of semiconductor lasers was advanced. Previous empirical studies with our project partners from the Leibniz Institute IHP – Innovations for High-Performance Microelectronics in Frankfurt (Oder) revealed that electronic designs that efficiently guide the electric current into the center of the optically active region by an aperture significantly reduce leakage currents and thus improve laser performance. Indeed, in [1] such an aperture was obtained as a solution of a PDE-constrained optimization problem based on the van Roosbroeck system, see Figure 2. The underlying cost functional aims at a trade-off in maximizing the optical emission and minimizing the electrical current. Moreover, in [2] in collaboration with RG 8 *Nonsmooth Variational Problems and Operator Equations*, the topology optimization of a strained optoelectronic device was studied using a phase-field approach with both the system of linear elasticity and the Helmholtz eigenvalue problem as PDE constraints.

Multiphase flows with free boundaries. The Weierstrass group develops mathematical methods for multiphase flows with a particular focus on free boundary problems, transport of mixtures and suspensions, and aims at their extension to applications in geosciences.

July 2018 saw the start of the newly granted project C09 "Dynamics of rock dehydration on multiple scales" within the DFG-funded CRC 1114 *Scaling Cascades on Multiple Scales*. Goal of this joint project of the petrologist Tim John (FU Berlin) and Marita Thomas is the development of a multiscale model that captures characteristic patterns of rocks that underwent subduction. During this process, chemical dehydration reactions are triggered, which release fluid that ultimately resurfaces by channel formation through the earth's mantle. As a combination of mathematics and experiment Andrea Zafferi (WIAS) and Konstantin Huber (FU Berlin) will investigate in their Ph.D. whether the arising patterns are scale invariant. To familiarize with the geophysical details and to discuss mechanisms that lead to the pattern characteristics, project C09 had a field trip to an outcrop in October 2018.

SFB 1114

Fig. 3: *C09 in Erro Tobbio, left to right: Konstantin Huber, Tim John, Johannes Vrijmoed (all FU Berlin), Marco Scambelluri (U Genova), Dirk Peschka, Andrea Zafferi, and Marita Thomas (all WIAS)*

A common mathematical problem in fluid flows is the presence of free interfaces. In this direction, the group works on extending known concepts for the modeling, simulation, and analysis of free boundary problems with respect to their thermodynamical treatment of interfaces and contact lines. A highlight of 2018 was the work on a *Variational approach to dynamic contact angles for thin films* [3], which provides the first fully developed thin-film gradient flow structure and a numerical algorithm with contact line dynamics based on a corresponding variational structure for the Stokes equation. Parts of this work on *Arbitrary Lagrangian–Eulerian* methods for finite-element methods lead to a joint contribution with Luca Heltai (SISSA) for the *deal.II FEM-library*.

In collaboration with Barbara Wagner from RG 7 and Andreas Münch (Oxford), a gradient flow model for flows of dense suspensions with free boundaries characterized by nonsmooth terms in the dissipation potential was developed. This provided the seed to extend the research towards the mathematical analysis for this kind of nonstandard rheology for suspension flow models with free boundaries and has lead to a successful grant proposal within the Berlin Mathematics Research Center MATH+. The new project was granted a 2-year position for a postdoctoral researcher and it aims at the development and justification of a unified continuum mechanical suspension flow model that allows for the transition from the dilute to the dense regime by making use of gradient and port-Hamiltonian structures, and by combining analytical tools with numerical methods investigated by Volker Mehrmann (TU Berlin) and experimental data generated by Matthias Rosenau (GFZ Potsdam).

MATH+

References

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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. B. Wagner, Full Professorship, June 13, University of Limerick, Department of Mathematics and Statistics, Ireland.

A.1.2 Awards and Distinctions

1. M. Hintermüller, *Chair of the Einstein Center for Mathematics Berlin*.
2. ———, *Member of* Matheon*'s Executive Board*.
3. ———, *Member of the Integrative Research Institute for the Sciences IRIS Adlershof of the Humboldt-Universität zu Berlin*.
4. ———, *Member of the Scientific Advisory Board of the INM – Leibniz-Institut für Neue Materialien, Saarbrücken*.
5. D. Hömberg, *Board of the European Consortium for Mathematics in Industry (ECMI)*.
6. ———, *Chair of Cost Action TD1409 (Mi-NET)*.
7. ———, *Vice Chair of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization*.
8. H.-Chr. Kaiser, *Deputy Spokesperson of the Representative Bodies for Disabled Employees of the Leibniz Association*.
9. M. Liero, *Junior Prize 2018 of the International Society for the Interaction of Mechanics and Mathematics (ISIMM)*.
10. ———, *Member of the Executive Board of the Einstein Center for Mathematics Berlin (Scientific Employee Representative)*.
11. A. Linke, *J. Tinsley Oden Faculty Fellowship of the Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin*, 2018.
12. A. Mielke, *Chair of the Prize Committee for the ICIAM Prizes 2019*.
13. ———, *Head of the Secretariat of the International Mathematical Union (IMU)*.
14. ———, *Member of* Matheon*'s Executive Board*.
15. ———, *Member of the Executive Board of the Einstein Center for Mathematics Berlin*.
16. ———, *Treasurer of IMU*.
17. M. Mittnenzweig, *GAMM Junior, Gesellschaft für Angewandte Mathematik und Mechanik*, 2018–2020.
18. D. Peschka, *Member of* Matheon's *Executive Board (Scientific Employee Representative)*.

A.1.3 Habilitations

1. A. LINKE, *Towards pressure-robust discretizations for the incompressible Navier–Stokes equations*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, January 10.

A.1.4 Defenses of Ph.D. Theses

1. P. GUSSMANN, *The small-deformation limit in elasticity and elastoplasticity in the presence of cracks*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, June 12.
2. V. AVANESOV, *Dynamics of high-dimensional covariance matrices*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, January 30.
3. C. BARTSCH, *A coupled stochastic-deterministic method for the numerical solution of population balance systems*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, August 28.
4. F. FLEGEL, *Spectral properties of the random conductance model*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 26.
5. M. KANTNER, *Modeling and simulation of electrically driven quantum dot based single-photon sources – From classical device physics to open quantum systems*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. U. Bandelow, September 4.
6. M. MITTNENZWEIG, *Entropy methods for quantum and classical evolution equtions*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, November 26.
7. S. PICKARTZ, *All-optical control of fiber solitons*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Priv.-Doz. Dr. U. Bandelow, May 18.
8. U. WILBRANDT, *Interactive subdomain methods for the Stokes–Darcy coupling*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, April 19.

A.1.5 Supervision of Undergraduate Theses

1. M. BRAND, *Ein Phasenfeldansatz für die schwingungsbasierte Topologieoptimierung* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 1.
2. A. CHMIELA, *Numerical methods for mixed integer nonlinear optimization problems* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, February 12.
3. M. EBELING-RUMP, *Topology optimization subject to additive manufacturing constraints* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, October 25.
4. M. GABRIEL, *Ordered stochastic processes* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 9.
5. M. KIRCHLER, *Efficient optimization algorithms for multi-class support vector machines* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, October 16.

6. M. Kirstein, *Gaussian surrogates for Bayesian inverse problems* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. D. Hömberg, Dr. M. Eigel, July 17.
7. M. König, *Optimierung des Durchsatzes mit kontinuierlicher Perkolation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, May 24.
8. A.M. Kruse, *Generalized Newton methods for convex l_1-regularization* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, March 5.
9. P.R. Kunze, *Optimales Routing auf einem Poisson-Delaunay-Graphen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 2.
10. S. Morgenstern, *Markov chain Monte Carlo for message routing* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, June 13.
11. C. Pech, *From finite to small strains in rate-independent damage processes* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. M. Thomas, July 2.
12. L. Scharff, *Stochastische Entscheidungsprobleme zur Vermeidung von Inferenz* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 27.
13. P. Schlicht, *Metastability for non-reversible Markov chains: Sharp asymptotics for metastable exit times and their distributions* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. M. Slowik, Prof. Dr. W. König, September 15.
14. J. Schmidt, *Große Abweichungen für die Selbstüberschneidungslokalzeit einer Irrfahrt* (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 29.
15. K. Sea Jin, *Stochastische Entscheidungsprobleme in Multihopsystemen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, November 13.
16. R. Thiele, *Reflektierte Brownsche Bewegung in einer wachsenden abgeschnittenen Weyl-Kammer* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 5.
17. S. Velemirovic, *Wright–Fisher model with frequency-dependent popolation size* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, January 2.
18. N. von Caprivi, *On a bi-level optimization problem arising from a gas market model under uncertainty* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Priv.-Doz. Dr. R. Henrion, June 12.
19. N. von Noroczynski, *Barzilai-Borwein und BFGS-Verfahren für unrestringierte Optimierungsprobleme im Vergleich* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, January 11.
20. A.D. Vu, *Homogenisierung mithilfe von Zweiskalenkonvergenz* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, July 12.
21. X. Wang, *Metastability in the Hopfield model with finitely many patterns* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. M. Slowik, Prof. Dr. W. König, December 13.

22. J. Weimer, *Estimation of point clouds via reproducing kernel methods* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 16.

23. N. Werner, *Ein Gibbs'sches Modell für Verkehrsfluss* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, December 7.

24. R. Young, *A comparison of a R-regularized Newton method and a proximal alternating linearized minimization scheme for sparse image reconstruction* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, December 17.

A.2 Grants[1]

European Union, Brussels

- **Seventh Framework Programme**

  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.

- **Marie Skłodowska-Curie Actions: Innovative Training Networks (ITN)**

  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.

  "ROMSOC – Reduced Order Modelling, Simulation and Optimization of Coupled systems" (in RG 8)

  The subproject "Optimal shape design of air ducts in combustion engines" (ROMSOC-ESR11) is treated in RG 8 jointly with Math. Tec GmbH, Austria, until March 4, 2021. The research aims to determine optimal shapes of regions of interest in order to minimize the number of suitable objectives subject to fluid flow.

- **Horizon 2020**

  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. Project: "Modeling, simulation analysis, and optimization of edge-emitting laser arrays with intracavity spatial filtering".

- **European Cooperation in Science & Technology (COST) Actions**

  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 (in RG 4).

[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

- **Mathematik für Innovationen** (Mathematics for innovations)

“Modellbasierte Abschätzung der Lebensdauer von gealterten Li-Batterien für die 2nd-Life Anwendung als stationärer Stromspeicher (MALLi ^{2})” (Model-based assessment of the life span of aged Li batteries for second-life use for stationary energy storage (MALLi ^{2} ; in RG 7)

The project ist coordinated by collaborators of RG 7. It aims to improve the lifetime estimation of lithium-ion batteries from electric vehicles for their continued use as stationary energy storage devices.

- **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.

- **Förderprogramm IKT 2020 – Forschung für Innovationen** (Funding programm for information and communication technologies 2020 – research and innovations)

“Berliner Zentrum für Maschinelles Lernen (BZML)” (Berlin Center for Machine Learning), Technische Universität Berlin

The new center aims at the systematic and sustainable expansion of interdisciplinary machine learning research, both in proven research constellations as well as in new, highly topical scientific objectives that have not yet been jointly researched. WIAS collaborates in the subproject “Adaptive Topologische Datenanalyse” (Adaptive topological data analysis; in RG 6).

- **Energy and Climate Fund of the German Federal Government**

Verbundvorhaben “LuCaMag – Wege zu sekundären Mg/Ca-Luft-Batterien” (joint project: LuCaMag – Ways to secondary Mg/Ca-air batteries; in RG 3 and RG 7)

From 2018 to 2020 WIAS (RG 3 and RG 7) participates in the joint project “Ways to secondary Mg/Ca-air batteries”. They work on the Subproject “Continuum based modeling”. The interdisciplinary project is coordinated by the Chair of Electrochemistry of Universität Bonn. Further partners are the Chair of Theoretical Chemistry of Universität Bonn, the Institute of Surface Chemistry and Catalysis of Universität Ulm, and the Center of Solar and Hydrogen Research (ZSW) in Ulm. WIAS supports the interpretation of experimental results by continuum based modeling and simulation. Further, WIAS plans to use results from measurements and quantum chemical computations performed by project partners to obtain parameters for the thermodynamically well founded electrolyte models recently developed in RG 7.

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

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

“MSim – Microelectronic Simulations” (May 1, 2017, to April 30, 2018) 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.

"rDesign – Robust Topology-Optimization for SME in Industry 4.0" (September 1, 2018, to August 31, 2019) is a spin-off in preparation of WIAS Berlin (RG 3). It is the aim of Dr. Johannes Neumann (WIAS), André Wilmes, Ph.D., and Abeed Visram, Ph.D. (both Imperial College) to productionize the robust topology optimization technology developed at WIAS and in the MATHEON SE13 research project.

The robust topology optimization technology allows for stochastically enabled automatic design creation with greatly improved robust responses in sub-optimal load configurations. The developed adaptive algorithms allow for much improved calculation efficiency and thus practically feasible compute times.

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, funded by the DFG since October 2014, has successfully been reviewed for the second phase, and the funding was extended until June 2022. The research center focuses on an efficient handling of gas transportation. The Weierstrass Institute participates in the subprojects "Wahrscheinlichkeitsrestriktionen in Gasmarktmodellen" (Chance constraints in models of gas markets; in RG 4) and "Parameter identification, sensor localization and quantification of uncertainties in switched PDE systems" (until 30.06.2019) resp. "Multicriteria optimization subject to equilibrium constraints at the example of gas markets" (from 01.07.2018, both 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)

  The prolongation to the third funding period of this center that started in 2011 begins in January 2019. The center 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, 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 (second funding period until June 30, 2022). WIAS members participate in the subprojects: B01 "Fault networks and scaling properties of deformation accumulation" (in RG 1, with FU Berlin and GFZ Potsdam), C02 "Interface dynamics: Bridging stochastic and hydrodynamic descriptions" (in RG 1, with FU Berlin), C05 "Effective models for interfaces with multiple scales" (in RG 1), C08 "Stochastic spatial coagulation particle processes" (in RG 5), and C09 "Dynamics of rock dehydration on multiple scales" (in WG1).

- **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 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 2018 on the analysis of branching processes in random environments on particular discret structures like the hypercube and random graphs with certain asymptotic degree structure.

- **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 "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 "Generalized Nash equilibrium problems with partial differential operators: Theory, algorithms and risk aversion", "Optimal control of elliptic and parabolic quasi-variational inequalities", and "Simulation and control of a nonsmooth Cahn–Hillard Navier–Stokes system with variable fluid densities", (all 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; in (RG 6)

- **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)

  "Analysis verbesserter Nernst-Planck-Poisson-Modelle für inkompressible, chemisch reagierende Elektrolyte" (Analysis of improved Nernst–Planck–Poisson models for incompressible electrolytic mixtures subject to chemical reactions; Dr. P.-E. Druet)

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 2018, 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:

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 "Hochschulkooperationen AIMS in Südafrika, Kamerun und Ghana in 2018–2022"
  "Berlin-AIMS Network in Stochastic Analysis", started in July 2018, jointly with HU Berlin, in RG 5.

- Programm Projektbezogener Personenaustausch (Project-Related Personal Exchange, PPP)
  "Emergent Dynamics in Systems of Coupled Excitable Units" (Cooperation wit Institute of Physics Belgrade; in RG 2)
- Three DAAD Fellowship holders (in RG 3 and RG 5); see page 176
- One DAAD-IAESTE Fellowship holder (International Association for the Exchange of Students for Technical Experience; in RG 1; see 176)

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 participated 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

- One Humboldt Research Fellowship holder (in RG 8); see page 176

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): Accounting for uncertainty in distribution networks (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:
  "The typical cell in anisotrophic tessellations" (15.11.2017–14.09.2018; in RG 5)
  "Data mobility in ad-hoc networks: Vulnerability and security" (01.07.2018–30.06.2019; in RG 5)
  "Coverage and mobility in infrastructure-augmented device-to device networks" (01.12.2018–30.11.2019; in RG 5)

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. ———, Editorial Board, Electronic Journal of Probability, Institute of Mathematical Statistics, Bethesda, USA.
8. R. Henrion, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
9. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
10. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
11. ———, Editorial Board, Mathematical Programming, Series A, Springer-Verlag, Heidelberg.
12. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
13. M. Hintermüller, Editorial Board, Interfaces and Free Boundaries, European Mathematical Society Publishing House, Zurich, Switzerland.
14. ———, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
15. ———, Editorial Board, ESAIM: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
16. ———, Editorial Board, Optimization Methods and Software, Taylor & Francis, Oxford, UK.
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. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
31. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, Netherlands.
32. M. Radziunas, Editorial Board, Mathematical Modelling and Analysis, Taylor and Francis Online, London, UK.
33. J.G.M. Schoenmakers, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
34. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
35. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
36. V. Spokoiny, Co-Editor, Stochastic Processes and their Applications, Elsevier, Amsterdam, Netherlands.
37. ———, Editor, Theory of Probability and its Applications, SIAM, Philadelphia, Pennsylvania, USA.
38. B. Wagner, Editorial Board, Journal of Engineering Mathematics, Springer-Verlag, Dordrecht, Netherlands.
39. ———, Editorial Board, SIAM Journal on Applied Mathematics, Society for Industrial and Applied Mathematics, Philadelphia, USA.
40. 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

MIA 2018 – Mathematics and Image Analysis
Berlin, January 15–17
Organized by: WIAS (RG 8), HU Berlin
Supported by: GdR MIA, Fraunhofer ITWM, HU Berlin, DFG, ECMath, WIAS

The MIA conference series was initiated in Paris in 2000, by the French Mathematics of Imaging group, GdR CNRS 2286 *Mathématiques de l'Imagerie et de ses Applications* (`http://gdr-mia.math.cnrs.fr`). It soon evolved to a meeting event between the French and German image processing communities – but speakers and participants were not restricted to these countries – and so it was decided to organize the conference alternatingly in France and in Germany. Thus, this was the first time that this highly reputed conference was held in Germany, and, in particular, in Berlin. The classic format of the MIA conference consists of 20–25 invited talks given by internationally recognized researchers in the broader field of applied mathematics for imaging, e.g., PDE's, Statistics, Sparsity, Variational methods, Inverse Problems, Optimization, Computer Vision, Machine Learning, and others. Moreover, the scientific programme of this year's conference was enhanced with a poster session open to young researchers as well as a Ph.D. thesis competition.

The 2018 MIA edition specifically focused on :
– Variational and optimization methods,
– image processing on manifolds and manifold-valued images,
– modeling and applications.

There were 21 invited speakers from 9 countries, and all in all 103 participants from Germany, Europe, and non-European institutions.

3rd Leibniz MMS Days
Leipzig, February 28 – March 2
Organized by: Leibniz Institute for Tropospheric Research (TROPOS), Leibniz Institute of Surface Engineering (IOM), WIAS
Supported by: Leibniz Association

The third Leibniz MMS Days were again an activity of the Leibniz Network "Mathematical Modeling and Simulation" (MMS) coordinated by WIAS.

The event brought together participants from varied fields from natural to social sciences. Fifty scientists from 20 scientific institutions 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.

The three keynote talks were given by:
– Neil Chue Hong (Software Sustainability Institute / U Edinburgh): "Managing research software development – better software, better research"
– Tijana Janjic Pfander (Deutscher Wetterdienst (DWD) / LMU München): "Challenges of atmospheric data assimilation"
– Klaus Kroy (U Leipzig): "Why is the desert not flat? The interesting physics of windblown sand."

A particular focus was also on computational and geophysical fluid dynamics, condensed matter, and statistics.

Workshop "9th Annual Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis"
Berlin, June 14–16
Organized by: WIAS (RG 6), TU Berlin, Oxford University
Supported by: DFG FOR 2042, European Research Council, WIAS

Running now for many years, the 9th Berlin-Oxford meeting on applied stochastic analysis took place at WIAS Berlin in Spring 2018. As in previous years, there is an emphasis on the powerful insights of pathwise analysis (Lyons' rough paths, Hairer's regularity structures, paracontrolled distributions à la Gubinelli–Imkeller–Perkowski), especially in the context of non-linear (stochastic) partial differential equations. Further included expected signatures with its applications to statistics and deep learning.

As in previous years, the three day workshop attracted more than 25 invited speakers, and around 80 participants, mostly early career researchers from Berlin, Oxford, and partnering research teams. Last not least, this workshop series fits perfectly into the new strategic partnership between Berlin and Oxford.

The workshop was jointly organized by WIAS group "Stochastic Algorithms and Nonparametric Statistics", Peter Friz (ERC and DFG funded, WIAS and TU Berlin), Michele Coghi (ECMath funded, WIAS), Terry Lyons (ERC funded, Oxford), and Torstein Kastberg Nilssen (DFG funded, TU Berlin).

Nonlinear Dynamics in Semiconductor Lasers (NDSL18)
Berlin, June 18–20
Organized by: WIAS (RG 2)
Supported by: SFB 787, WIAS

The workshop organized with the support of SFB 787 was focused on the discussion of novel technological trends and modeling approaches in optoelectronics. The aim of the three-day workshop was to bring together applied mathematicians, physicists, and engineers in order to provide them an opportunity to exchange knowledge and latest developments with their colleagues and young scientists by presenting their recent theoretical and experimental results in the field of nonlinear phenomena in optoelectronic devices. The subjects of the workshop included: dynamics of high-power tapered and broad area lasers and amplifiers, vertical cavity surface-emitting lasers, micro- and nanolasers, photonic crystal lasers, ring and multisection lasers, mode-locked lasers, lasers with delayed feedback, and synchronization of laser arrays. Special attention was focused on consideration of the field and carrier dynamics of quantum well and quantum dot lasers and amplifiers, investigation of spatial and temporal localized structures of light, application of the bifurcation theory and numerical methods to the analysis of optoelectronic devices, model reduction using the dynamical systems theory, and application of the singular perturbation theory in the field of nonlinear optics. The program featured 41 invited and contributed talks presented by speakers from 12 countries, and was attended by 52 registered participants.

Interplay of Random Media and Stochastic Interface Models (RMSI2018)
Berlin, June 25–27
Organized by: WIAS (RG 5) and TU Berlin
Supported by: ECMath, BMS, DFG

The workshop was devoted to Jean-Dominique Deuschel, one of the most well-known Berlin probabilists, on the occasion of his 60th birthday. It therefore featured topics from the main areas of his interest. Many of the talks concentrated on random motions in random media and on the search for new probabilistic structures emerging from many kinds of interaction between path and medium. Other talks reported on the description of stochastic fine properties of various types of random interfaces between different types of materials.

This three-day workshop featured about 17 speakers (some of which from Japan and the USA) and attracted about 60 participants from Berlin and various parts of Germany, even also from abroad. It took place in the Main Building of Technische Universität Berlin with coffee breaks being delivered in the beautiful "Lichthof", with the exception of the Tuesday, when it moved to the campus building at Hardenbergstraße.

This workshop was jointly organized by the WIAS Research Group RG 5 (Wolfgang König), Technische Universität Berlin (Martin Slowik), and University of Cambridge (Sebastian Andres).

WIAS-PGMO Workshop on Nonsmooth and Stochastic Optimization (NOSTOP2018)

Berlin, June 26
Organized by: WIAS (RG 4)
Supported by: Fondation Mathématique Jacques Hadamard, WIAS

The workshop is a follow up of the 2016 Workshop on Nonsmooth and Stochastic Optimization (NOSTOP2016). The aim of this workshop series is to bring together ideas from nonsmooth and stochastic optimization. Altogether, 26 scientists from six countries participated in the workshop. The talks were devoted to various aspects from variational analysis, optimal control, bilevel and stochastic optimization including applications to energy management (power, gas networks). Moreover, economic problems gave a background for new mathematical approaches.

MMS Summer School 2018 on Statistical Modeling and Data Analysis

Oberwolfach Research Institute for Mathematics, September 3–7
Organized by: WIAS
Supported by: Leibniz Association

Experimental or observational data of high or infinite dimensionality are getting common in institutes of all sections of the Leibniz Association. This creates an increasing demand for adequate modern data analysis techniques. At the same time, reproducibility of experiments and their statistical analyses lead to new requirements for good scientific practice and requests for open source and open science.

The first Ph.D. Summer School of the WIAS-led Leibniz Network "Mathematical Modeling and Simulation" addressed both topics in a way that provides knowledge transfer from mathematical and applied statistics into various scientific communities and helps to develop skills in R programming, statistical modeling, and reproducible data analysis.

The main topics that were treated were R programming and good scientific practice, modeling high-dimensional data, and statistical methods for functional data.

The five speakers were
Dr. Clara Happ (LMU Munich, AG Biostatistics): Functional data analysis
Dr. Jörg Polzehl (WIAS): Modeling high-dimensional data
Dr. Heidi Seibold (LMU Munich, Institute for Medical Information Processing, Biometry, and Epidemiology): R, Open Science, Reproducible Research
Almond Stöcker (LMU Munich, AG Biostatistics): Functional data analysis
Dr. Alexandra Suvorikova (WIAS): Mathematical statistics

AnaLysis of Evolutionary and compleX systems (ALEX 2018)

Berlin, September 24–28
Organized by: WIAS (RG 1 and WG1), U Stuttgart, and U Warwick
Supported by: DFG, CRC 910, CRC 1114, ECMath, U Stuttgart, WIAS

The workshop was organized by former Ph.D. students of Alexander Mielke: Guido Schneider (U Stuttgart), Florian Theil (U Warwick), Marita Thomas (WIAS, WG1), Matthias Liero, and Sina Reichelt (both WIAS, RG 1), and was held at WIAS and the Humboldt-Universität zu Berlin. New aspects of evolutionary PDEs were addressed with a wide range of applications in chemistry, biology, physics, and engineering. The focus was put on the following four main topics: gradient and Hamiltonian structures, variational methods for continuum mechanics, dynamical systems, and multiscale problems. Eleven keynote lectures and 27 invited talks were presented to 73 participants from 11 nations. Contributions included modeling of smart materials, multi-particle systems, interrelation between stochastics and PDEs, transition from discrete to continuum, reaction-diffusion systems, and quantum mechanics.

Fig. 1: *WIAS director Michael Hintermüller congratulates Alexander Mielke on his sixtieth birthday*

In the afternoon of the 26th, a special colloquium in honor of the 60th birthday of Alexander Mielke took place at the Humboldt-Universität zu Berlin. This colloquium featured, together with three excellent keynote lectures by Dorothee Knees (U Kassel), Ulisse Stefanelli (U Vienna), and Mark A. Peletier (TU Eindhoven) welcome addresses from the IMU office, the Forschungsverbund Berlin and the Berlin mathematics community. More than 100 participants attended this event.

SPP 1962 Annual Meeting

Sommerfeld, October 1–3
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 1 to 3 in Sommerfeld near Berlin. A total of 70 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 was given. Three of the attendees — Harbir Antil (George Mason University), Ekkehard Sachs (U Trier and Lawrence Livermore National Laboratory), and Claudia Schilligs (U Mannheim) — were plenary speakers specially chosen for the annual meeting, and each plenary speaker gave a talk of 45 minutes on the area of their expertise.

In addition, a meeting for principal investigators also took place where important matter related to the upkeep and continual improvement of SPP issues were discussed as well as the crucial upcoming mid-phase evaluation. 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' software course for the younger SPP members in 2019.

In summary, the meeting was very well attended and as before, participants expressed generally positive feedback regarding the event itself and the venue and location.

Young Researchers' Book Camp 2018

Berlin, October 4–5
Organized by: Veronika Karl (U Würzburg), Ailyn Stötzner (TU Chemnitz), Stephanie Thomas (U Kassel), and WIAS RG 8
Supported by: DFG-SPP 1962

The Young Researchers' Book Camp 2018 within the DFG Priority Programme 1962 *Non-smooth and Complementary-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* took place right after the Annual Meeting 2018 of the SPP. The organizers provided the chance to take the time to study a paper or part of a book in detail – not alone, but within a group of 3–5 motivated persons. There were four groups: Mathematical Programs with Complementarity Constraints (MPCC), Semismooth Newton, Variational Inequalities (VIs), and Clarke Subgradients. Working through a topic in this way generated fruitful discussions and improveded the learning effect for all 15 participants.

Applied Mathematics and Simulation for Semiconductors (AMaSiS 2018)

Berlin, October 8–10
Organized by: WIAS (RG 1 and RG 3), U Massachusetts
Supported by: DFG, ECMath, WIAS

The workshop was organized by Jürgen Fuhrmann, Annegret Glitzky, Hans-Christoph Kaiser, Thomas Koprucki, Matthias Liero (all WIAS), and Eric Polizzi (U Massachusetts). It dealt with modeling, mathematical analysis, and numerical schemes for the simulation of semiconductor devices and charge transport in electrolytes and other physical or biological systems. Due to the structural similarity of mathematical models and techniques for the numerical simulation of charge transport in semiconductors and electrolytes by generalized Poisson–Nernst–Planck systems, the workshop was also opened to the topic of electrolytes. The scientific focus was on the treatment of multiple scales, the interplay of electronic, optical, thermal, fluidic, and other effects in advanced device concepts and novel material systems.

The workshop was attended by 67 scientists from 29 institutions in Austria, Belgium, France, Germany, Great Britain, Israel, Italy, Poland, Switzerland, and the United States. The scientific program included 14 invited lectures, a tutorial on the eigenwert solver FEAST, 13 contributed talks, and the presentation of 13 posters.

Dynamics in Coupled Oscillator Systems
Berlin, November 19–21
Organized by: WIAS (RG 2), TU Berlin
Supported by: IRTG 1740, SFB 910, WIAS

The dynamics of coupled oscillators plays an important role in a variety of systems in nature and technology. Their ability to display complex self-organized dynamical phenomena makes them an important tool to explain the fundamental mechanism of emergent dynamics in coupled systems. The aim of the workshop was to discuss recent theoretical development in this field, including approaches from dynamical systems theory, statistical physics, and stochastics, as well as applications in various fields of science. The workshop received financial support from the Collaborative Research Center 910 *Control of Self-organizing Nonlinear Systems* and the International Research Training Group (IRTG) 1740. The program featured 25 invited and contributed talks presented by speakers from 8 countries, 13 poster presentations, and was attended by 59 registered participants.

13th International Workshop on Variational Multiscale and Stabilized Finite Elements (VMS 18)
Berlin, December 5–7
Organized by: WIAS (RG 3)
Supported by: DFG SPP 1679 *Dynamic Simulation of Interconnected Solids Processes*

The workshop aimed to bring together researchers who are working on different aspects of stabilized discretizations of convection-diffusion equations and incompressible flow problems. 15 talks were presented that discussed, e.g., recent results in the numerical analysis of stabilized discretizations, approaches for turbulent flow simulations, adaptive methods, and the efficient solution of the arising nonlinear and linear problems.

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

Workshop “Math for the Digital Factory”
Limerick, March 21–23
Organized by: Fraunhofer ITWM, MACSI, University of Limerick, WIAS (RG 4)
Supported by: Confirm Smart Manufacturing, ECMI, Fraunhofer ITWM, MACSI, MI-NET, Science Foundation Ireland, University of Limerick, WIAS

The second workshop of the ECMI Special Interest Group “Mathematics for the Digital Factory” took place in Limerick (March 21–23). More than 70 participants from 16 European countries discussed about maths for virtual product development, MSO of production systems, as well as recent energy optimization issues in robotics. Specific highlights were a public panel discussion on the position of mathematics within the future of digital manufacturing and a round table on mathematics in Horizon2020 and FP9.

A.4.3 Oberwolfach Workshops co-organized by WIAS

Interplay of Analysis and Probability in Applied Mathematics
Mathematisches Forschungsinstitut Oberwolfach, February 11–17
Organized by: Volker Betz (Darmstadt), Nicolas Dirr (Cardiff), Wolfgang König (RG 5), Florian Theil (Warwick)

This workshop continued to foster the collaboration between researchers working in analysis and probability, respectively. Some core areas, in which this happens with high success, belonged to the objectives of this meeting: stochastic homogenization of various quantities in random media and random operators, metastability in several particle models with stochastic input that are triggered by physics reasonings, emergence of macroscopic effects in large random structures like graphs or permutations. A main feature present was the exploration of the benefit of a high-level combination of methods from both fields: analysis and probability.

Challenges in Optimal Control of Nonlinear PDE-Systems
Mathematisches Forschungsinstitut Oberwolfach, April 8–14
Organized by: Michael Hintermüller (RG 8), Karl Kunisch (Graz), Günter Leugering (Erlangen), Elisabetta Rocca (Pavia)

The workshop focussed on various aspects of optimal control problems for systems of nonlinear partial differential equations. In particular, discussions around keynote presentations in the areas of optimal control of nonlinear/non-smooth systems, optimal control of systems involving nonlocal operators, shape and topology optimization, feedback control and stabilization, sparse control, and associated numerical analysis as well as design and analysis of solution algorithms were promoted. Moreover, also aspects of control of fluid structure interaction problems as well as problems arising in the optimal control of quantum systems were considered.

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

1. S. AMIRANASHVILI, scientific coordinator, *4th International Conference on Wave Interaction (WIN-2018)*, Johannes Kepler Universität Linz, Austria, April 3–7.
2. U. BANDELOW, member of the Program Committee, *18th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2018)*, The University of Hong Kong, China, November 5–9.
3. A. CAIAZZO, organizer of the Minisymposium "Multiscale In-silico Modelling of Cancer Biophysics and Therapy", *6th European Conference on Computational Mechanics, 7th European Conference on Computational Fluid Dynamics (ECCM-ECFD 2018)*, University of Glasgow, UK, June 11–15.
4. M. COGHI, co-organizer, *9th International Conference on Stochastic Analysis and Its Applications*, Universität Bielefeld, Fakultät für Mathematik, September 3–7.
5. M. EIGEL, co-organizer of the Minisymposia 96, 109, 122 "Low-Rank Approximations for the Forward- and the Inverse Problems I–III", *SIAM Conference on Uncertainty Quantification (UQ18)*, Garden Grove, USA, April 16–19.
6. P. FRIZ, co-organizer, *Pathwise SLE Berlin 2018*, Technische Universität Berlin, April 24–26.
7. ———, member of the Scientific Committee, *Stochastic Partial Differential Equations*, Centre International de Rencontres Mathématiques, Luminy, France, May 14–18.
8. ———, co-organizer, *Stochastic Methods in Finance and Physics*, National Technical University of Athens, Department of Mathematics, Heraklion, Greece, July 23–27.
9. ———, co-organizer, *Renormalisation in Quantum Field Theory and in Stochastic Partial Differential Equations: A Gentle Introduction and Some Recent Developments*, University of Cambridge, Isaac Newton Institute for Mathematical Science, UK, September 3–7.
10. ———, co-organizer, *10th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis*, University of Oxford, Mathematical Institute, UK, November 29 – December 1.
11. M. HINTERMÜLLER, organizer of the Session PP07 "DFG Priority Program 1962", *89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2018)*, Technische Universität München, March 19–23.
12. ———, co-organizer, *International Workshop on PDE-Constrained Optimization, Optimal Controls and Applications*, Sanya, China, December 10–14.
13. M. HINTERMÜLLER, K. PAPAFITSOROS, co-organizers of the Minisymposium MS5 "Learning and Adaptive Approaches in Image Processing", *SIAM Conference on Imaging Science*, Bologna, Italy, June 5–8.
14. D. HÖMBERG, organizer of the Minisymposium 26 "ECMI Special Interest Group: Maths for the Digital Factory", *The 20th European Conference on Mathematics for Industry (ECMI 2018)*, Budapest, Hungary, June 18–22.
15. ———, organizer of the Minisymposium 27 "MSO for Steel Production and Manufacturing", *The 20th European Conference on Mathematics for Industry (ECMI 2018)*, Budapest, Hungary, June 18–22.
16. O. HUBER, co-organizer, *SFB-TRR 154 Network Seminar on Equilibria and (Gas) Markets*, Energy Campus Nürnberg, November 26.
17. W. KÖNIG, co-organizer, *DFG-AIMS Workshop on Evolutionary Processes on Networks*, African Institute of Mathematical Sciences (AIMS), Kigali, Rwanda, March 20–24.

18. ———, organizer, *Meeting for the preparation of a priority programme on Mathematical Analysis of Disordered Geometric Systems*, Georg–August-Universität Göttingen, Göttingen, June 22.
19. ———, co-organizer, *Interplay of Random Media and Stochastic Interface Models (RMSI2018)*, Technische Universität Berlin, Institut für Mathematik, June 25–27.
20. Th. Koprucki, member of the Programme Committee, *11th Conference on Intelligent Computer Mathematics (CICM 2018), Workshop on Mathematical Models and Mathematical Software as Research Data (M3SRD)*, Johannes Kepler Universität Linz, Research Institute for Symbolic Computation (RISC), Hagenberg, Austria, August 13–17.
21. ———, member of the Steering Committee, *18th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2018)*, The Hong Kong University, China, November 5–9.
22. M. Landstorfer, organizer, *BMBF Workshop on MaLLi2*, VARTA, Ellwangen, November 5.
23. M. Liero, member of the Scientific Committee, *ECMath Colloquium "Nonsmooth Problems: Theory and Applications"*, Humboldt-Universität zu Berlin, Institut für Mathematik, January 26.
24. ———, co-organizer, *6th ECMath Colloquium "PDEs Meet Stochastics"*, Humboldt-Universität zu Berlin, Institut für Mathematik, July 6.
25. A. Mielke, co-organizer, *Berlin Dresden Prague Würzburg Workshop "Mathematics of Continuum Mechanics"*, Technische Universität Würzburg, Institut für Mathematik, November 29–30.
26. N. Rotundo, co-organizer of the Minisymposium "Charge Transport in Semiconductor Materials: Emerging and Established Mathematical Topics", *20th European Conference on Mathematics for Industry (ECMI 2018)*, Budapest, Hungary, June 18–22.
27. H. Si, member of the Program Committee (Co-Chairs), *International Symposium on IsoGeometric Analysis and Mesh Generation (IGA&Mesh) 2018*, Dalian, China, August 3–5.
28. ———, member of the Program Commitee (Co-Chair), *9th International Conference "Numerical Geometry, Grid Generation and Scientific Computing" (NUMGRID 2018)*, Russian Academy of Sciences, Federal Research Center of Information and Control, Moscow, Russian Federation, December 3–9.
29. V. Spokoiny, co-organizer, *New Frontiers in High-Dimensional Probability and Statistics*, National Research University Higher School of Economics, Faculty of Computer Science, Moscow, Russian Federation, February 23–24.
30. ———, co-organizer, *Structural Inference in High-Dimensional Models*, National Research University Higher School of Economics, Faculty of Computer Science, Moscow, Russian Federation, September 5–8.
31. ———, co-organizer, *Meeting in Mathematical Statistics 2018 "Mathematical Methods of Statistics"*, Fréjus, France, December 16–21.
32. V. Spokoiny, A. Suvorikova, co-organizers, *Statistical Optimal Transport*, Skolkovo Institute of Science and Technology, Moscow, Russian Federation, July 24–25.
33. M. Thomas, co-organizer of the Special Session 144 "Analytic Properties and Numerical Approximation of Differential Models arising in Applications", *The 12th AIMS Conference on Dynamical Systems, Differential Equations and Applications*, National Taiwan University, Taipeh, July 5–9.
34. B. Wagner, co-organizer of the Minisymposium 25 "Large-scale Effects of Local Structures in Complex Systems", *SIAM Conference on Nonlinear Waves and Coherent Structures*, Anaheim, USA, June 11–14.
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A.6 Publications

A.6.1 Monographs

[1] D. BELOMESTNY, J. SCHOENMAKERS, *Advanced Simulation-Based Methods for Optimal Stopping and Control: With Applications in Finance*, Macmillan Publishers Ltd., London, 2018, 364 pages.

Monographs (to appear)

[1] B. JAHNEL, W. KÖNIG, *Probabilistic Methods for Telecommunications*, Compact Textbooks in Mathematics, Birkhäuser.

A.6.2 Outstanding Contributions to Monographs

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A.6.3 Articles in Refereed Journals[3]

[1] P. COLLI, G. GILARDI, J. SPREKELS, *Optimal distributed control of a generalized fractional Cahn–Hilliard system*, Appl. Math. Optim., published online on 15.11.2018, https://doi.org/10.1007/s00245-018-9540-7.

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[37] J. FUHRMANN, C. GUHLKE, A. LINKE, CH. MERDON, R. MÜLLER, *Models and numerical methods for electrolyte flows*, Preprint no. 2525, WIAS, Berlin, 2018.

[38] J. FUHRMANN, C. GUHLKE, B. MATEJCZYK, R. MÜLLER, *Transport of solvated ions in nanopores: Asymptotic models and numerical study*, Preprint no. 2526, WIAS, Berlin, 2018.

[39] A. Glitzky, M. Liero, *Instationary drift-diffusion problems with Gauss–Fermi statistics and field-dependent mobility for organic semiconductor devices*, Preprint no. 2523, WIAS, Berlin, 2018.

[40] H. Heitsch, *On probabilistic capacity maximization in a stationary gas network*, Preprint no. 2540, WIAS, Berlin, 2018.

[41] H. Heitsch, N. Strogies, *Consequences of uncertain friction for the transport of natural gas through passive networks of pipelines*, Preprint no. 2513, WIAS, Berlin, 2018.

[42] D. Adelhütte, D. Assmann, T. González Grandón, M. Gugat, H. Heitsch, R. Henrion, F. Liers, S. Nitsche, R. Schultz, M. Stingl, D. Wintergerst, *Joint model of probabilistic-robust (probust) constraints with application to gas network optimization*, Preprint no. 2550, WIAS, Berlin, 2018.

[43] L. Adam, M. Branda, H. Heitsch, R. Henrion, *Solving joint chance constrained problems using regularization and Benders' decomposition*, Preprint no. 2471, WIAS, Berlin, 2018.

[44] A. Hantoute, R. Henrion, P. Pérez-Aros, *Subdifferential characterization of probability functions under Gaussian distribution*, Preprint no. 2478, WIAS, Berlin, 2018.

[45] R. Henrion, W. Römisch, *Problem-based optimal scenario generation and reduction in stochastic programming*, Preprint no. 2485, WIAS, Berlin, 2018.

[46] S. Hajian, M. Hintermüller, C. Schillings, N. Strogies, *A Bayesian approach to parameter identification in gas networks*, Preprint no. 2537, WIAS, Berlin, 2018.

[47] G. Dong, M. Hintermüller, K. Papafitsoros, *A physically oriented method for quantitative magnetic resonance imaging*, Preprint no. 2528, WIAS, Berlin, 2018.

[48] L. Adam, M. Hintermüller, D. Peschka, Th.M. Surowiec, *Optimization of a multiphysics problem in semiconductor laser design*, Preprint no. 2500, WIAS, Berlin, 2018.

[49] M. Carraturo, E. Rocca, E. Bonetti, D. Hömberg, A. Reali, F. Auricchio, *Additive manufacturing graded-material design based on phase-field and topology optimization*, Preprint no. 2553, WIAS, Berlin, 2018.

[50] J. Yu, D. Hömberg, Th. Petzold, S. Lu, *Temporal homogenization of a nonlinear parabolic system*, Preprint no. 2524, WIAS, Berlin, 2018.

[51] C. Cotar, B. Jahnel, Ch. Külske, *Extremal decomposition for random Gibbs measures*, Preprint no. 2546, WIAS, Berlin, 2018.

[52] P. Keeler, B. Jahnel, O. Maye, D. Aschenbach, M. Brzozowski, *Disruptive events in high-density cellular networks*, Preprint no. 2469, WIAS, Berlin, 2018.

[53] G. Botirov, B. Jahnel, *Phase transitions for a model with uncountable spin space on the Cayley tree: The general case*, Preprint no. 2490, WIAS, Berlin, 2018.

[54] Ch. Hirsch, B. Jahnel, A. Hinsen, E. Cali, *The typical cell in anisotropic tessellations*, Preprint no. 2557, WIAS, Berlin, 2018.

[55] E. Cali, T. En-Najjari, N.N. Gafur, Ch. Hirsch, B. Jahnel, R.I.A. Patterson, *Percolation for D2D networks on street systems*, Preprint no. 2479, WIAS, Berlin, 2018.

[56] G.R. Barrenechea, V. John, P. Knobloch, R. Rankin, *A unified analysis of Algebraic Flux Correction schemes for convection-diffusion equations*, Preprint no. 2475, WIAS, Berlin, 2018.

[57] A. Jha, V. John, *On basic iteration schemes for nonlinear AFC discretizations*, Preprint no. 2533, WIAS, Berlin, 2018.

[58] O. Klein, D. Davino, C. Visone, *On forward and inverse uncertainty quantification for models involving hysteresis operators*, Preprint no. 2561, WIAS, Berlin, 2018.

[59] P. Nestler, N. Schlömer, O. Klein, J. Sprekels, F. Tröltzsch, *Optimal control of semiconductor melts by traveling magnetic fields*, Preprint no. 2549, WIAS, Berlin, 2018.

[60] M. Landstorfer, *The dielectric constant of liquid electrolytes obtained from periodic homogenization theory*, Preprint no. 2531, WIAS, Berlin, 2018.

[61] ———, *A discussion of the reaction rate and the cell voltage of an intercalation electrode during discharge*, Preprint no. 2563, WIAS, Berlin, 2018.

[62] ———, *A Redlich–Kister type free energy model for Li-intercalation compounds with variable lattice occupation numbers*, Preprint no. 2560, WIAS, Berlin, 2018.

[63] R. Lasarzik, *Approximation and optimal control of dissipative solutions to the Ericksen–Leslie system*, Preprint no. 2535, WIAS, Berlin, 2018.

[64] ———, *Dissipative solution to the Ericksen–Leslie system equipped with the Oseen–Frank energy*, Preprint no. 2508, WIAS, Berlin, 2018.

[65] ———, *Measure-valued solutions to the Ericksen–Leslie model equipped with the Oseen–Frank energy*, Preprint no. 2476, WIAS, Berlin, 2018.

[66] ———, *Weak-strong uniqueness for measure-valued solutions to the Ericksen–Leslie model equipped with the Oseen–Frank free energy*, Preprint no. 2474, WIAS, Berlin, 2018.

[67] A. Linke, L.G. Rebholz, *Pressure-induced locking in mixed methods for time-dependent (Navier–)Stokes equations*, Preprint no. 2534, WIAS, Berlin, 2018.

[68] A. Mielke, J. Naumann, *On the existence of global-in-time weak solutions and scaling laws for Kolmogorov's two-equation model of turbulence*, Preprint no. 2545, WIAS, Berlin, 2018.

[69] A. Bacho, E. Emmrich, A. Mielke, *An existence result and evolutionary Gamma-convergence for perturbed gradient systems*, Preprint no. 2499, WIAS, Berlin, 2018.

[70] M. Mittnenzweig, *Hydrodynamic limit and large deviations of reaction-diffusion master equations*, Preprint no. 2521, WIAS, Berlin, 2018.

[71] L. Calatroni, K. Papafitsoros, *Analysis and optimisation of a variational model for mixed Gaussian and Salt & Pepper noise removal*, Preprint no. 2542, WIAS, Berlin, 2018.

[72] R.I.A. Patterson, D.R.M. Renger, *Large deviations of reaction fluxes*, Preprint no. 2491, WIAS, Berlin, 2018.

[73] D. Peschka, *Variational approach to contact line dynamics for thin films*, Preprint no. 2477, WIAS, Berlin, 2018.

[74] D. Peschka, N. Rotundo, M. Thomas, *Doping optimization for optoelectronic devices*, Preprint no. 2501, WIAS, Berlin, 2018.

[75] D. Peschka, M. Thomas, T. Ahnert, A. Münch, B. Wagner, *Gradient structures for flows of concentrated suspensions*, Preprint no. 2543, WIAS, Berlin, 2018.

[76] D. Peschka, S. Haefner, K. Jacobs, A. Münch, B. Wagner, *Signatures of slip in dewetting polymer films*, Preprint no. 2538, WIAS, Berlin, 2018.

[77] L. Antoine, P. Pigato, *Maximum likelihood drift estimation for a threshold diffusion*, Preprint no. 2497, WIAS, Berlin, 2018.

[78] A. Pimenov, S. Amiranashvili, A.G. Vladimirov, *Temporal dissipative solitons in a delayed model of a ring semiconductor laser*, Preprint no. 2552, WIAS, Berlin, 2018.

[79] A. Pimenov, A.G. Vladimirov, *Dynamics of an inhomogeneously broadened passively mode-locked laser*, Preprint no. 2551, WIAS, Berlin, 2018.

[80] A. Pimenov, J. Javaloyes, S.V. Gurevich, A.G. Vladimirov, *Light bullets in a time-delay model of a wide-aperture mode-locked semiconductor laser*, Preprint no. 2481, WIAS, Berlin, 2018.

[81] J. Polzehl, K. Papafitsoros, K. Tabelow, *Patch-wise adaptive weights smoothing*, Preprint no. 2520, WIAS, Berlin, 2018.

[82] M. Radziunas, J. Fuhrmann, A. Zeghuzi, H.-J. Wünsche, Th. Koprucki, C. Brée, H. Wenzel, U. Bandelow, *Efficient coupling of electro-optical and heat-transport models for broad-area semiconductor lasers*, Preprint no. 2558, WIAS, Berlin, 2018.

[83] A. Zeghuzi, M. Radziunas, H. Wenzel, H.-J. Wünsche, U. Bandelow, A. Knigge, *Modeling of current spreading in high-power broad-area lasers and its impact on the lateral far field divergence*, Preprint no. 2488, WIAS, Berlin, 2018.

[84] W.M. Klesse, A. Rathsfeld, C. Gross, E. Malguth, O. Skibitzki, L. Zealouk, *Fast scatterometric measurement of periodic surface structures in plasma-etching processes*, Preprint no. 2564, WIAS, Berlin, 2018.

[85] G. Hu, A. Rathsfeld, *Acoustic scattering from locally perturbed periodic surfaces*, Preprint no. 2522, WIAS, Berlin, 2018.

[86] H. Antil, C.N. Rautenberg, *Sobolev spaces with non-Muckenhoupt weights, fractional elliptic operators, and applications*, Preprint no. 2505, WIAS, Berlin, 2018.

[87] A. Ceretani, C.N. Rautenberg, *The Boussinesq system with mixed non-smooth boundary conditions and "do-nothing" boundary flow*, Preprint no. 2504, WIAS, Berlin, 2018.

[88] M. Redmann, *Energy estimates and model order reduction for stochastic bilinear systems*, Preprint no. 2503, WIAS, Berlin, 2018.

[89] D.R.M. Renger, *Gradient and Generic systems in the space of fluxes, applied to reacting particle systems*, Preprint no. 2516, WIAS, Berlin, 2018.

[90] R. Schlundt, *A multilevel Schur complement preconditioner with ILU factorization for complex symmetric matrices*, Preprint no. 2556, WIAS, Berlin, 2018.

[91] D. Belomestny, J.G.M. Schoenmakers, V. Spokoiny, Y. Tavyrikov, *Optimal stopping via deeply boosted backward regression*, Preprint no. 2530, WIAS, Berlin, 2018.

[92] H. Si, *On monotone sequences of directed flips, triangulations of polyhedra, and structural properties of a directed flip graph*, Preprint no. 2554, WIAS, Berlin, 2018.

[93] P. Nelson, R. Soares dos Santos, *Brownian motion in attenuated or renormalized inverse-square Poisson potential*, Preprint no. 2482, WIAS, Berlin, 2018.

[94] H. Stephan, A. Stephan, *Memory equations as reduced Markov processes*, Preprint no. 2496, WIAS, Berlin, 2018.

[95] E. Balteau, K. Tabelow, J. Ashburner, M.F. Callaghan, B. Draganski, G. Helms, F. Kherif, T. Leutritz, A. Lutti, Ch. Phillips, E. Reimer, L. Ruthotto, M. Seif, N. Weiskopf, G. Ziegler, S. Mohammadi, *hMRI – A toolbox for using quantitative MRI in neuroscience and clinical research*, Preprint no. 2527, WIAS, Berlin, 2018.

[96] A.G. Vladimirov, S.V. Gurevich, M. Tlidi, *Effect of Cherenkov radiation on localized states interaction*, Preprint no. 2480, WIAS, Berlin, 2018.

[97] M.G. Hennessy, A. Münch, B. Wagner, *Surface induced phase separation of a swelling hydrogel*, Preprint no. 2562, WIAS, Berlin, 2018.

[98] I. Bačić, S. Yanchuk, M. Wolfrum, I. Franović, *Noise-induced switching in two adaptively coupled excitable systems*, Preprint no. 2517, WIAS, Berlin, 2018.

A.7.2 Preprints/Reports in other Institutions

[1] N. Alia, V. John, S. Ollila, *Re-visiting the single-phase flow model for liquid steel ladle stirred by gas*, arXiv.1811.11535, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[2] V. Avanesov, *Structural break analysis in high-dimensional covariance structure*, arXiv:1803.00508, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[3] Ch. Bayer, R. Tempone, S. Wolfers, *Pricing American options by exercise rate optimization*, arXiv:1809.07300, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[4] C.A. Uribe, D. Dvinskikh, P. Dvurechensky, A. Gasnikov, A. Nedić, *Distributed computation of Wasserstein barycenters over networks*, arXiv:1803.02933, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[5] P. Dvurechensky, A. Gasnikov, E. Gorbunov, *An accelerated directional derivative method for smooth stochastic convex optimization*, arXiv:1804.02394, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[6] ———, *An accelerated method for derivative-free smooth stochastic convex optimization*, arXiv:1802.09022, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[7] P. Dvurechensky, A. Gasnikov, A. Kroshnin, *Computational optimal transport: Complexity by accelerated gradient descent is better than by Sinkhorn's algorithm*, arXiv:1802.04367, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[8] P. Dvurechensky, A. Gasnikov, F. Stonyakin, A. Titov, *Generalized mirror prox: Solving variational inequalities with monotone operator, inexact Oracle, and unknown Hölder parameters*, arXiv:1806.05140, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[9] A. Ivanova, P. Dvurechensky, A. Gasnikov, *Composite optimization for the resource allocation problem*, arXiv:1810.00595, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[10] P. Dvurechensky, D. Dvinskikh, A. Gasnikov, C.A. Uribe, A. Nedić, *Decentralize and randomize: Faster algorithm for Wasserstein barycenters*, arXiv:1806.03915, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[11] Y. Nesterov, A. Gasnikov, S. Guminov, P. Dvurechensky, *Primal-dual accelerated gradient descent with line search for convex and nonconvex optimization problems*, arXiv:1809.05895, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[12] I. Chevyrev, P. Friz, A. Korepanov, I. Melbourne, H. Zhang, *Multiscale systems, homogenization, and rough paths*, arXiv:1712.01343, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[13] P. Friz, P. Gassiat, P. Pigato, *Precise asymptotics: Robust stochastic volatility models*, arXiv:1811.00267, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[14] A. Koziuk, V. Spokoiny, *Instrumental variables regression*, arXiv:1806.06111v1, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[15] ———, *Toolbox: Gaussian comparison on Euclidean balls*, arXiv:1804.00601v1, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[16] N.R. Gauger, A. Linke, P. Schroeder, *On high-order pressure-robust space discretisations, their advantages for incompressible high Reynolds number generalised Beltrami flows and beyond*, arXiv:1808.10711, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[17] P. Mathé, *Bayesian inverse problems with non-commuting operators*, arXiv:1801.09540, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[18] B. Hofmann, St. Kindermann, P. Mathé, *Penalty-based smoothness conditions in convex variational regularization*, arXiv:1805.01320, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[19] A.D. McGuire, S. Mosbach, G. Reynolds, R.I.A. Patterson, E.J. Bringley, N.A. Eaves, J. Dreyer, M. Kraft, *Analysing the effect of screw configuration using a stochastic twin-screw granulation model*, Technical report no. 195, University of Cambridge, c4e-Preprint Series, Cambridge, UK, 2018.

[20] J.Y. Park, J. Polzehl, S. Chatterjee, A. Brechmann, et al., *Semiparametric modeling of time-varying activation and connectivity in task-based fMRI data*, Discussion paper, http://works.bepress.com/mfiecas/20, 2018.

[21] D. Belomestny, J.G.M. Schoenmakers, V. Spokoiny, Y. Tavyrikov, *Optimal stopping via reinforced regression*, arXiv:1808.02341v2, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[22] M. Boeckel, V. Spokoiny, A. Suvorikova, *Multivariate Brenier cumulative distribution functions and their application to non-parametric testing*, arXiv:1809.04090v1, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[23] F. Götze, A. Naumov, V. Spokoiny, V. Ulyanov, *Large ball probability, Gaussian comparison and anti-concentration*, arXiv:1708.08663v2, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[24] N. Puchkin, V. Spokoiny, *Adaptive multiclass nearest neighbor classifier*, arXiv:1804.02756, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[25] F. Bachoc, A. Suvorikova, J.-M. Loubes, V. Spokoiny, *Gaussian process forecast with multidimensional distributional entries*, arXiv:1805.00753v1, Cornell University Library, arXiv.org, Ithaca, USA, 2018.

[26] S. Slepneva, B. O'Shaughnessy, A.G. Vladimirov, S. Rica, G. Huyet, *Turbulent laser puffs*, arXiv:1801.05509, Cornell University Library, Ithaca, USA, 2018.

A.8 Talks and Posters

A.8.1 Main and Plenary Talks

1. U. Bandelow, *Control of ultrashort solitons in the regime of event horizons in nonlinear dispersive optical media*, XX Conference on Nonequilibrium Statistical Mechanics and Nonlinear Physics (MEDYFINOL 2018), December 3–7, Universidad de los Andes, Universidad de Mar del Plata, Hospital Italiano de Buenos Aires, Santiago, Chile, December 6.
2. P. Friz, *Rough path analysis of rough volatility*, 9-th International Workshop On Applied Probability, June 18–22, Eörvös Loránd University (ELU), Budapest, Hungary, June 18.
3. R. Henrion, *Optimization problems with probust constraints*, Colloquium & International Conference on Variational Analysis and Nonsmooth Optimization, June 28 – July 1, Martin-Luther-Universität Halle-Wittenberg, Halle, June 28.
4. M. Hintermüller, *Multiobjective optimization with PDE constraints*, 23rd International Symposium on Mathematical Programming (ISMP2018), July 1–6, Bordeaux, France, July 2.
5. D. Hömberg, *Mathematical challenges in steel manufacturing*, Second International Conference on Modern Mathematical Methods and High Performance Computing in Science and Technology (M3HPCST 2018), January 4–6, Inderprastha Engineering College (IPEC), Ghaziabad, India, January 4.
6. ———, *European collaboration in industrial and applied mathematics*, Conference "Mathematical Modelling in Metallurgical Industry", September 17–18, Kristiansand, Norway, September 18.
7. ———, *Knowledge exchange in mathematics – The European perspective*, 1st IMA Conference on Knowledge Exchange in the Mathematical Sciences, December 3–4, Aston University, Birmingham, UK, December 3.
8. B. Wagner, *Multi-scale problems of material design in sustainable energies*, SIAM Conference on Nonlinear Waves and Coherent Structures, June 11–14, Anaheim, USA, June 13.

A.8.2 Scientific Talks (Invited)

1. J. Sprekels, *Cahn–Hilliard systems with general fractional operators*, Workshop "Challenges in Optimal Control of Nonlinear PDE-Systems", April 9–13, Mathematisches Forschungsinstitut Oberwolfach, April 9.
2. ———, *Cahn–Hilliard systems with general fractional-order operators*, Workshop "Special Materials and Complex Systems" (SMACS 2018), June 18–22, University of Milan/University of Pavia, Gargnano, Italy, June 22.
3. A. Alphonse, *Directional differentiability for elliptic QVIs of obstacle type*, 89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2018), Session PP07 "DFG Priority Program 1962", March 19–23, Technische Universität München, March 20.
4. ———, *Directional differentiability for elliptic quasi-variational inequalities*, Workshop "Challenges in Optimal Control of Nonlinear PDE-Systems", April 8–14, Mathematisches Forschungsinstitut Oberwolfach, April 12.
5. ———, *Parabolic quasi-variational inequalities: Existence and sensitivity analysis*, 4th Central European Set-Valued and Variational Analysis Meeting (CESVVAM 2018), November 24, Philipps-Universität Marburg, November 24.
6. L. Andreis, *Self-sustained periodic behavior in interacting systems*, Random Structures in Neuroscience and Biology, March 26–29, Ludwig–Maximilians Universität München, Fakultät für Mathematik, Informatik und Statistik, Herrsching, March 26.

7. ———, *Networks of interacting components with macroscopic self-sustained periodic behavior*, Neural Coding 2018, September 9–14, University of Torino, Department of Mathematics, Italy, September 10.

8. ———, *A large-deviations approach to the multiplicative coagulation process*, Probability Seminar, Università degli Studi di Padova, Dipartimento di Matematica "Tullio Levi–Civita", Italy, October 12.

9. ———, *A large-deviations approach to the multiplicative coagulation process*, Seminar "Theory of Complex Systems and Neurophysics — Theory of Statistical Physics and Nonlinear Dynamics", Humboldt-Universität zu Berlin, Institut für Physik, October 30.

10. M.J. Arenas Jaén, *Modelling, simulation and optimization of inductive pre-heating for thermal cutting of steel plates*, The 20th European Conference on Mathematics for Industry (ECMI 2018), Minisymposium 27 "MSO for Steel Production and Manufacturing", June 18–22, Budapest, Hungary, June 19.

11. U. Bandelow, *Ultrashort solitons and their control in the regime of event horizons in nonlinear dispersive optical media*, George Stegeman Symposium, University of Central Florida, Orlando, USA, March 13.

12. ———, *Hierarchies of integrable NLS-type equations and selected solutions*, 4th International Conference on Wave Interaction (WIN-2018), Johannes Kepler Universität Linz, Austria, April 4.

13. ———, *Semiconductor laser instabilities and dynamics emerging from mode degeneracy*, International Workshop "Synthetic Non-Hermitian Photonic Structures: Recent Results and Future Challenges", August 13–17, Max Planck Institute for the Physics of Complex Systems, Dresden, August 14.

14. Ch. Bayer, *Smoothing the payoff for computation of basket options*, Stochastic Methods in Finance and Physics, July 23–27, National Technical University of Athens, Department of Mathematics, Heraklion, Greece.

15. ———, *Smoothing the payoff for computation of basket options*, Berlin-Paris Young Researchers Workshop Stochastic Analysis with Applications in Biology and Finance, May 2–4, Institut des Systèmes Complexes de Paris Ile-de-France (ISC-PIF), National Center for Scientific Research, Paris, France, May 3.

16. ———, *Short-time near-the-money skew in rough fractional volatility models*, 9-th International Workshop on Applied Probability, June 18–21, Eörvös Loránd University (ELU), Budapest, Hungary, June 19.

17. ———, *Smoothing the payoff for computation of basket options*, 13th International Conference in Monte Carlo & Quasi-Monte Carlo Methods in Scientific Computing, July 1–6, University of Rennes, Faculty of Economics, France, July 3.

18. I. Bremer, *Using an SQP-solver for nonlinear optimization under probabilistic constraints*, 100th Meeting of the GOR Working Group "Real World Mathematical Optimization", April 12–13, Regenstauf, April 12.

19. N. Buzun, *Sein's method*, Haindorf Seminar 2018, January 24–27, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, Hejnice, Czech Republic, January 26.

20. A. Caiazzo, *A penalty-free Nitsche method for the Stokes, Darcy and Brinkman problems*, Universität Augsburg, Lehrstuhl für Numerische Mathematik, May 15.

21. ———, *Towards the personalization of (1D) blood-flow simulations*, University of Amsterdam, Computational Science Lab, Netherlands, September 21.

22. ———, *Robust open boundary conditions and efficient data assimilation in multiscale hemodynamics*, International Symposium "Modeling, Simulation and Optimization of the Cardiovascular System", October 22–24, Universität Magdeburg, October 22.

23. ———, *Mathematical modeling and simulations of geothermal reservoirs*, Leibniz-Institut für Angewandte Geophysik, Hannover, November 7.

24. ———, *Multiscale and reduced-order modeling of biphasic materials with application to tissue elastography*, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Numerische Simulation, November 23.

25. L. Capone, *Induction hardening of cam profiles: Modeling, simulation, and optimization*, The 20th European Conference on Mathematics for Industry (ECMI 2018), Minisymposium 27 “MSO for Steel Production and Manufacturing”, June 18–22, Budapest, Hungary, June 19.

26. M. Coghi, *Mean field limit of interacting filaments for 3D Euler equations*, Bielefeld-Edinburgh-Swansea Stochastic Spring, March 26–28, Universität Bielefeld, Fakultät für Mathematik, March 27.

27. ———, *Non-local stochastic scalar conservation laws*, Bielefeld Stochastic Afternoon, Universität Bielefeld, Fakultät für Mathematik, October 16.

28. ———, *Pathwise McKean–Vlasov theory*, 10th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, November 29 – December 1, University of Oxford, Mathematical Institute, UK, December 1.

29. W. Dreyer, *Thermodynamics and kinetic theory of non-Newtonian fluids*, Technische Universität Darmstadt, Mathematische Modellierung und Analysis, June 13.

30. P. Dvurechensky, *Faster algorithms for (regularized) optimal transport*, Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, March 30.

31. ———, *Faster algorithms for (regularized) optimal transport*, Grenoble Optimization Days 2018, June 28–29, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, France, June 29.

32. ———, *Computational optimal transport: Accelerated gradient descent vs. Sinkhorn’s algorithm*, Statistical Optimal Transport, July 24–25, Skolkovo Institute of Science and Technology, Moscow, Russian Federation, July 25.

33. M. Eigel, *Aspects of adaptive Galerkin FE for stochastic direct and inverse problems*, Workshop “Surrogate Models for UQ in Complex Systems” (UNQW02), February 5–9, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, February 7.

34. M. Eigel, *Adaptive Galerkin FEM for stochastic forward and inverse problems*, Optimisation and Numerical Analysis Seminars, University of Birmingham, School of Mathematics, UK, February 15.

35. ———, *Adaptive tensor methods for forward and inverse problems*, SIAM Conference on Uncertainty Quantification (UQ18), Minisymposium 122 “Low-Rank Approximations for the Forward- and the Inverse Problems III”, April 16–19, Garden Grove, USA, April 19.

36. F. Flegel, *Spectral homogenization vs. localization in the barrier model*, Symposium on the occasion of the 60th birthday of Igor Sokolov, Bernstein Center for Computational Neuroscience Berlin, Humboldt-Universität zu Berlin, February 26.

37. ———, *Spectral homogenization vs. localization in the random conductance model*, Seminar Angewandte Analysis, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, March 9.

38. ———, *Localization vs. homogenization in the random conductance model*, Forschungsseminar Analysis, Technische Universität Chemnitz, June 6.

39. ———, *Spectral localization vs. homogenization in the random conductance model*, Seminar of SFB/CRC 1060 Bonn, Rheinische Friedrich-Wilhelms-Universität Bonn, June 12.

40. ———, *Spectral localization vs. homogenization in the random conductance model*, Oberseminar Stochastik, Universität zu Köln, Mathematisches Institut, June 14.

41. ———, *Spectral localization vs. homogenization in the random conductance model*, Oberseminar Wahrscheinlichkeitstheorie, Ludwigs-Maximilians-Universität München, July 9.

42. Th. Frenzel, *Slip-stick motion via a wiggly energy model and relaxed EDP-convergence*, Workshop “Variational Methods for the Modelling of Inelastic Solids”, February 5–9, Mathematisches Forschungsinstitut Oberwolfach, February 8.

43. P. FRIZ, *From rough paths and regularity structures to short dated option pricing under rough volatility*, Workshop on Mathematical Finance and Related Issues, Osaka University, Nakanoshima Center, Japan, March 15.

44. ———, *Stepping stoch vol and related topics*, 25th Global Derivatives Trading & Risk Management 2018, Volatility Modelling & Trading, May 14–18, Lisbon, Portugal, May 16.

45. ———, *Analysis of rough volatility via rough paths / regularity structures*, METE – Mathematics and Economics: Trends and Explorations. A conference celebrating Mete Soner's 60th birthday and his contributions to Analysis, Control, Finance and Probability, June 4–8, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, June 5.

46. ———, *Varieties of signature tensors*, Workshop on Stochastic Analysis, Geometry and Statistics, June 21–22, Imperial College London, UK, June 22.

47. ———, *Rough paths, stochastics and PDE's*, ECMath Colloquium, July 6, Humboldt-Universität zu Berlin, July 6.

48. J. FUHRMANN, *Computational assessment of the derivation of the Butler–Volmer kinetics as a limit case of the Nernst–Planck equations with surface reactions*, Workshop "Numerical Optimization of the PEM Fuel Cell Bipolar Plate", Zentrum für Solarenergie- und Wasserstoff-Forschung (ZSW), Ulm, March 20.

49. ———, *Towards finite volume based PDE simulations with Julia*, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, December 19.

50. A. GLITZKY, *Electrothermal feedback in organic LEDs*, Workshop "Numerical Optimization of the PEM Fuel Cell Bipolar Plate", March 20, Zentrum für Solarenergie- und Wasserstoff-Forschung (ZSW), Ulm, March 20.

51. M. HEIDA, *On convergences of the square root approximation scheme to the Fokker–Planck operator*, Workshop "Interplay of Analysis and Probability in Applied Mathematics", February 11–17, Mathematisches Forschungsinstitut Oberwolfach, February 13.

52. ———, *On convergence of the square root approximation scheme to the Fokker–Planck operator*, Technische Universität Berlin, Institut für Mathematik, May 14.

53. ———, *On convergence of the square root approximation scheme to the Fokker–Planck operator*, Oberseminar "Optimierung", Humboldt-Universität zu Berlin, Institut für Mathematik, May 29.

54. ———, *Mathematische Mehrskalenmethoden in Natur und Technik*, Seminar "Angewandte Analysis", Universität Konstanz, Institut für Mathematik, October 31.

55. H. HEITSCH, *A probabilistic approach to optimization in gas transport*, 2nd Conference on Mathematics of Gas Transport (MoG-2), October 10–11, Konrad-Zuse-Zentrum für Informationstechnik Berlin, October 10.

56. R. HENRION, *Verification and comparison of the calmness of generalized equations in original and enhanced form*, International Workshop on Optimization and Variational Analysis, January 10–11, Termas de Cauquenes, Chile, January 11.

57. ———, *Maximization of free capacities in gas networks with random load*, Conference "Variational Analysis – Challenges in Energy", June 4–6, Castro Urdiales, Spain, June 4.

58. ———, *M-stationary conditions for MPECs in finite dimension (Part 1+2)*, 2 talks, SPP 1962 Summer School on Complementarity Problems in Applied Mathematics: Modeling, Analysis, and Optimization, July 30 – August 1, Technische Universität Dortmund, July 31.

59. ———, *Perspectives in probabilistic programming under continuous random distributions*, Workshop "New Directions in Stochastic Optimisation", August 19–25, Mathematisches Forschungsinstitut Oberwolfach, August 20.

60. ———, *Probabilistic programming with applications*, Universidad Miguel Hernández de Elche, Instituto Centro de Investigación Operativa, Spain, September 13.

61. ———, *Optimization problems under probabilistic constraints*, 3rd Russian-German Conference on Multi-Scale BioMathematics: Coherent Modeling of Human Body System, November 7–9, Lomonosov Moscow State University, Russian Federation, November 8.

62. ———, *Dynamic chance constraints under continuous random distribution*, PGMO DAYS 2018, Session 1E "Stochastic Optimization", November 20–21, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF'Lab Paris-Saclay, Palaiseau, France, November 21.

63. ———, *Lipschitz properties and their moduli for constraint mappings*, 4th Central European Set-Valued and Variational Analysis Meeting (CESVVAM 2018), November 24, Philipps-Universität Marburg, November 24.

64. A. Hinsen, *Vulnerability and security in ad-hoc networks*, Universität Osnabrück, Fachbereich Mathematik/Informatik, December 11.

65. M. Hintermüller, *Semismooth Newton methods in PDE constrained optimization*, 2 talks, Advanced Training in Mathematics Schools "New Directions in PDE Constrained Optimisation", March 12–16, National Centre for Mathematics of IIT Bombay and TIFR, Mumbai, Bombay, India, March 14.

66. ———, *Recent advances in non-smooth and complementarity-based distributed parameter systems*, 89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2018), Session PP07 "DFG Priority Program 1962", March 19–23, Technische Universität München, March 20.

67. ———, *Nonsmooth structures in PDE constrained optimization*, Mathematisches Kolloquium, Universität Bielefeld, Fakultät für Mathematik, June 7.

68. ———, *Generalised Nash equilibrium problems with partial differential equations*, Search Based Model Engineering Workshop, August 7–9, King's College London, UK, August 7.

69. ———, *Automated regularization parameter choice rule in image processing*, Workshop "New Directions in Stochastic Optimisation", August 19–25, Mathematisches Forschungsinstitut Oberwolfach, August 23.

70. ———, *Structural total variation regularization with applications in inverse problems*, International Conference on Scientific Computing, December 5–8, Department of Mathematics, The Chinese University of Hong Kong, China, December 8.

71. ———, *Multiobjective optimization with PDE constraints*, International Workshop on PDE-Constrained Optimization, Optimal Controls and Applications, December 10–14, Sanya, China, December 13.

72. D. Hömberg, *European collaboration in industrial and applied mathematics*, Inderprastha Engineering College, Ghaziabad, India, January 5.

73. ———, *European collaboration in industrial and applied mathematics*, Salzburg Mathematics Colloquium, Universität Salzburg, Fachbereich Mathematik, Austria, May 17.

74. ———, *Temporal homogenization of a nonlinear parabolic system*, The 20th European Conference on Mathematics for Industry (ECMI 2018), Minisymposium 15 "Electromagnetic Problems Arising in Industry: Modelling and Numerical Techniques", June 18–22, Budapest, Hungary, June 18.

75. ———, *Maths for digital factory*, University of Southern Denmark, The Maersk Mc-Kinney Moller Institute, Odense, Denmark, October 12.

76. B. Jahnel, *Gibbsian representation for point processes via hyperedge potentials*, Workshop on Transformations and Phase Transitions, January 29–31, Ruhr-Universität Bochum, Fakultät für Mathematik, Bochum, January 30.

77. ———, *Continuum percolation for Cox point processes*, Universität Osnabrück, Fachbereich Mathematik/Informatik, February 1.

78. ———, *Dynamical Gibbs-non-Gibbs transitions for continuous spin models*, DFG-AIMS Workshop on Evolutionary Processes on Networks, March 20–24, African Institute of Mathematical Sciences (AIMS), Kigali, Rwanda, March 21.

79. ———, *Attractor properties for irreversible and reversible interacting particle systems*, Random Structures in Neuroscience and Biology, March 26–29, Ludwig–Maximilians Universität München, Fakultät für Mathematik, Informatik und Statistik, Herrsching, March 29.

80. ———, *Continuum percolation for Cox point processes*, Seminar, Universität Potsdam, Institut für Mathematik, April 13.

81. ———, *Telecommunication models in random environments*, BIMoS Day, Berlin International Graduate School in Model and Simulation based Research, Technische Universität Berlin, May 23.

82. ———, *Percolation for Cox point processes*, Geometry and Scaling of Random Structures, July 16–27, Centre International de Mathématiques Pures et Appliquées (CIMPA), School and X Escuela Santaló, ICM Rio Satellite Workshop, Buenos Aires, Argentina, July 18.

83. ———, *Attractor properties for irreversible and reversible interacting particle systems*, ICM 2018 Satellite Conference: Topics in Mathematical Physics, July 26–31, Institute of Mathematics and Statistics, University of São Paulo, Institute of Physics, Brazil, July 27.

84. ———, *Dynamical Gibbs-non-Gibbs transitions for the continuum Widom–Rowlinson model*, Seminar der AG Stochastik, Technische Universität Darmstadt, Fachbereich Mathematik, September 21.

85. ———, *Spatial stochastic models with applications in telecommunications*, 4 talks, Summer School 2018 "Combinatorial Structures in Geometry", September 24–27, Universität Osnabrück, Institut für Mathematik (DFG GK 1916), September 24–27.

86. ———, *Attractor properties for irreversible and reversible interacting particle systems*, Ibn Zohr University, Agadir, Morocco, September 28.

87. ———, *Gibbsian representation for point processes via hyperedge potentials*, Universität Potsdam, Institut für Mathematik, October 10.

88. V. John, *Finite elements for scalar convection-dominated equations and incompressible flow problems – A never ending story?*, International Conference of Boundary and Interior Layers (BAIL 2018), June 18–22, University of Strathclyde, Glasgow, Scotland, UK, June 18.

89. ———, *Angewandte Mathematik für Strömungssimulationen*, Martin-Luther-Universität Halle, Fachbereich Mathematik, October 27.

90. ———, *Variational Multiscale (VMS) methods for the simulation of turbulent incompressible flows*, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, November 14.

91. W. König, *The principal part of the spectrum of random Schrödinger operators in large boxes*, Rhein-Main Kolloquium Stochastik, Goethe-Universität Frankfurt am Main, January 26.

92. ———, *Random message routing in highly dense multi-hop networks*, DFG-AIMS Workshop on Evolutionary Processes on Networks, March 20–24, African Institute of Mathematical Sciences (AIMS), Kigali, Rwanda, March 21.

93. ———, *Large deviations theory and applications*, 2 talks, Classical and Quantum Dynamics of Interacting Particle Systems, Universität zu Köln, Mathematisches Institut, Köln, June 15.

94. ———, *A large-deviations approach to the multiplicative coalescent*, Workshop on High-dimensional Phenomena in Probability — Fluctuations and Discontinuity (Research Training Group 2131), September 24–28, Ruhr-Universität Bochum, September 28.

95. Th. Koprucki, *Numerical methods for drift-diffusion equations*, Matheon 11th Annual Meeting "Photonic Devices", February 8–9, Konrad-Zuse-Zentrum für Informationstechnik Berlin, February 8.

96. A. Koziuk, *Gaussian comparison on a family of Euclidean balls*, Haindorf Seminar 2018, January 23–27, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, Hejnice, Czech Republic, January 26.
97. Z. Lakdawala, *Mathematics meets industry – Modeling and simulation of plain and porous media*, Habib University, Dhanani School of Science and Engineering, Karachi, Pakistan, November 27.
98. ———, *Multiscale modeling of filtration processes*, Quaid-i-Azam University, Department of Mathematics, Islamabad, Pakistan, November 29.
99. M. Landstorfer, *Homogenization methods for electrochemical systems*, Workshop "Numerical Optimization of the PEM Fuel Cell Bipolar Plate", Zentrum für Solarenergie- und Wasserstoff-Forschung (ZSW), Ulm, March 20.
100. ———, *Modelling and simulation of porous battery electrodes with multi-scale homogenisation techniques*, 6th European Conference on Computational Mechanics, 7th European Conference on Computational Fluid Dynamics (ECCM-ECFD 2018), June 11–15, Glasgow, UK, June 14.
101. ———, *Thermodynamic modeling of electrolytes and their boundary conditions to electrodes*, AMaSiS 2018: Applied Mathematics and Simulation for Semiconductors, October 8–10, WIAS, Berlin, October 9.
102. ———, *Continuum thermodynamic modelling of electrolytes*, BMBF Kickoff Meeting LuCaMag, Bonn, November 7.
103. ———, *Modelling and simulation of porous battery electrodes with multi-scale homogenisation techniques*, Solid State Electrochemistry Symposium, November 12–14, Helmut-Schmidt-Universität, Hamburg, November 13.
104. R. Lasarzik, *Generalised solutions to the Ericksen–Leslie model describing liquid crystal flow*, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, June 7.
105. M. Liero, *Feel the heat—Modeling of electrothermal feedback in organic devices*, A Joint Meeting of the Society for Natural Philosophy and the International Society for the Interaction of Mathematics and Mechanics "Mathematics & Mechanics: Natural Philosophy in the 21st Century", June 24–27, University of Oxford, Mathematical Institute, UK, June 25.
106. ———, *On entropy-transport problems and the Hellinger–Kantorovich distance*, IFIP TC 7 Conference on System Modelling and Optimization, Minisymposium "Optimal Transport and Applications", July 26–27, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, July 27.
107. A. Linke, *On the role of the Helmholtz–Leray projector for a novel pressure-robust discretization theory for the incompressible Navier–Stokes equations*, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, January 23.
108. ———, *On the role of the Helmholtz–Leray projector for a novel pressure-robust discretization theory for the incompressible Navier–Stokes equations*, Workshop "Finite Element Exterior Calculus (FEEC) and High Order Methods", June 4–6, University of Oslo, Faculty of Mathematics and Natural Sciences, Norway, June 6.
109. ———, *User talk: Pressure-robust space discretization for the incompressible Navier–Stokes equations*, 2nd NGSolve User Meeting, July 4–6, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, July 5.
110. ———, *On the role of the Helmholtz–Leray projector for a novel pressure-robust discretization theory for the incompressible Navier–Stokes equations*, Clemson University, Department of Mathematical Sciences, South Carolina, USA, August 17.
111. C. Löbhard, *Analysis, algorithms and applications for the optimal control of variational inequalities*, European Women in Mathematics (EWM) General Meeting 2018, Minisymposium 9 "Nonsmooth PDE-constrained Optimization: Problems and Methods", September 3–7, Karl-Franzens-Universität Graz, Austria, September 7.

112. O. MARQUARDT, *Electronic properties of semiconductor nanostructures – Eight band k.p and beyond*, Nanostructures Seminar, Beijing Institute of Nanoenergy and Nanosystems (BINN), Chinese Academy of Sciences, China, April 12.

113. ———, *Modelling the electronic properties of polytype heterostructure (synopsis)*, QuantumWise A/S, Kgs. Lyngby, Denmark, August 21.

114. M. MARSCHALL, *Bayesian inversion with adaptive low-rank approximation*, Analysis, Control and Inverse Problems for PDEs – Workshop of the French-German-Italian LIA (Laboratoire International Associe) COPDESC on Applied Analysis, November 26–30, University of Naples Federico II and Accademia Pontaniana, Italy, November 29.

115. P. MATHÉ, *Complexity of linear ill-posed problems in Hilbert space*, Stochastisches Kolloquium, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, February 7.

116. ———, *Bayesian inverse problems with non-commuting operators*, Chemnitz September of Applied Mathematics 2018, Chemnitz Symposium on Inverse Problems, September 27–28, Technische Universität Chemnitz, Fakultät für Mathematik, September 28.

117. ———, *Relating posterior contraction for direct and inverse Bayesian problems by the modulus of continuity*, International Conference on Inverse Problems, October 12–14, Fudan University, School of Mathematical Sciences, Shanghai, China, October 13.

118. ———, *Complexity of linear ill-posed problems in Hilbert space*, University of Cyprus, Department of Mathematics and Statistics, Nicosia, Cyprus, December 7.

119. M. MAURELLI, *A McKean–Vlasov SDE with reflecting boundaries*, CASA Colloquium, Eindhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, January 10.

120. ———, *Sanov theorem for Brownian rough paths and an application to interacting particles*, Università di Roma La Sapienza, Dipartimento di Matematica Guido Castelnuovo, Italy, January 18.

121. ———, *McKean–Vlasov SDEs with irregular drift: Large deviations for particle approximation*, University of Oxford, Mathematical Institute, UK, March 5.

122. A. MIELKE, *Global existence for finite-strain viscoplasticity*, Workshop “Variational Methods for the Modelling of Inelastic Solids”, February 5–9, Mathematisches Forschungsinstitut Oberwolfach, February 6.

123. ———, *Construction of effective gradient systems via EDP convergence*, Workshop on Mathematical Aspects of Non-Equilibrium Thermodynamics, March 5–7, Rheinisch-Westfälische Technische Hochschule Aachen, March 6.

124. ———, *EDP-convergence: Gamma-convergence for gradient systems in the sense of the energy-dissipation principle*, 89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2018), Section S14 “Applied Analysis”, March 19–23, Technische Universität München, March 20.

125. ———, *Finding limiting dissipative potentials via EDP convergence*, Applied Mathematics Seminar, Università di Pavia, Dipartimento di Matematica, Italy, April 23.

126. ———, *Entropy and gradient structures for quantum Markov semigroups and couplings to macroscopic thermodynamical systems*, Nonlinear Mechanics Seminar, University of Bath, Mathematical Sciences, UK, May 22.

127. ———, *Entropy-induced geometry for classical and quantum Markov semigroups*, Mathematisches Kolloquium, Technische Universität Darmstadt, Fachbereich Mathematik, June 6.

128. ———, *On notions of evolutionary Gamma convergence for gradient systems*, Workshop “Gradient Flows: Challenges and New Directions”, September 10–14, International Centre for Mathematical Sciences (ICMS), Edinburgh, UK, September 13.

129. ———, *Coarse graining of energy and dissipation*, Festkolloquium zu Ehren von Martin Brokate, November 8–10, Technische Universität München, Zentrum Mathematik, Garching, November 9.

130. ———, *EDP convergence and optimal transport*, Workshop "Optimal Transportation and Applications", November 12–15, Scuola Normale Superiore, Università di Pisa, Università di Pavia, Pisa, Italy, November 13.

131. ———, *Energy, dissipation, and evolutionary Gamma convergence for gradient systems*, Kolloquium "Applied Analysis", Universität Bremen, December 18.

132. R. Müller, *Modeling and simulation of electrolyte transport in nanopores*, Center for Computational Engineering, Rheinisch-Westfälische Technische Hochschule Aachen, May 8.

133. ———, *Dynamics of electrochemical interfaces*, Asymptotic Behavior of Systems of PDE arising in Physics and Biology: Theoretical and Numerical Points of View (ABPDE III), August 28–31, Université de Lille I, France, August 30.

134. K. Papafitsoros, *A function space framework for structural total variation regularization with applications in inverse problems*, VI Latin American Workshop on Optimization and Control (LAWOC 18), September 3–7, Quito, Ecuador, September 4.

135. R.I.A. Patterson, *Large deviations for reaction fluxes*, Séminaire EDP, Modélisation et Calcul Scientifique (commun ICJ & UMPA), École Normale Supérieure de Lyon (CNRS), France, July 12.

136. D. Peschka, *Steering pattern formation during dewetting with interface and contact lines properties*, The 20th European Conference on Mathematics for Industry (ECMI 2018), Minisymposium 38 "ECMI Special Interest Group: Material Design and Performance in Sustainable Energies", June 18–22, Budapest, Hungary, June 21.

137. P. Pigato, *Faits stilisés et modélisation de la volatilité*, École Polytechnique, Université Paris-Saclay, Département de Mathématiques Appliquées, Palaiseau, France, April 20.

138. ———, *Short dated option pricing under rough volatility*, Berlin-Paris Young Researchers Workshop Stochastic Analysis with applications in Biology and Finance, May 2–4, Institut des Systèmes Complexes de Paris Ile-de-France (ISC-PIF), National Center for Scientific Research, Paris, France, May 4.

139. ———, *Faits stilisés et modélisation de la volatilité*, Seminaire, Institut de Science Financière et d'Assurances, Université Lyon 1, France, May 14.

140. ———, *Estimation of piecewise-constant coefficients in a stochastic differential equation*, The 40th Conference on Stochastic Processes and their Applications (SPA 2018), University of Gothenburg, Göteborg, Sweden, June 13.

141. ———, *Asymptotic analysis of rough volatility models*, Seminar of the Research Training Group 2131, Ruhr-Universität Bochum, June 25.

142. ———, *Asymptotic analysis of rough volatility models*, Probability Seminar, L'Università di Milano-Bicocca, Dipartimento di Matematica e Applicazioni, Italy, July 13.

143. ———, *Precise asymptotics of rough stochastic volatility models*, University of Trento, Department of Mathematics, November 16.

144. ———, *Density and tube estimates for diffusion processes under Hormander-type conditions*, Séminaire (de Calcul) Stochastique, Université de Strasbourg, Institut de Recherche Mathématique Avancée, France, November 23.

145. ———, *Some elements of statistics and modeling for financial markets*, University of Trento, Department of Mathematics, Italy, December 19.

146. J. Polzehl, *High resolution magnetic resonance imaging experiments – Lessons in nonlinear statistical modeling*, 3rd Leibniz MMS Days, February 28 – March 2, Wissenschaftszentrum Leipzig, March 1.

147. ———, *Modeling high dimensional data*, 2 talks, Leibniz MMS Summer School 2018 on Statistical Modeling and Data Analysis, September 3–7, Leibniz MMS Network, Mathematisches Forschungsinstitut Oberwolfach, September 3–7.

148. ———, *Towards in-vivo histology of the brain – Some statistical contributions*, CMRR Seminar, University of Minnesota, Center for Magnetic Resonance Research (CMRR), Minneapolis, USA, October 15.

149. M. Radziunas, *Intelligent solution for complex problems*, Research Seminar of the Faculty of Science and Engineering, Macquarie University, Sydney, Australia, July 4.

150. ———, *Modeling, simulation, and analysis of nonlinear dynamics in semiconductor lasers*, Research Seminar of the Faculty of Science and Engineering, Macquarie University, Sydney, Australia, July 24.

151. ———, *Modeling and simulation of high-power broad-area semiconductor lasers with optical feedback from different external cavities*, 26th International Semiconductor Laser Conference (ISLC 2018), September 16–19, IEEE Photonics Society, Santa Fe, USA, September 16.

152. C.N. Rautenberg, *Optimization problems with quasi-variational inequality constraints*, Workshop "Challenges in Optimal Control of Nonlinear PDE-Systems", April 8–14, Mathematisches Forschungsinstitut Oberwolfach, April 11.

153. ———, *On the optimal control of quasi-variational inequalities*, 23rd International Symposium on Mathematical Programming (ISMP2018), Session 221 "Optimization Methods for PDE Constrained Problems", July 1–6, Bordeaux, France, July 3.

154. ———, *Dissipative and non-dissipative evolutionary quasi-variational inequalities with derivative constraints*, Joint Meeting of the Italian Mathematical Union, the Italian Society of Industrial and Applied Mathematics and the Polish Mathematical Society, Session 14 "Nonlinear Variational Methods with Applications", September 17–20, Wroclaw, Poland, September 19.

155. ———, *Evolutionary quasi-variational inequalities: Applications, theory, and numerics*, 5th International Conference on Applied Mathematics, Design and Control: Mathematical Methods and Modeling in Engineering and Life Sciences, November 7–9, San Martin National University, Buenos Aires, Argentina, November 9.

156. M. Redmann, *Beyond the theory of ordinary differential equations*, Seminar of the Department of Mathematics and Computer Science, University of Southern Denmark, Odense, February 22.

157. ———, *Solving linear parabolic rough partial differential equations*, 13th German Probability and Statistics Days 2018, February 27 – March 2, Albert-Ludwigs-Universität Freiburg, Abteilung für Mathematische Stochastik, March 1.

158. ———, *Solving stochastic partial differential equations*, Universität Greifswald, Institut für Mathematik und Informatik, April 19.

159. ———, *Solving parabolic rough partial differential equations using regression*, 13th International Conference in Monte Carlo & Quasi-Monte Carlo Methods in Scientific Computing, July 1–6, University of Rennes, Faculty of Economics, France, July 5.

160. S. Reichelt, *Pulses in FitzHugh–Nagumo systems with rapidly oscillating coefficients*, SIAM Annual Meeting, Minisymposium 101 "Multiscale Analysis and Simulation on Heterogeneous Media", July 9–13, Society for Industrial and Applied Mathematics, Oregon Convention Center (OCC), Portland, USA, July 12.

161. D.R.M. Renger, *Large deviations for reaction fluxes*, Università degli Studi dell'Aquila, Dipartimento di Ingegneria e Scienze dell'Informazione e Matematica, L'Aquila, Italy, January 10.

162. ———, *Large deviations for reaction fluxes*, Workshop on Transformations and Phase Transitions, January 29–31, Ruhr-Universität Bochum, Fakultät für Mathematik, January 29.

163. ———, *Gradient and GENERIC structures from flux large deviations*, POLYPHYS Seminar, Eidgenössische Technische Hochschule Zürich, Department of Materials, Zürich, Switzerland, March 28.

164. ———, *Gradient and Generic structures in the space of fluxes*, Analysis of Evolutionary and Complex Systems (ALEX2018), September 24–28, WIAS Berlin, September 27.

165. N. Rotundo, *On a thermodynamically consistent coupling of quantum system and device equations*, The 20th European Conference on Mathematics for Industry (ECMI 2018), Minisymposium "Mathematical Modeling of Charge Transport in Graphene and Low Dimensional Structures", August 18 – June 22, Budapest, Hungary, June 19.

166. ———, *Consistent modeling of optoelectronic semiconductors via gradient structures*, Congress of the Italian Society of Applied and Industrial Mathematics (SIMAI), Minisymposium MS-23 "Mathematical Modeling of Charge Transport in Low Dimensional Structures (Part II)", July 2–6, Sapienza Università di Roma, Faculty of Civil and Industrial Engineering, Cosenza, Italy, July 3.

167. H. Si, *Challenges in 3D unstructured mesh generation and adaptation*, Challenges in the Computational Modeling of Beijing's Air Pollution and Traffic, March 19–23, Beijing University of Technology, China, March 22.

168. ———, *Challenges in 3D unstructured mesh generation and adaptation*, The Second Chinese International Conference on CFD, July 17–21, China Aerodynamics Research and Development Center, Mianyang, Sichuan, China, July 20.

169. ———, *Unstructured mesh generation and its applications*, University of Cambridge, Bullard Laboratories, UK, October 18.

170. ———, *An algorithm to triangulate 3D non-convex polyhedra without Steiner points*, 9th International Conference "Numerical Geometry, Grid Generation and Scientific Computing" (NUMGRID 2018), December 3–9, Russian Academy of Sciences, Federal Research Center of Information and Control, Moscow, Russian Federation, December 3.

171. ———, *Advances in unstructured mesh generation and adaptation*, International Workshop on Numerical Analysis with Applications in Medium Imaging and Computer Visions, Minisymposium "Computer Vision and Applications", December 10–14, International Consortium of Chinese Mathematicians in Computational and Applied Mathematics (ICCM-CAM), Shing-Tung Yau Center of the Southeast University, Nanjing, China, December 13.

172. R. Soares dos Santos, *Random walk on random walks*, University of Groningen, Johann Bernoulli Institute for Mathematics and Computer Science, Netherlands, February 14.

173. ———, *Random walk on random walks*, Oberseminar Mathematische Stochastik, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, Münster, July 4.

174. V. Spokoiny, *Adaptive nonparametric clustering*, Multiscale Problems in Materials Science and Biology: Analysis and Computation, January 8–12, Tsinghua University, Yau Mathematical Sciences Center, Sanya, Hainan, China, January 10.

175. ———, *Inference for spectral projectors*, Workshop "Statistical Inference for Structured High-dimensional Models", March 11–16, Mathematisches Forschungsinstitut Oberwolfach, March 14.

176. ———, *Gaussian process forecast with multidimensional distributional input*, 4th Conference of the International Society for Nonparametric Statistics, June 11–15, University of Salerno, Italy, June 15.

177. ———, *Bootstrap confidence sets for spectral projectors of sample covariance*, 12th International Vilnius Conference on Probability Theory and Mathematical Statistics and 2018 IMS Annual Meeting on Probability and Statistics, July 2–6, Vilnius University, Lithuanian Mathematical Society and the Institute of Mathematical Statistics, Lithuania, July 5.

178. ———, *Structured nonparametric and high-dimensional statistics*, 2018 Joint Meeting of the Korean Mathematical Society and the German Mathematical Society, October 3–6, Korean Mathematical Society, Seoul, Korea (Republic of), October 5.

179. ———, *Prior impact in Bayesian inference*, International Seminar & Workshop: "Stochastic Dynamics on Large Networks: Prediction and Inference", October 15–16, Max-Planck-Institut für Physik komplexer Systeme, Dresden, October 15.

180. ———, *Large ball probability with applications to statistical inference*, 6th Princeton Day of Statistics, Princeton University, Department of Operations Research and Financial Engineering, USA, November 9.

181. ———, *Manifold learning: Theory and applications*, Pennsylvania State University, Department of Mathematics, State College, USA, November 14.

182. ———, *Large ball probability with applications in statistics*, Mathematical Workshop of the School of Applied Mathematics and Computer Science, Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, November 30.

183. B. Stemper, *Pricing under rough volatility*, Premia Meeting, Centre de recherche INRIA Paris, France, March 12.

184. A. Suvorikova, *Gaussian process forecast with multidimensional distributional input*, Haindorf Seminar 2018, January 23–27, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, Hejnice, Czech Republic, January 25.

185. ———, *Construction of non-asymptotic confidence sets in 2-Wasserstein space*, Structural Learning Seminar, Skolkovo Institute of Science and Technology, Moscow, Russian Federation, May 10.

186. ———, *Central limit theorem for barycenters in 2-Wasserstein space*, Ruhr-Universität Bochum, Fakultät für Mathematik, Lehrstuhl für Stochastik, May 30.

187. ———, *CLT for barycenters in 2-Wasserstein space*, Mass TransportationTheory: Opening Perspectives in Statistics, Probability and Computer Science, June 3–10, Universidad de Valladolid, Departamento de Estadística e Investigación Operativa, Spain, June 5.

188. ———, *Central limit theorem for Wasserstein barycenters of Gaussian measures*, 4th Conference of the International Society for Nonparametric Statistics, June 11–15, University of Salerno, Italy, June 15.

189. K. Tabelow, *Structural adaptation for noise reduction in magnetic resonance imaging*, SIAM Conference on Imaging Science, Minisymposium MS5 "Learning and Adaptive Approaches in Image Processing", June 5–8, Bologna, Italy, June 5.

190. M. Thomas, *Analysis and simulation for a phase-field fracture model at finite strains based on modified invariants*, Analysis Seminar, University of Brescia, Department of Mathematics, Italy, May 10.

191. ———, *Optimization of the radiative emission for mechanically strained optoelectronic semiconductor devices*, 9th International Conference "Inverse Problems: Modeling and Simulation" (IPMS 2018), Minisymposium M16 "Inverse and Control Problems in Mechanics", May 21–25, The Eurasian Association on Inverse Problems, Malta, May 24.

192. ———, *Analysis and simulation for a phase-field fracture model at finite strains based on modified invariants*, Workshop "Special Materials and Complex Systems" (SMACS 2018), June 18–22, University of Milan/University of Pavia, Gargnano, Italy, June 18.

193. ———, *Rate-independent evolution of sets & applications to damage and delamination*, PDEs Friends, June 21–22, Politecnico di Torino, Dipartimento di Scienze Matematiche "Giuseppe Luigi Lagrange", Italy, June 22.

194. ———, *Analysis for the discrete approximation of damage and fracture*, Applied Analysis Day, June 28–29, Technische Universität Dresden, Chair of Partial Differential Equations, June 29.

195. ———, *Analytical and numerical approach to a class of damage models*, The 12th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 75 "Mathematics and Materials: Models and Applications", July 5–9, National Taiwan University, Taipeh, Taiwan, Province Of China, July 6.

196. ———, *Gradient structures for flows of concentrated suspensions*, The 12th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Special Session 18 “Emergence and Dynamics of Patterns in Nonlinear Partial Differential Equations and Related Fields”, July 5–9, National Taiwan University, Taipeh, Taiwan, Province Of China, July 7.

197. ———, *Analysis for the discrete approximation of gradient-regularized damage models*, Workshop “Women in Mathematical Materials Science”, November 5–6, Universität Regensburg, Fakultät für Mathematik, November 6.

198. ———, *Analytical and numerical aspects of damage models*, Berlin Dresden Prague Würzburg Workshop “Mathematics of Continuum Mechanics”, November 29–30, Technische Universität Würzburg, Institut für Mathematik, November 30.

199. W. van Zuijlen, *A Hamilton–Jacobi point of view on mean-field Gibbs-non-Gibbs transitions*, Workshop on Transformations and Phase Transitions, January 29–31, Ruhr-Universität Bochum, Fakultät für Mathematik, Bochum, January 30.

200. ———, *Eigenvalues of the Anderson Hamiltonian with white noise potential in 2D*, Leiden University, Institute of Mathematics, Leiden, Netherlands, May 1.

201. ———, *Mass-asymptotics for the parabolic Anderson model in 2D*, 10th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, November 29 – December 1, University of Oxford, Mathematical Institute, Oxford, UK, November 29.

202. ———, *Mass-asymptotics for the parabolic Anderson model in 2D*, Statistical Mechanics Seminar, University of Warwick, Department of Statistics, Coventry, UK, December 6.

203. A.G. Vladimirov, *Time-delay modeling of short pulse generation in lasers*, Annual International Conference „Days on Diffraction 2018”, June 4–8, Steklov Mathematical Institute, St. Petersburg, Russian Federation, June 6.

204. ———, *Time-delay systems in multimode laser dynamics*, 675. WE-Heraeus-Seminar „Delayed Complex Systems”, July 2–5, Physikzentrum Bad Honnef, July 4.

205. ———, *Delay models in nonlinear laser dynamics*, Dynamics Days Europe 2018, September 3–7, Loughborough University, UK, September 6.

206. B. Wagner, *Yield stress in concentrated suspensions*, Mathematical Nanosystems Workshop, January 17–18, California NanoSystems Institute at UCLA, Los Angeles, USA, January 18.

207. ———, *Multiple scales in thin liquid films*, UCLA Guest Lecture, University of California, Department of Mathematics, Los Angeles, USA, January 25.

208. ———, *Thin film models for an active gel*, 89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2018), Session S02 “Biomechanics”, March 19–23, Technische Universität München, March 22.

209. ———, *Multiscale modelling of suspensions and how it fits into the UL context*, University of Limerick, Department Mathematics & Statistics, Ireland, June 7.

210. ———, *Signatures of slip in thin film flows*, SIAM Conference on Nonlinear Waves and Coherent Structures, Minisymposium MS25 “Large-scale Effects of Local Structures in Complex Systems”, June 11–14, Anaheim, USA, June 13.

211. ———, *Modeling microstructures for light harvesting surfaces*, The 20th European Conference on Mathematics for Industry (ECMI 2018), Minisymposium 38 “ECMI Special Interest Group: Material Design and Performance in Sustainable Energies”, June 18–22, Budapest, Hungary, June 21.

212. ———, *Modeling microstructures for light harvesting surfaces*, European Women in Mathematics (EWM) General Meeting 2018, Minisymposium “Mathematics in Industry”, Karl-Franzens-Universität Graz, Austria, September 7.

213. M. Wolfrum, *Dynamics of coupled oscillator systems and their continuum limits*, Kolloquium der Arbeitsgruppe Modellierung, Numerik, Differentialgleichungen, Technische Universität Berlin, Institut für Mathematik, June 12.

214. ———, *Phase solitons in DDEs with large delay*, 14th IFAC Workshop on Time Delay Systems, June 28–30, Budapest University of Technology and Economics, Hungary, June 29.

215. A. Zafferi, *Regularity results for a thermodynamically consistent non-isothermal Cahn–Hilliard model*, Summer School “Dissipative Dynamical Systems and Applications”, September 3–7, University of Modena, Department of Physics, Informatics and Mathematics, Italy, September 6.

A.8.3 Talks for a More General Public

1. L. Blank, *Das (Mathematik-) Studium*, Girls’ Day, WIAS Berlin, April 26.

2. W. König, *Murphys Gesetz, tippende Affen und die Unendlichkeit der Wahrscheinlichkeit*, MathInside – Mathematik ist überall, Urania, Berlin, January 23.

3. ———, *Stochastische Geometrie für Telekommunikationsnetzwerke*, 2 talks, Tag der Wissenschaften 2018, Weinberg-Gymnasium Kleinmachnow, Kleinmachnow, November 20.

4. S. Reichelt, *Achilles und die Schildkröte*, Girls’ Day, WIAS Berlin, April 26.

5. H. Stephan, *Endliche Kardinal- und Ordinalzahlen: Unterschiede und Widersprüche zwischen Mathematik und Realität am Beispiel der Zahlen*, Tag der Mathematik 2018, Technische Universität Berlin, April 21.

6. ———, *Von Primzahlen und Pseudoprimzahlen*, Tag der Mathematik 2018, Technische Universität Berlin, April 21.

A.8.4 Posters

1. R. Ahrens, F. Anker, C. Bartsch, A. Voigt, V. Wiedmeyer, K. Sundmacher, V. John, S. Le Borne, *Advanced numerical methods for the simulation of population balance systems*, 6th International Conference on Population Balance Modelling (PBM2018), Ghent University, Belgium, May 7–9.

2. C. Bartsch, V. John, R.I.A. Patterson, *A new mixed stochastic-deterministic simulation approach to particle populations in fluid flows*, 6th International Conference on Population Balance Modelling (PBM2018), Ghent University, Belgium, May 7–9.

3. D.H. Doan, J. Fuhrmann, A. Glitzky, Th. Koprucki, M. Liero, *On van Roosbroeck systems with Gauss–Fermi statistics*, Applied Mathematics and Simulation for Semiconductors (AMaSiS 2018), WIAS Berlin, October 8–10.

4. P. Dvurechensky, *Universal method for variational inequalities with Holder-continuous monotone operator*, MIA 2018 – Mathematics and Image Analysis, Humboldt-Universität zu Berlin, January 15–17.

5. ———, *Computational optimal transport: Complexity by accelerated gradient descent is better than by Sinkhorn’s algorithm*, The 35th International Conference on Machine Learning (ICML 2018), Stockholm, Sweden, July 9–15.

6. P. Dvurechensky, D. Dvinskikh, *Decentralize and randomize: Faster algorithm for Wasserstein barycenters*, Thirty-Second Conference On Neural Information Processing Systems, Montréal, Canada, December 3–8.

7. M. Eigel, R. Gruhlke, *Domain decomposition for random high-dimensional PDEs*, Workshop “Reducing Dimensions and Cost for UQ in Complex Systems”, Cambridge, UK, March 5–9.

8. S. Eydam, *Mode locking in systems of globally coupled phase oscillators*, Dynamics Days Europe, Loughborough, UK, September 3–7.

9. ———, *Mode-locking in systems of globally coupled phase oscillators*, International Conference on Control of Self-Organizing Nonlinear Systems, Warnemünde, September 9–13.
10. C. Cancès, C. Chainais-Hillairet, J. Fuhrmann, B. Gaudeul, *Numerical schemes for a reduced case of an improved Nernst–Planck–Poisson model*, Applied Mathematics and Simulation for Semiconductors (AMaSiS 2018), WIAS Berlin, October 8–10.
11. J. Fuhrmann, A. Linke, Ch. Merdon, C. Guhlke, R. Müller, *Models and numerical methods for electroosmotic flow including finite ion size effects*, Workshop on Ion Exchange Membranes for Energy Applications (EMEA2018), Bad Zwischenahn, June 26–28.
12. J. Fuhrmann, A. Linke, Ch. Merdon, C. Guhlke, R. Müller, *Models and numerical methods for electroosmotic flow including finite ion size effects*, Applied Mathematics and Simulation for Semiconductors (AMaSiS 2018), WIAS Berlin, October 8–10.
13. R. Gruhlke, *Stochastic domain decomposition and application in heterogeneous material*, 3rd GAMM AGUQ Workshop on Uncertainty Quantification 2018, Technische Universität Dortmund, March 12–14.
14. M. Hintermüller, M. Holler, K. Papafitsoros, *A function space framework for structural total variation regularization in inverse problems*, MIA 2018 – Mathematics and Image Analysis, Humboldt-Universität zu Berlin, January 15–17.
15. M. Landstorfer, *Modelling and simulation of porous electrodes with multi-scale homogenization technique*, ModVal 2018, 15th Symposium on Modeling and Experimental Validation of Electrochemical Energy Devices, Aarau, Switzerland, April 12–13.
16. ———, *Modellbasierte Abschätzung der Lebensdauer von gealterten Li-Batterien für die 2nd-Life Anwendung als stationärer Stromspeicher*, BMBF-Statusseminar zur Förderrichtlinie Mathematik, Bonn, November 19–20.
17. A. Maltsi, Th. Koprucki, T. Niermann, T. Streckenbach, K. Tabelow, J. Polzehl, *Computing TEM images of semiconductor nanostructures*, Applied Mathematics and Simulation for Semiconductors (AMaSiS 2018), WIAS Berlin, October 8–10.
18. M. Marschall, *Bayesian inversion and adaptive low-rank tensor decomposition*, 3rd GAMM AGUQ Workshop on Uncertainty Quantification 2018, Technische Universität Darmstadt, March 12–14.
19. ———, *Bayesian inversion and adaptive low-rank tensor decomposition*, Workshop “UQ for Inverse Problems in Complex Systems”, Cambridge, UK, April 9–13.
20. H.-J. Mucha, *Multivariate statistische Auswertung von archäometrischen Messwerten von Mammut-Elfenbein*, Tagung Archäometrie und Denkmalpflege 2018, Deutsches Elektronen-Synchrotron DESY, Hamburg, March 20–24.
21. R. Müller, J. Fuhrmann, C. Guhlke, B. Matejczyk, *Dimension reduction of improved Nernst–Planck models for charged nanopores*, Asymptotic Behavior of Systems of PDE Arising in Physics and Biology: Theoretical and Numerical Points of View (ABPDE III), Lille, France, August 28–31.
22. P. Farrell, D. Peschka, *Challenges for drift-diffusion simulations of semiconductors: A comparative study of different discretization philosophies*, Applied Mathematics and Simulation for Semiconductors (AMaSiS 2018), WIAS Berlin, October 8–10.
23. A. Pimenov, *Analysis of temporal localized structures in a time delay model of a ring laser*, 675. WE-Heraeus Seminar: Delayed Complex Systems 2018, Bad Honnef, July 2–5.
24. C.N. Rautenberg, *Spatially distributed parameter selection in Total Variation (TV) models*, MIA 2018 – Mathematics and Image Analysis, Humboldt-Universität zu Berlin, January 15–17.
25. St.-M. Stengl, *Uncertainty quantification of the Ambrosio–Tortorelli approximation in image segmentation*, MIA 2018 – Mathematics and Image Analysis, Humboldt-Universität zu Berlin, January 15–17.

26. A. Stephan, *Rigorous derivation of the effective equation of a linear reaction system with different time scales*, 3rd Berlin Dresden Prague Würzburg Workshop “Mathematics of Continuum Mechanics”, Würzburg, November 29–30.
27. A. Suvorikova, *Statistical inference with optimal transport*, Spring School “Structural Inference 2018” and Closing Workshop, FOR 1735 “Structural Inference in Statistics”, Lübbenau, March 4–9.
28. M. Thomas, *Dynamics of rock dehydration on multiple scales*, Begutachtung SFB 1114: Scaling Cascades in Complex Systems, Freie Universität Berlin, February 27–28.
29. S. Tornquist, *Towards the analysis of dynamic phase-field fracture*, 3rd Berlin Dresden Prague Würzburg Workshop “Mathematics of Continuum Mechanics”, Würzburg, November 29–30.
30. M. Wolfrum, *Phase-sensitive excitability of a limit cycle*, International Conference on Control of Self-Organizing Nonlinear Systems, Warnemünde, September 9–13.
31. A. Zafferi, *Flows of concentrated suspensions in geosciences*, 3rd Berlin Dresden Prague Würzburg Workshop “Mathematics of Continuum Mechanics”, Würzburg, November 29–30.

A.9 Visits to other Institutions[5]

1. N. Alia, Outokumpu Stainless OY, Tornio, Finland, May 2 – June 1.
2. L. Andreis, Università degli Studi di Padova, Dipartimento di Matematica "Tullio Levi–Civita", Padova, Italy, October 5–14.
3. ———, Università degli Studi di Torino, Dipartimenti di Matematica, Torino, Italy, December 3–7.
4. Ch. Bayer, Institut National de Recherche en Informatique et en Automatique, Paris, France, January 26 – February 1.
5. ———, King Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences and Engineering Division, Thuwal, Saudi Arabia, April 19–29.
6. ———, City University of New York, Baruch College, USA, November 18–23.
7. ———, King Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences and Engineering Division, Thuwal, Saudi Arabia, December 7–17.
8. L. Capone, Outokumpu Stainless OY, Tornio, Finland, May 3 – June 1.
9. P. Dvurechensky, Université Catholique de Louvain, Institut Multidisciplinaire pour la Modélisation et l'Analyse Quantitative (IMAQ), Louvain-la-Neuve, Belgium, March 19–23.
10. ———, Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russian Federation, March 27 – April 6.
11. ———, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russian Federation, July 24 – August 7.
12. ———, Maastricht University, School of Business and Economics, Netherlands, October 8–12.
13. M. Eigel, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, February 12–21.
14. S. Eydam, Institute of Physics Belgrade, Serbia, October 4–18.
15. F. Flegel, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, March 5–9.
16. ———, Universität zu Köln, Mathematisches Institut, Köln, June 12–15.
17. J. Fuhrmann, Université de Lille, Centre Européen pour les Mathématiques, France, May 13 – June 9.
18. R. Henrion, Miguel Hernández University of Elche, Center of Operations Research, Spain, September 10–15.
19. D. Hömberg, Fudan University, School of Mathematical Sciences, Shanghai, China, January 8–12.
20. ———, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, January 22 – February 9.
21. ———, November 10–23.
22. B. Jahnel, Universität Osnabrück, Institut für Mathematik, September 24–28.
23. V. John, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, March 11–16.
24. ———, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, October 22–25.
25. ———, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, November 12–16.

[5] Only stays of more than three days are listed.

26. Z. Lakdawala, Lahore University of Management Sciences, School of Science & Engineering, Pakistan, November 5–24.
27. ———, Habib University, School of Science and Engineering, Karachi, Pakistan, November 25–28.
28. A. Linke, Aix Marseille Université, Institut de Mathématiques, France, April 3–6.
29. ———, Clemson University, Department of Mathematical Sciences, South Carolina, USA, August 14–21.
30. ———, University of Texas at Austin, Institute for Computational Engineering and Sciences, USA, September 14–28.
31. O. Marquardt, Chinese Academy of Sciences, Beijing Institute of Nanoenergy and Nanosystems (BINN), China, April 9–17.
32. P. Mathé, Technische Universität Chemnitz, Fachbereich Mathematik, September 24–28.
33. ———, Fudan University, School of Mathematical Sciences, Shanghai, China, October 4–20.
34. ———, University of Cyprus, Department of Mathematics and Statistics, Nicosia, Cyprus, December 4–11.
35. M. Maurelli, Eindhoven University of Technology, Department of Mathematics and Computer Science, Institute for Complex Molecular Systems, Netherlands, February 26 – March 2.
36. A. Mielke, Università di Pavia, Dipartimento di Matematica, Italy, April 23–27.
37. ———, University of Bath, Mathematical Sciences, UK, May 19–25.
38. M. Mittnenzweig, Weizmann Institute of Science, Feinberg Graduate School, Revohot, Israel, April 28 – June 2.
39. R.I.A. Patterson, University of Cambridge, Faculty of Mathematics, Cambridge, UK, July 21 – August 6.
40. D. Peschka, On-site examination of the stages of geological rock dehydration, Bosio, Italy, September 29 – October 3.
41. P. Pigato, Université Paris-Dauphine, Centre de Recherche en Mathématiques de la Décision (CEREMADE), France, May 22–25.
42. J. Polzehl, University of Minnesota, School of Statistics, Minneapolis, USA, September 20 – October 18.
43. M. Radziunas, Macquarie University, Faculty of Science and Engineering, Sydney, Australia, June 28 – July 26.
44. J. Rehberg, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, September 27 – October 5.
45. D.R.M. Renger, Università degli Studi dell'Aquila, Dipartimento di Ingegneria e Scienze dell'Informazione e Matematica, L'Aquila, Italy, January 7–15.
46. N. Rotundo, University of Calabria, Department of Physics, Cosenza, Italy, July 23–27.
47. ———, October 22–26.
48. H. Si, Beijing Computational Science Research Center, Applied and Computational Mathematics, Beijing, China, March 12–16.
49. ———, Beijing Institute for Scientific and Engineering Computing, Applied and Computational Mathematics, China, March 19–24.
50. ———, Beijing Computational Science Research Center, Applied and Computational Mathematics, Beijing, China, March 26–30.
51. ———, Beijing Computational Science Research Center, Applied and Computational Mathematics, China, July 23 – August 2.

52. ———, Dalian University of Technology, International School of Information Science & Engineering, China, August 6–13.
53. ———, University of Cambridge, Bullard Laboratories, UK, October 16–19.
54. ———, Zhejiang University, Center for Engineering & Scientific Computation, Hangzhou, China, November 19 – December 1.
55. R. Soares dos Santos, University of Groningen, Johann Bernoulli Institute for Mathematics and Computer Science, Groningen, Netherlands, February 13–16.
56. ———, Leiden University, Institute of Mathematics, Leiden, Netherlands, April 22–26.
57. V. Spokoiny, National Research University Higher School of Economics, Faculty of Computer Science, Moscow, Russian Federation, February 22–28.
58. ———, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, PreMoLab, Moscow, Russian Federation, May 21–26.
59. ———, Skolkovo Institute of Science and Technology, Moscow, Russian Federation, July 17–28.
60. ———, National Research University Higher School of Economics, Moscow, Russian Federation, September 3–25.
61. ———, Moscow Institute of Physics and Technology (MIPT), PreMoLab, Dolgoprudny, Russian Federation, October 26–30.
62. ———, Pennsylvania State University, Department of Mathematics, State College, USA, November 11–15.
63. ———, National Research University Higher School of Economics, Moscow, Russian Federation, November 28 – December 2.
64. A. Suvorikova, Russian Academy of Sciences, Kharkevich Institute for Information Transmission Problems, Moscow, Russian Federation, December 18, 2017 – January 5, 2018.
65. ———, National Research University Higher School of Economics, Moscow, Russian Federation, May 9–25.
66. ———, Ruhr-Universität Bochum, Fakultät für Mathematik, Lehrstuhl für Stochastik, May 29 – June 30.
67. ———, Skolkovo Institute of Science and Technology, Moscow, Russian Federation, July 23–27.
68. ———, National Research University Higher School of Economics, Moscow, Russian Federation, July 30 – August 10.
69. M. Thomas, University of Brescia, Department of Mathematics, Italy, May 7–11.
70. ———, University of Pavia, Department of Mathematics, Italy, June 12–16.
71. ———, On-site examination of the stages of geological rock dehydration, Bosio, Italy, September 29 – October 3.
72. ———, Universität Kassel, Fachbereich Mathematik und Naturwissenschaften, November 30 – December 3.
73. P. Vágner, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, August 13–19.
74. ———, December 18–21.
75. W. van Zuijlen, Leiden University, Institute of Mathematics, Leiden, Netherlands, December 22, 2017 – January 2, 2018.
76. ———, August 1–8.
77. ———, University of Warwick, Department of Statistics, Coventry, UK, December 2–7.
78. B. Wagner, University of California, Department of Mathematics, Los Angeles, USA, January 19–28.

79. ———, University of Oxford, Mathematical Institute, UK, November 19–23.

80. M. Wolfrum, Institute of Physics Belgrade, Center for the Study of Complex Systems, Scientific Computing Laboratory, Serbia, October 4–11.

81. A. Zafferi, On-site examination of the stages of geological rock dehydration, Bosio, Italy, September 29 – October 3.

A.10 Academic Teaching[6]

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), 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. B. Jahnel, *Analysis I und Lineare Algebra für Ingenieurwissenschaften* (lecture), Technische Universität Berlin, 4 SWS.
13. V. John, *Numerik IV: Finite-Elemente-Methoden II (Strömungsmechanik)* (lecture), Freie Universität Berlin, 2 SWS.
14. ———, *Numerik IV: Finite-Elemente-Methoden II (Strömungsmechanik)* (practice), Freie Universität Berlin, 2 SWS.
15. O. Klein, *Mathematische Modellierung von Hystereseeffekten* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
16. ———, *Mathematische Modellierung von Hystereseeffekten* (practice), Humboldt-Universität zu Berlin, 1 SWS.
17. W. König, *Analysis I für Mathematikerinnen und Mathematiker* (lecture), Technische Universität Berlin, 4 SWS.
18. J. Blath, W. König, *Stochastic Processes in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
19. M. Liero, *Optimaler Transport und Wasserstein-Gradientenflüsse* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
20. ———, *Optimaler Transport und Wasserstein-Gradientenflüsse* (practice), Humboldt-Universität zu Berlin, 1 SWS.

[6] SWS = semester periods per week

21. O. Marquardt, *Mathematisch-physikalische Grundlagen, Screen Based Media (BA)* (lecture), Beuth Hochschule für Technik Berlin, 2 SWS.
22. M. Maurelli, *Fortgeschrittene Themen der Stochastik – Regularization by Noise* (lecture), Technische Universität Berlin, 2 SWS.
23. Ch. Merdon, *Numerik partieller Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
24. A. Mielke, *Analysis III* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
25. J.G.M. Schoenmakers, *Stochastische Finanzmathematik I* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
26. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
27. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
28. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
29. M. Thomas, *Nichtlineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
30. ———, *Nichtlineare partielle Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
31. B. Wagner, *Asymptotische Analysis* (lecture), Technische Universität Berlin, 4 SWS.
32. M. Wolfrum, B. Fiedler, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

Summer Semester 2018

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. U. Bandelow, S. Amiranashvili, *Nichtlineare Dynamik in der Photonik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
3. Ch. Bayer, A. Papapantoleon, *Fortgeschrittene Themen der Finanzmathematik: Computational Finance* (lecture), Technische Universität Berlin, 2 SWS.
4. P.-É. Druet, O. Klein, *Höhere Analysis II / Partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
5. ———, *Höhere Analysis II / Partielle Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
6. P. Farrell, *Numerik II* (lecture), Technische Universität Hamburg-Harburg, 2 SWS.
7. ———, *Numerik von gewöhnlichen Differentialgleichungen* (lecture), Technische Universität Hamburg-Harburg, 2 SWS.
8. P. Friz, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
9. ———, *Quantitative Finance* (seminar), Technische Universität Berlin, 2 SWS.
10. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
11. A. Glitzky, A. Mielke, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
12. M. Heida, *An Introduction to Homogenization Theory* (lecture), Technische Universität Berlin, 2 SWS.

13. M. Hintermüller, *Optimierung bei partiellen Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
14. 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.
15. D. Hömberg, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
16. B. Jahnel, W. König, *Räumliche stochastische Modelle für Telekommunikation* (lecture), Technische Universität Berlin, 2 SWS.
17. ———, *Räumliche stochastische Modelle für Telekommunikation* (seminar), Technische Universität Berlin, 2 SWS.
18. V. John, *Numerical Methods in Fluid Dynamics* (lecture), Freie Universität Berlin, 2 SWS.
19. ———, *Numerical Methods in Fluid Dynamics* (practice), Freie Universität Berlin, 2 SWS.
20. T. Keil, *Optimierung bei partiellen Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
21. W. König, *Analysis II für Mathematikerinnen und Mathematiker* (lecture), Technische Universität Berlin, 4 SWS.
22. M. Liero, *Mehrdimensionale Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
23. ———, *Mehrdimensionale Variationsrechnung* (practice), Humboldt-Universität zu Berlin, 2 SWS.
24. A. Linke, *Analysis 1 (Mathematik für Physiker I)* (lecture), Freie Universität Berlin, 4 SWS.
25. O. Marquardt, *Brückenkurs Physik (10 two-hour lectures from March 25 to 29, 2018)* (lecture), Beuth Hochschule für Technik Berlin, – SWS.
26. D.R.M. Renger, *Konvexe Analysis* (lecture), Technische Universität Berlin, 2 SWS.
27. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
28. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
29. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
30. M. Wolfrum, B. Fiedler, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

Winter Semester 2018/2019

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. Ch. Bayer, P. Friz, *Fortgeschrittene Themen der Finanzmathematik: Rough Volatility* (lecture), WIAS Berlin/Technische Universität Berlin, 4 SWS.
3. J.A. Brüggemann, *Nonlinear Optimization* (practice), Humboldt-Universität zu Berlin, 2 SWS.
4. M. Eigel, *Uncertainty Quantification and Statistical Learning* (lecture), Technische Universität Berlin, 2 SWS.
5. P. Farrell, *Numerik partieller Differentialgleichungen* (lecture), Technische Universität Hamburg-Harburg, 2 SWS.

6. ———, *Numerische Mathematik I* (lecture), Technische Universität Hamburg-Harburg, 2 SWS.
7. P. Friz, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
8. J. Fuhrmann, *Wissenschaftliches Rechnen* (lecture), Technische Universität Berlin, 4 SWS.
9. A. Glitzky, A. Mielke, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
10. M. Heida, *Nonlinear Functional Analysis* (lecture), Technische Universität Berlin, 4 SWS.
11. M. Hintermüller, *Nichtlineare Optimierung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
12. 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.
13. ———, *Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 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. W. König, *Analysis III für Mathematikerinnen und Mathematiker* (lecture), Technische Universität Berlin, 4 SWS.
17. O. Marquardt, *Grundlagen der medizinischen Messtechnik* (lecture), Beuth Hochschule für Technik Berlin, 2 SWS.
18. ———, *Brückenkurs Physik für Elektrotechnik und Mechatronik (10 two-hour lectures from Sept. 24 to 28, 2018)* (seminar), Beuth Hochschule für Technik Berlin, – SWS.
19. B. Moreau, *Computational Fluid Dynamics* (practice), Beuth Hochschule für Technik Berlin, 2 SWS.
20. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
21. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
22. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
23. 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. Adamyan, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 "High Dimensional Non Stationary Time Series", Berlin, January 1 – December 31.
2. N. Ahmed, American University of the Middle East, Mathematics Department, Kuwait, August 7–17.
3. A.A. Al-Eryani, Friedrich-Alexander-Universität Erlangen-Nürnberg, Professur für Wissensrepräsentation und -verarbeitung, Erlangen, July 11 – August 31.
4. I. Bačić, University of Belgrade, Institute of Physics Belgrade, Scientific Computing Laboratory, Serbia, June 4–24.
5. ———, November 4–30.
6. N. Baldin, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, Cambridge, UK, April 16–25.
7. L. Banz, Universität Salzburg, Fachbereich Mathematik, Austria, May 14–18.
8. S. Bechtel, Technische Universität Darmstadt, Fachbereich Mathematik, February 25 – March 2.
9. N. Berger, Technische Universität München, Fakultät für Mathematik, Garching b. München, July 17–20.
10. N. Berglund, Université d'Orléans, Institut Denis Poisson, France, July 4–12.
11. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, June 26 – July 1.
12. ———, September 28 – October 2.
13. L. Bonifacius, Technische Universität München, Center for Mathematical Sciences, Garching, March 5–16.
14. G. Botirov, National University of Uzbekistan, Mathematical Analysis, Tashkent, Uzbekistan, February 1–28.
15. A. Ceretani, Humboldt-Universität zu Berlin, Institut für Mathematik, August 20 – December 31.
16. P. Colli, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, May 21–26.
17. P. Das, EFD Induction AS, Skien, Norway, November 6, 2017 – January 31, 2018.
18. ———, May 2 – June 30.
19. ———, October 31 – November 3.
20. ———, November 19, 2018 – January 23, 2019.
21. F. Dassi, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, February 20 – March 6.
22. O. D'Huys, Aston University, Engineering and Applied Science, Birmingham, UK, February 25 – March 18.
23. K. Doku-Amponsah, University of Ghana, School of Physical and Mathematical Sciences, Department of Statistics and Actuarial Science, Legon-Accra, Ghana, November 26 – December 22.
24. G. Dong, Humboldt-Universität zu Berlin, Institut für Mathematik, September 1, 2017 – December 31, 2018.

[7] Only stays of more than three days are listed.

25. A. Drewitz, Universität zu Köln, Mathematisches Institut, July 24 – August 2.
26. D. Dvinskikh, Moscow Institute of Physics and Technology, Department of Control and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, August 21–31.
27. K. Efimov, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – December 31.
28. M. Egert, Université Paris-Sud, Laboratoire de Mathématiques, Orsay, France, February 26 – March 2.
29. R. Eisenberg, Rush University, Department of Physiology & Biophysics, Chicago, USA, October 2–6.
30. M.C. Ferris, The University of Wisconsin, Computer Sciences and Statistics, Madison, USA, June 18–21.
31. I. Franovic, University of Belgrade, Institute of Physics Belgrade, Belgrade, Serbia, June 4–24.
32. ———, November 4–30.
33. S. Ganesan, Indian Institute of Science, Department of Computational and Data Sciences, Bangalore, India, August 27 – September 3.
34. A. Gasnikov, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, January 9 – February 8.
35. ———, October 10–22.
36. M.J. Gisbert, Universidad Miguel Hernández de Elche, Instituto Centro de Investigación Operativa, Alicante, Spain, February 1 – May 4.
37. B. Grund, University of Minnesota, School of Statistics, Minneapolis, USA, June 11–29.
38. ———, July 3–13.
39. S. Hajian, Humboldt-Universität zu Berlin, Institut für Mathematik, April 29, 2016 – September 30, 2018.
40. E.J. Hall, Rheinisch-Westfälische Technische Hochschule Aachen, Fachgruppe Mathematik, Aachen, November 12–16.
41. B. Hamoudi, King Abdullah University of Science and Technology, Department of Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, May 7–11.
42. M. Heinkenschloss, Rice University, Department of Computational and Applied Mathematics, Houston, Texas, USA, October 17–21.
43. L. Heltai, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, January 22 – March 16.
44. ———, October 30 – November 12.
45. ———, December 3–7.
46. D. Heydecker, University of Cambridge, Faculty of Mathematics, Cambridge, UK, March 19–25.
47. Ch. Hirsch, Aalborg University, Department of Mathematical Sciences, Denmark, September 7–10.
48. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, Chemnitz, March 5–9.
49. J. Holley, Robert Bosch GmbH, April 1, 2017 – March 31, 2020.
50. G. Hu, Beijing Computational Science Research Center, China, June 4–29.
51. O. Huber, Humboldt-Universität zu Berlin, Institut für Mathematik, October 8, 2018 – October 8, 2022.
52. T. Iliescu, Virginia Polytechnic Institute and State University, Department of Mathematics, Blacksburg, USA, June 25–29.
53. K. Ito, North Carolina State University, Department of Mathematics, Raleigh, USA, September 5–12.

54. A. Jüngel, Technical University of Vienna, Institute for Analysis and Scientific Computing, Research Group Partial Differential Equations and Dynamical Systems, Austria, May 7–10.
55. D. Kamzolov, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, October 10–22.
56. A. Kebaier, Université Paris 13, Laboratoire Analyse, Géométrie et Applications, Villetaneuse, France, January 20–23.
57. Y. Klochkov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, January 1 – December 31.
58. D. Knees, Universität Kassel, Institut für Mathematik, June 9–14.
59. M. Kraft, University of Cambridge, Department of Chemical Engineering and Biotechnology, UK, August 20 – September 7.
60. A. Kruger, Federation University Australia, School of Science, Engineering and Information Technology, Centre for Informatics and Applied Optimization (CIAO), Ballarat, Australia, September 16–20.
61. Ch. Kuhn, Technische Universität Kaiserslautern, Fachbereich Maschinenbau und Verfahrenstechnik, October 15–18.
62. G. Lelong, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, St. Martin d’Hères, France, April 9–12.
63. U. Leonhardt, Weizmann Institute of Science, Department of Physics of Complex Systems, Rehovot, Israel, May 16–20.
64. M.M. Malamud, Peoples’ Friendship University of Russia, S.M. Nikol’skii Mathematical Institute, Moscow, Russian Federation, November 10–19.
65. P. Mangold, Université Paris-Saclay, École Polytechnique, Centre de Mathématiques Appliquées, Palaiseau, France, April 16 – July 20.
66. M. Maurelli, University of York, Department of Mathematics, York, UK, September 28 – October 5.
67. E. Meca, University of Cordoba, Agronomy Department, Spain, March 25–29.
68. H. Meinlschmidt, Johann-Radon-Institute for Computational and Applied Mathematics, Optimization and Optimal Control, Linz, Austria, November 12–20.
69. V. Miloš, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, September 10–14.
70. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, June 4–8.
71. ———, June 25 – July 31.
72. ———, August 29 – September 30.
73. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica (DMI), Italy, August 20–30.
74. M.T. Nair, Indian Institute of Technology Madras, Department of Mathematics, Chennai, India, September 17–24.
75. A. Naumov, National Research University Higher School of Economics, International Laboratory of Stochastic Algorithms and High-Dimensional Inference, Moscow, Russian Federation, October 22–26.
76. M.J. Neilan, University of Pittsburgh, Department of Mathematics, USA, April 10–13.
77. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, December 3–7.

78. Ch. Onyi, Nnamdi Azikiwe University Awka, Department of Mathematics, Awka, Nigeria, September 26, 2017 – December 31, 2018.

79. M. Patriarca, University of Rome Tor Vergata, Electronic Engineering Department, Rome, Italy, March 6–9.

80. M. Peters, Eidgenössische Technische Hochschule Zürich, Department of Biosystems Science and Engineering (D BSSE), Basel, Switzerland, June 11–15.

81. N. Petrelis, Université de Nantes, Laboratoire Jean Leray, UFR Sciences et Techniques, Nantes, France, May 7–18.

82. S. Popov, University of Campinas — UNICAMP, Institute of Mathematics, Statistics and Scientific Computation, Campinas, Brazil, December 4, 2018 – January 24, 2019.

83. S. Ramesh Babu, SSAB Europe Oy, Raahe, Finland, January 8–23.

84. ———, December 10–20.

85. A. Rasheed, Lahore University of Management Sciences, Department of Mathematics, Pakistan, January 2–14.

86. J.F. Rodrigues, University of Lisbon, Department of Mathematics, Portugal, January 21–27.

87. ———, April 30 – May 31.

88. P.-F. Rodriguez, University of California, Los Angeles (UCLA), Department of Mathematics, Los Angeles, USA, June 18–30.

89. F.J. Romero Hinrichsen, ETH Zurich, Department of Mathematics, Switzerland, May 27 – June 1.

90. F. Schäfer, California Institute of Technology, Department of Computing and Mathematical Sciences, Pasadena, California, USA, May 27 – June 9.

91. G. Schimperna, Università di Pavia, Dipartimento di Matematica, Italy, September 24–28.

92. A. Schlüter, Technische Universität Kaiserslautern, Fachbereich Maschinenbau und Verfahrenstechnik, October 15–18.

93. L. Shen, University of the Chinese Academy of Sciences, School of Mathematical Sciences, Beijing, China, June 10–15.

94. J. Shewchuk, University of California at Berkeley, Computer Science Division, California, USA, November 6–17.

95. Z. Shi, Tsinghua University, Department of Mathematical Sciences, Beijing, China, June 18–24.

96. J. Sieber, University of Exeter, College of Engineering, Mathematics and Physical Sciences, Exeter, UK, October 15–19.

97. M. Staudigl, Maastricht University, School of Business and Economics (SBE), Netherlands, December 10–13.

98. E. Stepanov, Russian Academy of Sciences, Steklov Institute, St. Petersburg, Russian Federation, October 22–26.

99. Y. Sun, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, October 18, 2017 – September 30, 2018.

100. ———, October 1, 2018 – September 30, 2019.

101. A. Suvorikova, Universität Potsdam, Institut für Mathematik, Potsdam OT Golm, September 1, 2018 – August 31, 2019.

102. R.F. Tempone, King Abdullah University of Science and Technology, Department of Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, May 7–11.

103. ———, November 5–8.

104. J. ten Thije Boonkkamp, Eindhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, November 25–30.

105. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, October 22–25.

106. D. Turaev, Imperial College London, Department of Mathematics, UK, July 8–15.

107. M. Willatzen, Technical University of Denmark, Department of Photonics Engineering, Kgs. Lyngby, Denmark, June 27–30.

108. S. Wolfers, King Abdullah University of Science and Technology, Department of Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, May 7–11.

109. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, May 20–24.

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. M. Akbas, Duzce University, Department of Mathematics, Turkey, DAAD scholarship of the programme “Research Grants – One-Year Grants”, January 17 – September 30.
3. G. Botirov, National University of Uzbekistan, Institute of Mathematics, Tashkent, Ukraine, DAAD Fellowship, February 1–28.
4. A. Fiebach, Berlin, EXIST Business Start-up Grant, Federal Ministry for Economic Affairs and Energy, June 1, 2017 – April 30, 2018.
5. K. Gärtner, Berlin, EXIST Business Start-up Grant, Federal Ministry for Economic Affairs and Energy, May 1, 2017 – April 30, 2018.
6. A. Jha, New Delhi, India, Berlin Mathematical School, October 1, 2017 – December 31, 2018.
7. L. Kamenski, Berlin, EXIST Business Start-up Grant, Federal Ministry for Economic Affairs and Energy, May 1, 2017 – April 30, 2018.
8. Ch. Kwofie, University of Energy and Natural Ressources, Ghana, DAAD Fellowship, February 1, 2018 – June 30, 2021.
9. J. Neumann, Berlin, EXIST Business Start-up Grant, September 1, 2018 – August 31, 2019.
10. Ch. Onyi, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School, October 1, 2017 – December 31, 2018.
11. A. Stephan, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School, January 1 – September 30.
12. H. Sun, Renmin University of China, Institute for Mathematical Sciences, Peking, China, Humboldt Research Fellowship, February 1, 2017 – January 31, 2018.
13. P. Vagner, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, Erasmus+ Traineeship, February 1, 2017 – February 28, 2018.
14. A. Visram, Berlin, EXIST Business Start-up Grant, September 1, 2018 – August 31, 2019.
15. A. Wilmes, Berlin, EXIST Business Start-up Grant, September 1, 2018 – August 31, 2019.

A.11.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. L. Adamyan, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, International Research Training Group 1792 "High Dimensional Non Stationary Time Series Analysis", doctoral candidate, January 1 – December 31.
2. P. Das, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. D. Hömberg, doctoral candidate, January 1 – December 31.
3. T. González Grandón, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. R. Henrion, doctoral candidate, January 1, 2016 – January 30, 2019.
4. J. Holley, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. M. Hintermüller, Robert Bosch GmbH, doctoral candidate, January 1 – December 31.
5. A. Jha, Freie Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. V. John, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
6. 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.
7. Ch. Onyi, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, Berlin Mathematical School, doctoral candidate, January 1 – December 31.
8. A. Stephan, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, Institut für Mathematik, supervisor: Prof. Dr. A. Mielke, Berlin Mathematical School, doctoral candidate, January 1 – September 30.
9. Y. Sun, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, Berlin Mathematical School, doctoral candidate, January 1 – December 31.

A.12 Guest Talks

1. A. AGAZZI, Duke University, Mathematics Department, North Carolina, USA, *Large deviations and recurrence for chemical reaction networks*, October 25.
2. M. AKBAS, Duzce University, Department of Mathematics, Turkey, *The analogue of grad-div stabilization in DG methods for incompressible flows: Limiting behavior and extension to tensor-product meshes*, September 13.
3. I. BAČIĆ, University of Belgrade, Institute of Physics Belgrade, Scientific Computing Laboratory, Serbia, *Stochastic dynamics in systems of adaptively coupled active rotators*, June 11.
4. N. BALDIN, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, Cambridge, UK, *Optimal link prediction with matrix logistic regression*, April 25.
5. L. BANZ, Universität Salzburg, Fachbereich Mathematik, Austria, *A posteriori error estimates for hp-dual mixed finite elements by implicit reconstruction*, May 16.
6. S. BARTELS, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, *Finite element methods for nonsmooth problems and application to a problem in optimal insulation*, January 19.
7. S. BECHTEL, Technische Universität Darmstadt, Fachbereich Mathematik, *Quantitative estimates for parabolic operators in $L^q(]0,T[;X)$*, February 28.
8. N. BERGLUND, Université d'Orléans, Institut Denis Poisson, France, *Metastable dynamics of Allen–Cahn SPDEs on the torus*, July 9.
9. L. BERLYAND, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, *Free boundary PDE models of active gels*, June 27.
10. F. BESOLD, Berlin, *Adaptive clustering using kernel density estimators*, September 11.
11. C. BETKEN, Universität Osnabrück, Fachbereich Mathematik/Informatik, *Dynamic random graphs: Sedentary random waypoint and preferential attachment models*, December 19.
12. TH. BOCKLITZ, Leibniz-Institut für Photonische Technologien, Spektroskopie/Bildgebung, Jena, *Machine learning of molecular sensitive spectral and image data*, November 16.
13. M. CARO, Aalto University, Department of Applied Physics, Finland, *Growth of amorphous carbon simulated with a machine-learning based interatomic potential*, June 29.
14. P. COLLI, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, *A Cahn–Hilliard system with convection and dynamic boundary conditions: Well-posedness and optimal velocity control*, May 23.
15. ———, *Shape memory alloys, phase-field models, Cahn–Hilliard systems*, October 24.
16. F. DASSI, Politecnico di Milano, Laboratory for Modeling and Scientific Computing MOX, Italy, *Recent advancements of the Virtual Element Method in 3D*, March 1.
17. P. DEURING, Université du Littoral "Côte d'Opale", Centre Universitaire de la Mi-Voix, Calais, France, *Stabilitäts- und Fehlerschranken einer FE-FV-Diskretisierung von Konvektions-Diffusionsgleichung: Exponentielle Abhängigkeit von Parametern*, April 18.
18. O. D'HUYS, Aston University, Engineering and Applied Science, Birmingham, UK, *Dynamics of delay-coupled networks with time-varying connections*, March 6.
19. K. DOKU-AMPONSAH, University of Ghana, Department of Statistics and Actuarial Science, Legon-Accra, Ghana, *Joint large deviation result for empirical measures of the random geometric graphs*, December 12.
20. A. DREWITZ, Universität zu Köln, Mathematisches Institut, Köln, *Phase transitions in some percolation models with long-range correlations on general graphs*, July 26.

21. M. Egert, Université Paris-Sud, Laboratoire de Mathématiques, Orsay, France, *How half-order time derivatives help us to better understand parabolic equations*, February 28.
22. M. Evans, Technische Universität Berlin, Institut für Mathematik, *Surfaces and tangling*, June 14.
23. L. Feierabend, Zentrum für BrennstoffzellenTechnik (ZBT), Abteilung Mikrosysteme und Strömungsmechanik, *Model development for flowing slurry electrodes in zinc-air batteries*, May 3.
24. M.C. Ferris, University of Wisconsin-Madison, Computer Sciences Department and Wisconsin Institute for Discovery, Madison, USA, *Modelling 100 percent renewable electricity*, June 20.
25. A. Gasnikov, Moscow Institute of Physics and Technology, Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, *Recent developments of accelerated gradient descent, part I*, January 16.
26. ———, *Recent developments of accelerated gradient descent, part II*, February 1.
27. ———, *Unified view on accelerated methods for structural convex optimization problems*, October 16.
28. C. Geiersbach, Universität Wien, Institut für Statistik und Operations Research, Austria, *A projected stochastic gradient algorithm for optimization with random elliptic PDE constraints*, May 17.
29. J. Giesselmann, RWTH Aachen, Center for Computational Engineering Science, *Modelling error estimates and model adaptation in compressible flows*, January 23.
30. A.C. Goessmann, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, *Representing crystals for kernel-based learning of their properties*, November 13.
31. L. Goubergrits, Charité – Universitätsmedizin Berlin, Labor für Biofluidmechanik, *Modelling and simulation for treatment planning: CFD methods for valve treatment*, June 20.
32. E.J. Hall, Rheinisch-Westfälische Technische Hochschule Aachen, Fachgruppe Mathematik, Aachen, *Causality and Bayesian network PDE for multiscale representations of porous media*, November 13.
33. G. Hu, Beijing Computational Science Research Center, China, *Outgoing radiation conditions for the Helmholtz equation in inhomogeneous periodic media*, June 19.
34. O. Huber, Philipps-Universität Marburg, Fakultät für Mathematik und Computerwissenschaften, *Solving optimisation problems with optimal value function via reformulations*, November 24.
35. O. Huber, Humboldt-Universität zu Berlin, Institut für Mathematik, *Using reformulations in nonsmooth mathematical programming: The examples of friction contact problems and optimal value functions*, December 19.
36. T. Iliescu, Virginia Polytechnic Institute and State University, Department of Mathematics, Blacksburg, USA, *Physically-constrained data-driven correction for reduced order modeling of fluid flows*, June 26.
37. K. Ito, North Carolina State University, Department of Mathematics, Raleigh, USA, *Semismooth Newton method for variational inequalities and MPEC*, September 10.
38. A. Jüngel, Technical University of Vienna, Institute for Analysis and Scientific Computing, Research Group Partial Differential Equations and Dynamical Systems, Austria, *Cross-diffusion systems with entropy structure*, May 9.
39. Y. Klochkov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, *On uniform Hanson–Wright type inequalities for sub-Gaussian entries*, November 27.
40. T. Kluth, Universität Bremen, Center for Industrial Mathematics, *Model-based magnetic particle imaging*, January 11.
41. D. Knees, Universität Kassel, Institut für Mathematik, *Rate-independent processes with time-discontinuous data*, June 11.

42. S. Ko, Oxford University, Mathematical Institute, UK, *Analysis and approximation of incompressible chemically reacting non-Newtonian fluids*, June 6.
43. A. Kruger, Federation University Australia, School of Science, Engineering and Information Technology, Centre for Informatics and Applied Optimization (CIAO), Ballarat, Australia, *Extremal principle revisited*, September 18.
44. Ch. Kuhn, Technische Universität Kaiserslautern, Fachbereich Maschinenbau und Verfahrenstechnik, *Phase field modelling of fracture – from a mechanics point of view*, October 16.
45. U. Leonhardt, Weizmann Institute of Science, Department of Physics of Complex Systems, Rehovot, Israel, *Fiber-optical analogue of Hawking radiation*, May 17.
46. M. Löffler, University of Cambridge, Centre for Mathematical Sciences, UK, *Spectral thresholding for Markov chain transition operators*, December 5.
47. G. Lube, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *Why exactly divergence-free H(div)-conforming FEM for transient incompressible flows?*, January 11.
48. J. Machalová, Palacky University Olomouc, Department of Mathematical Analysis and Applications of Mathematics, Czech Republic, *Contact problem solution for nonlinear beam and foundation by CVM*, December 11.
49. J. Mankau, Technische Universität Dresden, Institut für Mathematik, *A descent step algorithm based on generalized gradients on sets*, July 4.
50. A. Marciniak-Czochra, Universität Heidelberg, Institut für Angewandte Mathematik, *Post-Turing tissue pattern formation: Insights from mathematical modelling*, November 12.
51. E. Meca, University of Cordoba, Agronomy Department, Spain, *Localized instabilities in phase-changing systems: The effect of elasticity*, March 27.
52. H. Meinlschmidt, Johann-Radon-Institute for Computational and Applied Mathematics, Optimization and Optimal Control, Linz, Austria, *Maximal regularity in optimal control for quasilinear parabolic evolution equations*, November 14.
53. E. Meneses Rioseco, Leibniz-Institut für Angewandte Geophysik, Geothermik & Informationssysteme, Hanover, *Modeling, simulation and optimization of geothermal reservoir – THMC (thermo-hydraulical, mechanical, chemical) processes involved*, July 11.
54. V. Miloš, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, *Thermodynamics and electrochemical impedance spectroscopy – 1D model of YSZ electrolyte and triple phase boundary interface*, September 13.
55. M.T. Nair, Indian Institute of Technology Madras, Department of Mathematics, Chennai, India, *An inverse problem in parabolic PDEs*, September 18.
56. A. Naumov, National Research University Higher School of Economics, International Laboratory of Stochastic Algorithms and High-Dimensional Inference, Moscow, Russian Federation, *Gaussian approximations for maxima of large number of quadratic forms of high-dimensional random vectors*, October 23.
57. M.J. Neilan, University of Pittsburgh, Department of Mathematics, USA, *Inf-sup stable Stokes pairs on barycentric refinements producing divergence-free approximations*, April 12.
58. O. Öktem, KTH Royal Institute of Technology, Department of Mathematics, Stockholm, Sweden, *Recent advances in using machine learning for image reconstruction*, April 10.
59. G. Panasenko, University of Lyon, Mathematical Mechanics and Inverse Problems, France, *Asymptotic analysis of wave propagation in a laminated beam with contrasting stiffness of the layers*, May 29.
60. M. Peters, Eidgenössische Technische Hochschule Zürich, Department of Biosystems Science and Engineering (D BSSE), Basel, Switzerland, *Uncertainty quantification for elliptic PDEs*, June 12.

61. N. Petrelis, Université de Nantes, Laboratoire Jean Leray, UFR Sciences et Techniques, Nantes, France, *Scaling limit of the Interacting partially directed self-avoiding walk at criticality*, May 17.

62. J. Pfefferer, TU München, Zentrum Mathematik, Garching, *hp-finite elements for fractional diffusion*, June 18.

63. S. Popov, University of Campinas — UNICAMP, Institute of Mathematics, Statistics and Scientific Computation, Campinas, Brazil, *Two-dimensional random interlacements, conditional SRW, and the cryptocurrencies*, December 5.

64. S. Praetorius, Technische Universität Dresden, Fakultät für Mathematik, Institut für Wissenschaftliches Rechnen, *From individual motion to collective cell migration*, May 8.

65. A. Rasheed, Lahore University of Management Sciences, Department of Mathematics, Pakistan, *Influence of magnetic field on dendrites during solidification of binary mixtures*, January 11.

66. J.F. Rodrigues, University of Lisbon, Department of Mathematics, Portugal, *Evolutionary quasi-variational and variational inequalities with constraints on the derivatives*, May 30.

67. F.J. Romero Hinrichsen, ETH Zurich, Department of Mathematics, Switzerland, *Dynamical super-resolution with applications to ultrafast ultrasound*, May 28.

68. Th. Ruf, Universität Augsburg, *On a variational approach to the nonlinear wave equation*, February 2.

69. F. Schäfer, California Institute of Technology, Department of Computing and Mathematical Sciences, Pasadena, California, USA, *Compression, inversion, and approximate PCA of dense kernel matrices at near-linear computational complexity*, May 30.

70. M. Schienle, Karlsruher Institut für Technologie, Lehrstuhl für Ökonometrie, *Determination of vector error correction models for different types of high-dimensionality*, November 28.

71. A. Schlüter, Technische Universität Kaiserslautern, Fachbereich Maschinenbau und Verfahrenstechnik, *Phase field modelling of fracture – from a mechanics point of view*, October 16.

72. L. Shen, University of the Chinese Academy of Sciences, School of Mathematical Sciences, Beijing, China, *Implicitizing rational tensor product surfaces using the resultant of three moving planes*, June 14.

73. J. Shewchuk, University of California at Berkeley, Computer Science Division, California, USA, *Higher-quality tetrahedral mesh generation for domains with small angles by constrained Delaunay refinement*, November 15.

74. Z. Shi, Tsinghua University, Department of Mathematical Sciences, Beijing, China, *Low dimensional manifold model for image processing*, June 20.

75. A.L. Shilnikov, Georgia State University, Neuroscience Institute, Department of Mathematics & Statistics, Atlanta, USA, *Torus bifurcations in slow fast systems*, January 11.

76. E. Sinibaldi, Italian Institute of Technology, Center for Micro-BioRobotics, Pontedera, Italy, *Selected modeling approaches for biomedical applications and biorobotics tools*, February 1.

77. J. Starke, Universität Rostock, Institut für Mathematik, Rostock, *Multiscale analysis of collective behavior in particle systems*, June 5.

78. E. Stepanov, Russian Academy of Sciences, Steklov Institute, St. Petersburg, Russian Federation, *Hybrid control in a model from molecular biology: Between continuous and discrete*, October 24.

79. W. Sun, Technische Universität Berlin, Institut für Mathematik, *On the asymptotic distribution of nucleation times of polymerization processes*, November 21.

80. Y. Sun, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, *Complete graph based online change point detection*, December 4.

81. R.F. Tempone, King Abdullah University of Science and Technology, Department of Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, *Multilevel and Multi-index Monte Carlo methods for the McKean–Vlasov equation*, November 6.

82. J. ten Thije Boonkkamp, Eindhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, *Flux vector approximation schemes for systems of conservation laws*, November 29.

83. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, Romania, *Optimal control methods in shape optimization*, October 23.

84. ———, *Implicit parametrizations and applications in optimization and control*, October 24.

85. M. Timme, Technische Universität Dresden, Center for Advancing Electronics Dresden, *Network dynamics as an inverse problem*, May 8.

86. A. Tóbiás, Technische Universität Berlin, Institut für Mathematik, *Signal to interference ratio percolation for Cox point processes*, November 7.

87. D. Turaev, Imperial College London, Department of Mathematics, UK, *On positive metric entropy conjecture*, July 12.

88. M. Varga, Technische Universität Dresden, Institut für Mathematik, *Stochastic unfolding and homogenization*, April 18.

89. D. Walter, Technische Universität München, Zentrum Mathematik, Garching bei München, *Sparse sensor placement for inverse problems: From finite to infinite dimensional parameters*, June 5.

90. S. Waters, University of Oxford, Mathematical Institute, UK, *Fluid dynamical models for tissue engineering*, April 23.

91. K. Welker, Universität Trier, Fachbereich IV – Mathematik, *Constrained shape optimization problems in shape spaces*, June 13.

92. M. Willatzen, Technical University of Denmark, Department of Photonics Engineering, Kgs. Lyngby, Denmark, *Strain and symmetry effects in Bi_2Se_3 thin films using the* $\mathbf{k} \cdot \mathbf{p}$ *method*, June 29.

93. B. Witzigmann, Universität Kassel, Computational Electronics and Photonics Group, *Carrier injection efficiency and impurity modeling in III-nitride LEDs*, September 3.

94. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Inverse problems of determining moving sources in diffusion equations*, May 22.

95. A. Yochelis, Ben-Gurion University of the Negev, The Jacob Blaustein Institutes for Desert Research (BIDR), Beer-Sheva, Israel, *From solvent free to dilute electrolytes: A unified continuum approach*, October 16.

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 **A**daptive **W**eights **C**lustering. 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 **A**daptive **W**eights **S**moothing 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).

More information: https://www.wias-berlin.de/software/aws/

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/

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 semiconductor 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: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@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.

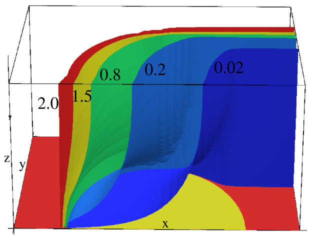
Please find more information under http://cmg.cds.iisc.ac.in/parmoon/.

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. G. Matthies (TU Dresden).

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



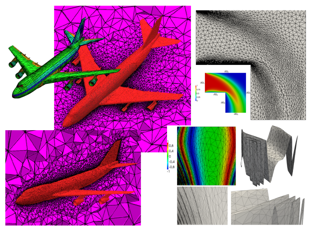
Concentration isosurfaces in a thin-layer flow cell (`pdelib`)

`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/.

TetGen (contact: H. Si, phone: +49 30/20372-446, e-mail: hang.si@wias-berlin.de)



Adapted tetrahedral meshes and anisotropic meshes for numerical methods and scientific computation

`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).