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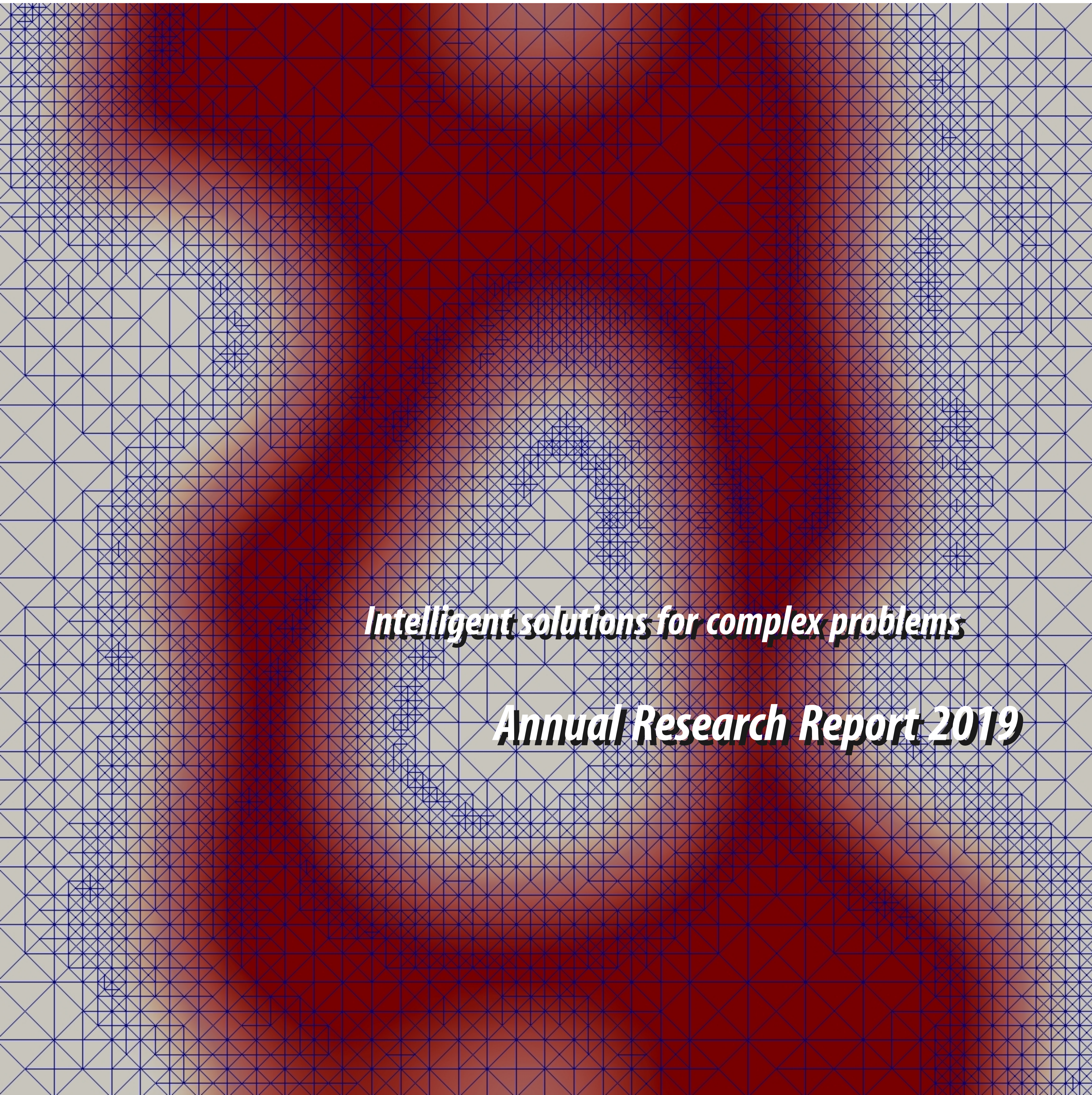
Weierstrass Institute for Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2019

Cover figure: Zoom-in view on the phase-field for representing a two-phase fluid at a time instance during an optimal control process. *Red* respectively *grey* represent pure fluid phases while the *light red* transition layer belongs to a mixed fluid state. Along with the phase-field quantity, the associated dynamically adapted finite element mesh (blue lines) for numerical computations is shown.

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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 2019. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2019. Following five 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

In January 2019, 15 research projects with WIAS PIs started under the umbrella of the Berlin Cluster of Excellence MATH+, and first very promising results were already presented during the first MATH+ Day in mid December. WIAS is proud to be among the five cooperation partners of MATH+, with its Director, Prof. Michael Hintermüller one of its three spokespersons. In addition, two DFG Priority Programs which will be coordinated by members of our Institute got successfully evaluated, SPP 2265 *Random Geometric Systems* coordinated by Prof. Wolfgang König and SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* (prolongation), by Prof. Michael Hintermüller. These facts and many more projects within other priority programs, collaborative research centers, the BMBF, and other funding organizations clearly demonstrate our Institute's central position in Applied Mathematics in Germany and beyond.

For the winter semester 2020/2021, WIAS colleagues and others were granted a Thematic Einstein Semester on *Energy-based Mathematical Methods for Reactive Multiphase Flows* by the Einstein Foundation Berlin in the framework of MATH+.

It is also one of the strengths of our Institute to shape next generation researchers and leading figures in mathematics. Not only have several early career WIAS members successfully applied for DFG / MATH+ grants, but WIAS is also proud to host one of the new Leibniz Junior Research Groups which succeeded in the always tough annual Leibniz internal excellence competition. The new Leibniz Group LG 5 *Numerical Methods for Innovative Semiconductor Devices*, started, headed by Dr. Patricio Farrell, in January 2020 as an independent temporary research unit on the Flexible Research Platform of WIAS. Additionally, the WIAS internal Young Scientist Grants Program and the WIAS Female Master's Students Program were initiated in 2019.

Our Institute ran an impressive number of high-calibre workshops at WIAS. I think it is fair to say that ICCOPT, the International Conference on Continuous Optimization 2019, was our main conference event with about 840 scientific contributions and 1000 participants. All of these events have received extraordinarily positive feedback from the international community. This is a very important contribution to the international outreach of our Institute. In addition to the workshops in Berlin, WIAS members (co-)organized numerous scientific meetings throughout the world.

Besides the large number of invited lectures held by WIAS members at international meetings and research institutions, and the many renowned visitors from abroad hosted by the institute, last year's positive development is again best reflected by the acquisition of grants: altogether, 41 additional co-workers (+ 8 outside WIAS; Dec. 31, 2019) were financed from third-party funds.

Led by WIAS, the MaRDI – Mathematical Research Data Initiative – group for establishing a mathematics consortium within NFDI, the BMBF's National Research Data Initiative, has been another major project which has kept us busy throughout the entire year. The project was very well presented in mid December in front of an international review panel in Bonn. The final result will be published in June 2020.

Since January 2011, the Secretariat of the International Mathematical Union (IMU) has been permanently based at WIAS. The Secretariat's staff, headed by the WIAS Authorized Representative and IMU Treasurer Prof. Alexander Mielke, has served mathematics and mathematicians all over the world ever since.

Our "Work and Family" team led our Institute through another very successful re-audit in the *audit berufundfamilie*. With this certificate, we document our commitment to a sustainable family- and life-phase-conscious personnel policy, which is also a major contribution for making our Institute a highly attractive workplace.

Like the previous years, 2019 has proven to be a busy and fruitful year for the institute with 106 preprints in the WIAS Preprints Series, 122 articles in refereed journals, two monographs, and 3.6 million euros provided by grants. For further information please refer to the facts-and-figures part of this report.

In the WIAS-coordinated Leibniz Network "Mathematical Modeling and Simulation" (MMS), 34 institutes from all sections of the Leibniz Association work together. On March 20 to 22, 2019, the 4th Leibniz MMS Days took place in Kühlungsborn, supported by the member Leibniz Institute of Atmospheric Physics IAP. Also the Leibniz MMS Summer School in October 2019 on „Modern Programming Languages for Science and Statistics: R and Julia" at the Mathematical Research Institute at Oberwolfach was a big success.

Of course, our Institute continued also in 2019 its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. We cooperate in MATH+ and in many other projects. Six leading members of WIAS, including the director and his deputies, held WIAS-funded special chairs at the Berlin universities. And there was again a manifold of teaching activities of our members.

Finally, let me – like in every year – 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. This concept, in combination with hard, continuing work on scientific details, eventually leads to success.

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

Berlin, in March 2020

M. Hintermüller

P.S. Please find our new image film "Mathematics is everywhere" under
`https://www.wias-berlin.de/transfer/movies/WIAS_MASTER_EN_EN.mp4`.

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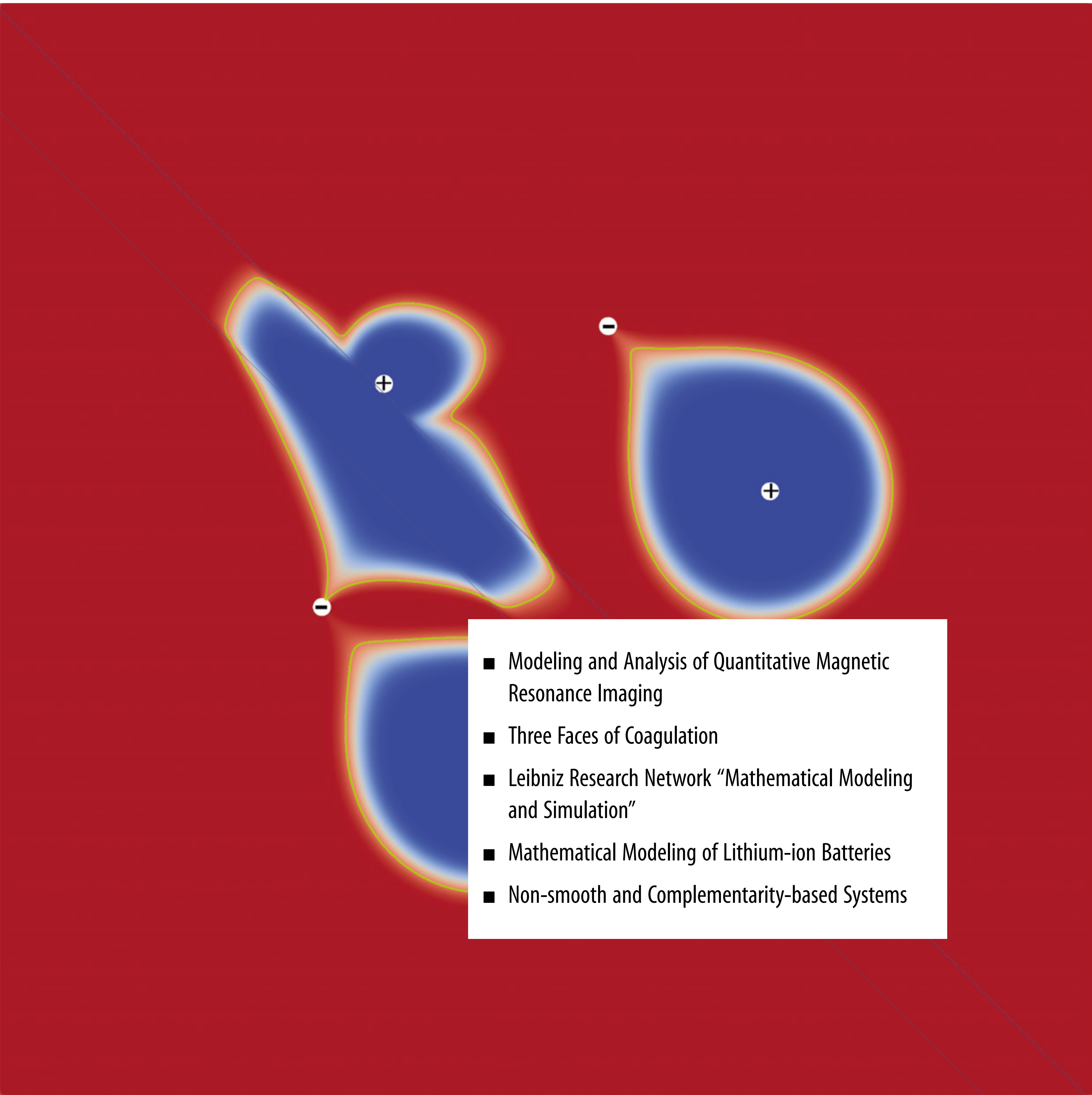
1 Scientific Highlights



- Modeling and Analysis of Quantitative Magnetic Resonance Imaging
- Three Faces of Coagulation
- Leibniz Research Network “Mathematical Modeling and Simulation”
- Mathematical Modeling of Lithium-ion Batteries
- Non-smooth and Complementarity-based Systems

1.1 Modeling and Analysis of Quantitative Magnetic Resonance Imaging

Kostas Papafitsoros and Karsten Tabelow

In the Annual Research Report 2014 of the Weierstrass Institute we reported on the role of adaptive methods for noise characterization and noise reduction for enabling in-vivo histology using magnetic resonance imaging (MRI), see Figure 1.

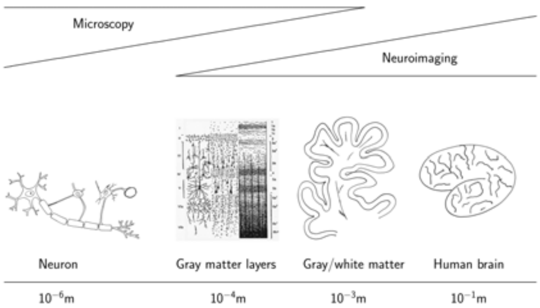


Fig. 1: *Bridging the gap between ex-vivo histology-based microscopy images and in-vivo neuroimaging. It is expected that this requires quantitative imaging methods in connection with biophysical models (model-based imaging), cf. the Annual Research Report 2014.*

The methods were dedicated to diffusion MRI, an imaging modality inferring on the directionally dependent diffusion constant of water within the tissue. The technique allows for examining structural properties of the tissue because diffusion is basically free in the direction of elongated structures and typically hindered perpendicular to this direction. The corresponding anisotropy can, e.g., be described by a scalar quantity: the fractional anisotropy (FA). Since diffusion MRI for a given diffusion direction measures the diffusion constant, it is a *quantitative* method. In recent years, a number of other quantitative MRI methods that aim to determine local physical quantities instead of weighted images in arbitrary units optimized for tissue contrast have emerged; see Figure 2.

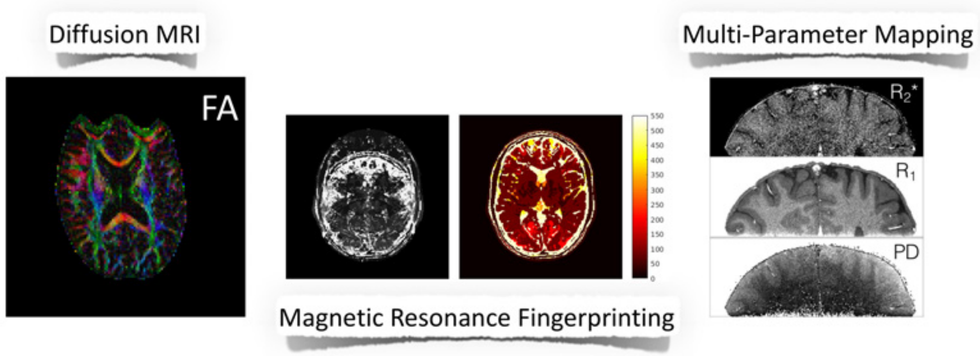


Fig. 2: *Different quantitative magnetic resonance imaging (qMRI) methods aim to infer on characteristics related to physical characteristics instead of weighted images in arbitrary units optimized for tissue contrast*

Among them is multi-parameter mapping (MPM), which uses a special multi-echo sequence to determine relaxation rates R_1, R_2^* of the spin excitation, and the proton density PD, respectively. Another one is magnetic resonance fingerprinting (MRF), which acquires sequences of low-quality

MR images and uses dictionary learning to reconstruct high-resolution quantitative maps of $T_1 = 1/R_1$, $T_2 = 1/R_2^\star$, and other parameters.

Improved methods for quantitative MRI

Here, we report on two contributions to the modeling and analysis of quantitative MRI data: a new adaptive noise reduction method applied to data from MPM sequences, and an integrated physics-based approach inspired from the recently introduced MRF method.

Patch-wise structural adaptive smoothing (PAWS) for multi-parameter mapping. An MPM sequence acquires multi-echo data with different weightings (defined by acquisition parameters and denoted by T_1w, PDw, and MTw) in order to infer on quantitative parameters such as the relaxation rates R_1, $R_2^\star$, the proton density PD, and the magnetization transfer MT. In the so-called *ESTATICS model* (Weiskopf et al., Front Neurosci. 8 (2014), pp. 278, doi: 10.3389/fnins.2014.00278), the signal S, which depends on the echo time TE, is described by using indicator functions I for the different weightings by four parameters

$$S = (S_{T1} \cdot I_{T1w} + S_{PD} \cdot I_{PDw} + S_{MT} \cdot I_{MTw}) \cdot e^{-R_2^\star \cdot TE}, \tag{1}$$

from which the quantitative maps can be calculated.

In order to introduce the patch-wise structural adaptive smoothing algorithm, let us assume that data $Y_i \in \mathcal{Y}$ is observed at positions $x_i = (x_{i_1}, \dots, x_{i_d})$ in a bounded subset $\mathcal{X}$ of a rectangular grid in a d-dimensional metric space ($d = 3$ for MPM data). Let $\mathcal{X}_G$ denote the set of grid points in $\mathcal{X}$. We assume Y_i to be distributed as $Y_i \sim P_{\theta_i}$, where P_{θ_i}, with density $p(y, \theta_i)$, depends on some local parameter θ_i (typically from $\mathbb{R}^p$) and is a probability distribution with support in $\mathcal{Y}$ from some parametric (typically exponential) family $P_{\theta_i} \in \mathcal{P}_\Theta$.

The smoothing algorithm relies on a structural assumption which is formulated such that there exists a partitioning $\mathcal{X} = \bigcup_{n=1,\dots,N} \mathcal{X}_n$ into N subsets with $\mathcal{X}_n \cap \mathcal{X}_l = \emptyset$ if $n \neq l$, and $\theta_i \equiv \theta_j$ if $x_i \in \mathcal{X}_n$ and $x_j \in \mathcal{X}_n$ for some n. Literally speaking, we assume that within any subset $\mathcal{X}_n$, the parameter θ as a function of x is constant.

The method employs both a distance $\delta(x_i, x_j)$ in design space, e.g., the Euclidean distance for $\mathcal{X} \subset \mathbb{R}^d$

$$\delta(x_i, x_j) = ||x_i - x_j||_2,$$

as well as a distance $\eta(\theta_i, \theta_j)$ in parameter space

$$\eta(\theta_i, \theta_j) = \mathcal{KL}(P_{\theta_i}, P_{\theta_j}) = \int_{\mathcal{Y}} p(y, \theta_i) \log \frac{p(y, \theta_i)}{p(y, \theta_j)} dy,$$

e.g., the Kullback–Leibler divergence between the probability distributions with parameters θ_i and θ_j at locations x_i and x_j, respectively. Henceforth, we abbreviate locations with indices i and j.

Adaptive weights smoothing uses an iterative scheme with a sequence of increasing bandwidths $h^{(k)}$ for steps $k = 0, \dots, k^\star$ alternating the computation of weighted maximum likelihood (i.e., l) estimates

$$\hat{\theta}_i^{(k)} = \arg\max_\theta l(Y, W_i^{(k)}; \theta) = \arg\max_\theta \sum_{j \in \mathcal{X}_G} w_{ij}^{(k)} \log(p(Y_j, \theta))$$

and the determination of adaptive weighting schemes $W_i^{(k)} = \{w_{ij}^{(k)}, j \in \mathcal{X}_G\}$. Specifically, the weights $w_{ij}^{(k)}$ at iteration step k are given as the product of two terms: a kernel weight $K_{\text{loc}}(l_{ij}^{(k)})$ with $l_{ij}^{(k)} = \left(\delta(x_i, x_j)/h^{(k)}\right)^2$ and $K_{\text{stat}}(s_{ij}^{(k)})$ depending on $s_{ij}^{(k)} = N_i^{(k-1)} \cdot \eta(\hat{\theta}_i^{(k-1)}, \hat{\theta}_j^{(k-1)})/\lambda$ denoted as statistical penalty for two kernel functions K_{loc} and K_{stat}. The term $N_i^{(k-1)} = \sum_j w_{ij}^{(k-1)}$ serves as a proxy for the variance reduction achieved for $\hat{\theta}_i^{(k-1)}$. Note that the noise variance σ^2 typically enters the function η and needs to be known or has to be estimated.

Patch-wise adaptive smoothing generalizes this concept by using vectorized values in vicinities of the locations for comparison in design space instead of the data at locations i and j, only. In order to formalize the basic idea, we introduce a local patch, or vicinity, $V_i = \{v_l(i) | \, ||v_l(i) - i||_1 \leq s\}$ of a design point i; see Figure 3. It contains all $n_s = (2s+1)^d$ grid points $x_{v_l(i)}$ within a d-dimensional cube of side length $2s$. The index $l = 1, \ldots, n_s$ varies over the locations $v_l(i)$ in the patch V_i. We denote by Y_{V_i} the vectorized data $(Y_{v_1(i)}, \ldots, Y_{v_{n_s}(i)})$.

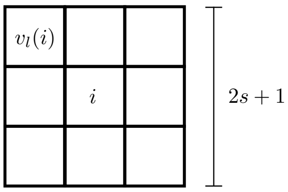


Fig. 3: *Schematic example of a patch V_i of size s of a location i. It contains all locations $v_l(i)$ with a maximum l_1-distance of s from i.*

The patch-wise adaptive weights smoothing (PAWS) procedure introduced in [1] employs a new form of the statistical penalty $s_{ij}^{(k)}$ based on patches V_i. The variability of the estimates $\hat{\theta}_i$ at iteration step k depends on the (local) weighting schemes $W_i^{(k)}$. This is taken into account in the definition of the statistical penalty $s_{ij}^{(k)}$ by the use of the sum of weights $N_i^{(k)}$. Depending on the unknown underlying structure $\mathcal{X}_n$, the variability of the estimates $\hat{\theta}_{v_l(i)}$ may vary considerably over grid points $v_l(i) \in V_i$. Thus, when we extend the definition $s_{ij}^{(k)}$ to comparisons between patches, it should consider the accuracy of the parameter estimates reflected by $N_{v_l(i)}$ as achieved in former iteration steps. We define a suitable statistical penalty for PAWS by

$$\tilde{s}_{ij}^{(k)} = \max_{l=1,\ldots,n_s} s_{v_l(i)\, v_l(j)}^{(k)}.$$

Taking the maximum over all locations $l = 1, \ldots, n_s$ in the patch enables to balance spatial differences in the variance of the estimates.

The method can then be applied to the parameter estimates

$$\vec{S}^{(0)} = \left(\hat{S}_{T1}^{(0)}, \hat{S}_{PD}^{(0)}, \hat{S}_{MT}^{(0)}, \hat{R}_2^{\star(0)}\right)^\top$$

from the ESTATICS model for MPM data. Additionally, voxelwise estimates $\hat{\Sigma}$ for the covariance matrix of the parameter estimates are available. Specifically, for each iteration step $k = 1, \ldots, k^\star$ we define as usual adaptive weights $w_{ij}^{(k)}$ for all pairwise voxel locations i and j with the statistical penalty

$$s_{ij}^{(k)} = N_i^{(k-1)} \cdot \left(\vec{S}_i^{(k-1)} - \vec{S}_j^{(k-1)}\right)^\top \hat{\Sigma}_i^{-1} \left(\vec{S}_i^{(k-1)} - \vec{S}_j^{(k-1)}\right) \tag{2}$$

based on the estimates $\vec{S}_i^{(k-1)}$ and $\vec{S}_j^{(k-1)}$ and the sum of weights $N_i^{(k-1)} = \sum_j w_{ij}^{(k-1)}$ from the previous step. For $k = 1$ use $N_i^{(0)} \equiv 1$. We finally calculate new estimates $\vec{S}^{(k)}$

$$\vec{S}_i^{(k)} = \sum_j w_{ij}^{(k)} \vec{S}^{(0)} / \sum_j w_{ij}^{(k)} \tag{3}$$

and stop the iteration at $k = k^\star$ to obtain the final smoothed maps $\vec{S}^{(k^\star)}$. From those (implicitly) smoothed R_1, PD, and MT-maps can be calculated; see Figure 4.

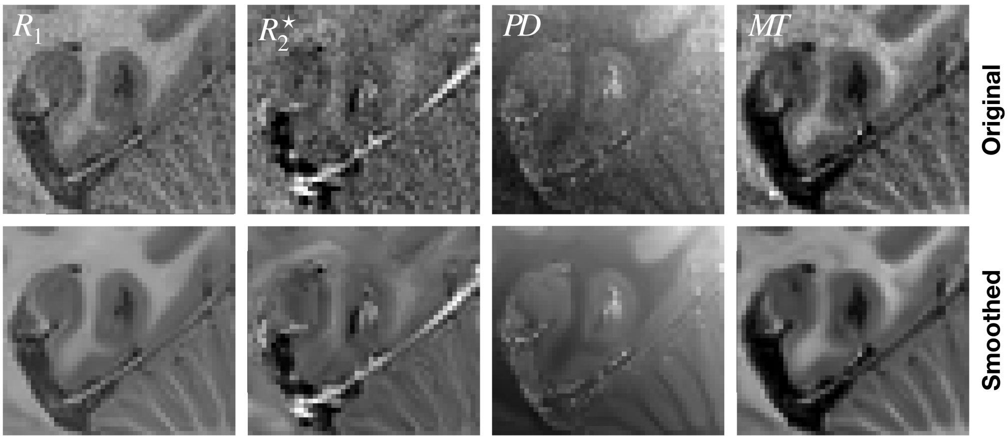


Fig. 4: *Comparison of un-smoothed and smoothed quantitative maps. The patch-wise adaptive smoothing. The procedure is able to reduce the noise in the maps without blurring fine anatomical structures.*

Magnetic resonance fingerprinting and integrated physics-based models. In 2013, a promising new technique for quantitative MRI to infer on $T_1 = 1/R_1$ or $T_2 = 1/R_2$, named *magnetic resonance fingerprinting*, was introduced and gained considerable attention [2]. In that method, a database (dictionary) consisting of all trajectories (fingerprints) of the evolution of the magnetization m of the bulk nuclear spins is built in an offline phase. Each fingerprint is obtained by solving the Bloch equations

$$\frac{\partial m}{\partial t}(t) = m(t) \times \gamma B(t) - \left(\frac{m_x(t)}{T_2}, \frac{m_y(t)}{T_2}, \frac{m_z(t) - m_{eq}}{T_1} \right) \tag{4}$$

for some preselected combination of parameter values, typically those of relaxation times $T_1 = 1/R_1$, $T_2 = 1/R_2$, but also others such as, e.g., the off-resonance frequency. The external magnetic field B that is used to compute the solutions of (4) is exactly the one that corresponds to the excitation scheme of a given MRI experiment (radio pulses, excitation flip angles, repetition, and echo times). During the MRI experiment, a sequence of L magnetization images are reconstructed, corresponding to L read-out times. These reconstructions rely on the pseudoinverse of the Fourier transform. As a result, they suffer from severe artifacts. However, the evolution of the magnetization of a specific voxel along the series of the L reconstructed magnetization images can be assumed to correspond (approximately) to the solution of Bloch equations with parameters that correspond to this specific voxel. Hence, the second step of MRF matches the recorded trajectory of each voxel to a fingerprint in the precomputed dictionary, typically, through minimizing a least-squares distance. In this way, the parameter values that correspond to the “best” fingerprint are then assigned to that very voxel.

Another approach [3] was introduced by the research group RG 8 *Nonsmooth Variational Problems*

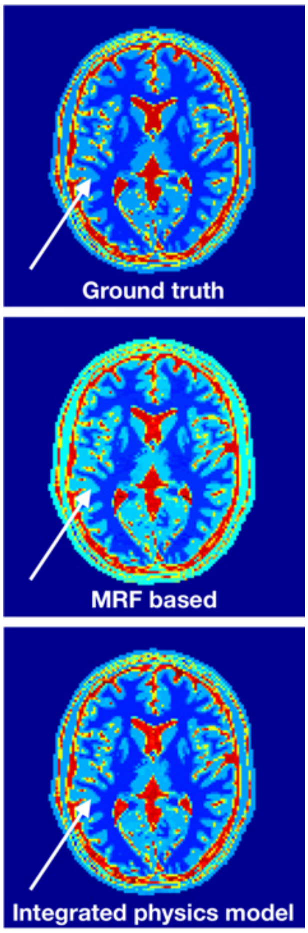


Fig. 5: *Improved reconstruction of the T_1 map using the integrated physics-based model (5) – note how the T_1 value in the brain grey matter better fits the ground truth compared to MRF*

and Operator Equations within the recently completed CH12 project on "Advanced magnetic resonance imaging: Fingerprinting and geometric quantification" in the Einstein Center for Mathematics Berlin ECMath. Instead of the two-step procedure described above (i.e., reconstruction of the magnetization and matching to the dictionary), a single-step, dictionary-free model for estimating the T_1, T_2 values has been analyzed and implemented. The proposed model relies on a single nonlinear operator equation which, in compact form, reads

$$P\mathcal{F}(\rho T_{x,y} M(\theta)) = D. \tag{5}$$

Here, D denotes the detected signal, modeled as an element in $\left(L^2(K)^2\right)^L$, K being the Fourier space. The operator P is a subsampling operator of the Fourier transform $\mathcal{F}$. Furthermore, $M(\theta) \in \left(L^2(\Omega)^3\right)^L$ denotes the (pointwise) solution map of the Bloch equations (4) for $\theta = (T_1, T_2) \in (L^\infty(\Omega))^2$. Here, $\Omega \subset \mathbb{R}^2$ models a thin tissue slice that is to be imaged. This solution map can be approximated in a simple way at read-out times if specific flip angle sequence patterns are considered. For example, in the inversion recovery balanced steady-state free precession (IR-bSSFP) flip angle sequence (which was also considered in [3]), the magnetization M can be explicitly computed in a recursive way, as a function of θ.

In view of the subsampling and noisy data D^δ, in order to solve (5) robustly, one turns to a projected *Levenberg–Marquardt* (L-M) iterative method which, after denoting $\mathbf{x} := (\rho, \theta)$ and $Q(\mathbf{x}) := P\mathcal{F}(\rho T_{x,y} M(\theta))$, reads for $n = 0, 1, 2, \ldots$

$$\tilde{D}_n^\delta = D^\delta - Q(\mathbf{x}_n), \tag{6}$$

$$\mathbf{h}_n^\delta = \operatorname*{argmin}_{\mathbf{h}} \left\| Q'(\mathbf{x}_n)\mathbf{h} - \tilde{D}_n^\delta \right\|^2_{(L^2(K)^2)^L} + \lambda_2 \|\mathbf{h}\|^2_{(L^2(\Omega))^3}, \tag{7}$$

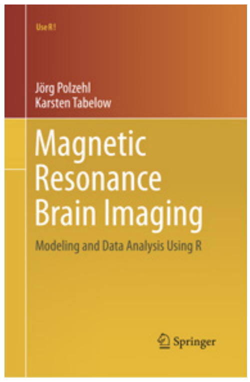
$$\mathbf{x}_{n+1} = P_{C_{ad}}(\mathbf{x}_n + \mathbf{h}_n^\delta). \tag{8}$$

Here, $P_{C_{ad}}$ denotes a projection to a feasible set C_{ad} (typically a bound-constrained set) that corresponds to the values for θ that are meaningful for the human tissue. In [3], Fréchet differentiability for the map Q was shown and a suitable initialization strategy was devised for θ, which is essential for the meaning and successful application of the L–M method (6)–(8). The method gives improved results for the quantification of T_1, T_2 parameters over MRF and its improved variants, e.g., the BLIP method in [4], see, for instance, Figure 5 where it leads to more accurate assignments of T_1 values (improved contrast and more accurate in grey and white matter areas) in a simulated brain slice image.

Informed learning approach for quantitative MRI. Extensions of the integrated physics-based approach described above are currently an active field of research at WIAS within the project EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization" in Emerging Field 3 (Model-based Imaging) of the Berlin Mathematics Research Center MATH+. The project aims to capture a more general MRI setting, in particular, excitation sequences for which an explicit solution map of the Bloch equations cannot be obtained but can nevertheless be learned by a neural network. More details can be found on page 93 of the present report.

In summary, the new methods for MPM or MRF developed at WIAS allow for the more accurate estimation of physical parameters, such as the relaxation times T_1 or $T_2^\star$ (T_2) in quantitative magnetic resonance imaging improving accuracy for neuroscientific studies.

New methods and Open Science



Methods such as the patch-wise structural adaptive smoothing described above are part of analysis pipelines for MRI data. A successful transfer of new methods into applications also requires the availability of implementations as in the WIAS Software collection for NeuroScience; see also page 180. Those reference implementations were done within R, a free software environment for statistical computing and graphics. We recently published a monograph [5] on “Magnetic Resonance Brain Imaging” where full analysis pipelines for functional and diffusion MRI as well as MPM are described in R. In an attempt for Open Science, the book is fully reproducible, i.e., all results and figures can be automatically created from the sources by the code applied to openly accessible data.

However, the neuroscience community often relies on other software environments such as the statistical parametric mapping (SPM) software for Matlab. It is thus essential to integrate new methods also into those tool chains. While within the published monograph, we establish this via the standardized medical imaging formats, we are also part of a large European consortium for creating the Open Source `hmri-Toolbox` for SPM [6], which is specifically dedicated to quantitative imaging for in-vivo histology. To foster Open Science, the publication has been accompanied by the publication of a reference dataset [7], which is essential for developing new methods in the field.

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1.2 Three Faces of Coagulation

Robert I. A. Patterson

Coagulation has been a topic at WIAS since at least 1997, when WIAS Preprint no. 361 appeared with the title “Convergence of a Nanbu type method for the Smoluchowski equation”. The Smoluchowski equation is a mathematical description of how particles in a large population moving in a well-mixed container grow by coagulating, that is, sticking together, upon collision. The topic has been of constant interest at WIAS since 1997, and the three sections of this contribution will each highlight one recent application of the expertise of the institute in this field.

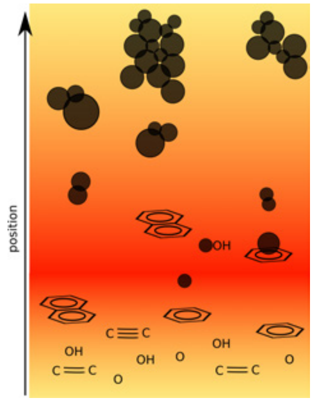

Fig. 1: *Combustion produces hexagonal molecules that form small soot particles and then coagulate further to produce aggregates*

In the first application, the Smoluchowski equation is assumed to be a good model (mathematical approximation of the real world), and stochastic particle systems are used as a computational tool for generating approximate solutions in situations of engineering interest. One example where these stochastic particle systems are used computationally [2] is illustrated in Figure 1. In the second application, theoretical studies of stochastic coagulating particle systems very similar to those used in the first application enable us to prove new large deviations results about a family of random graphs or networks. Finally, we see that some rather complex dependency structures in a model of an ideal gas have sizes that follow coagulation dynamics and can be successfully analyzed using a mixture of techniques developed for random graph and coagulation problems. The basic object for this final application is the collision cluster, which is illustrated in Figure 2 for five molecules moving sideways and colliding as time advances to form two collision clusters.

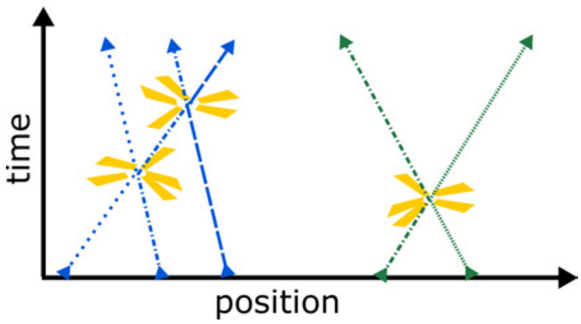

Fig. 2: *Color-coded clusters of colliding gas molcules in one dimension*

Coagulation and computation

Preprint 361 mentioned above was about a method for using a computer to calculate concentrations of particles of different sizes after they have had the opportunity to coagulate. The authors assumed that the Smoluchowski equation was a good mathematical description for large collections of small particles moving and coagulating. There were sophisticated mathematical grounds for expecting the Smoluchowski equation to be useful in a wide range of applications. The usefulness of the Smoluchowski equation can also be seen from the range of practical problems where it has successfully been applied. For example, stochastic numerical methods similar to those introduced in Preprint 361 were developed [2] for the simulation of soot particle formation in flames as illustrated in Figure 1.

The development of stochastic numerical techniques for simulating systems of coagulating particles described by the Smoluchowski equation and their application to problems from chemical engineering is an ongoing topic at WIAS [1]. It is interesting to observe that the stochastic particle systems used numerically to compute solutions to the Smoluchowski equation are themselves algorithmic realizations of systems of coagulating computational particles. Indeed, one can think of the simulation method as a realization of an idealized, stochastic model of the physical system, although strictly it is just an approximation method for the Smoluchowski equation.

Coagulation and connected components

Graphs are ubiquitous mathematical structures, for example, they are used at WIAS in the study of communication networks [5]. Formally, a graph is a collection of points, known as "vertices", some of which are joined together by edges (the lines in Figure 3). In a communication network, the vertices might be people or electronic devices, and edges would correspond to actual or at least possible connections.

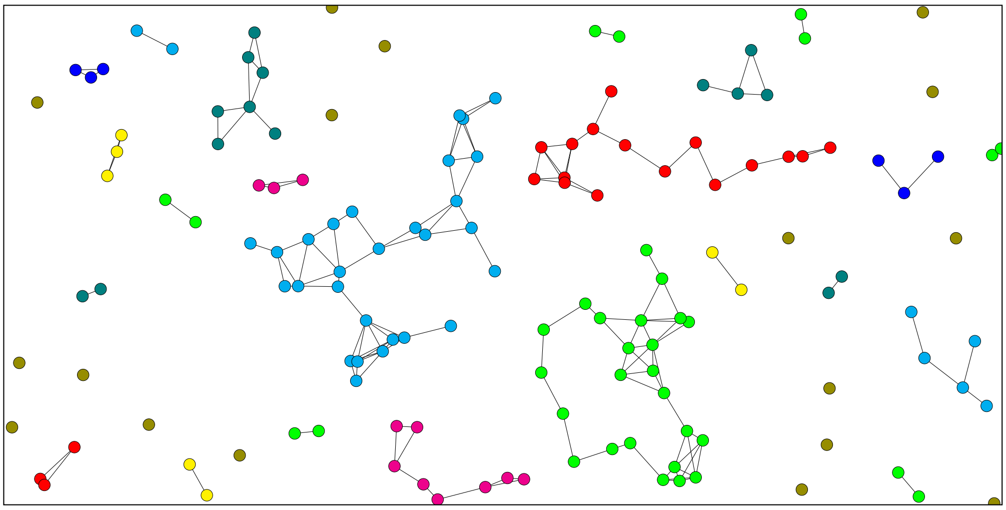

Fig. 3: *A spatial graph with points shown as colored discs and connections as black lines; points are color-coded to highlight* connected components *which are groups of points joined to each other by lines at some fixed time*

A connected component of a graph is a collection of vertices with their adjoining edges such that every pair of vertices in the component are connected by a sequence of edges, and it is not possible to add further vertices from the original graph without destroying this property. In other words, it is a maximal set of connected vertices and edges. See the color coding in Figure 3 for an illustration in the case of a spatial graph with short edges. The illustration is for a spatial graph in two dimensions, but it is also possible to consider more abstract graphs where the points are not located in physical space and the connected components are still well defined, although rather hard to picture.

An initially surprising observation is that in a simple dynamic model for an abstract graph—a fixed set of points where edges are continually being added independently of all other edges—the sizes of the connected components have the same dynamics as coagulating particles. At WIAS, we have exploited this fact to extend results initially formulated in the context of a stochastic coagulating particle system to the connected component sizes of random graphs.

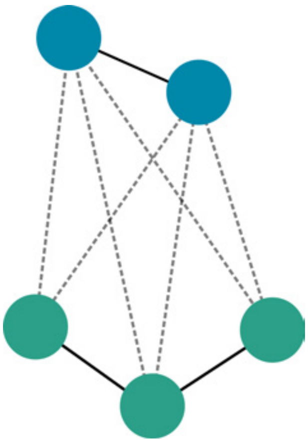

Fig. 4: The number of possible (dashed line) connections between the blue and green connected components is 2×3

Consider a graph with N vertices starting with no edges and where every missing edge has an independent creation probability of approximately $\Delta t/N$ for a short time interval Δt and edges are never removed. To merge a connected component of size n with one of size m, an edge must be created with an end in each component.

There are $n \times m$ possible edges joining a component of size n with one of size m, see Figure 4 for a simple example, so the probability of the components merging is roughly $nm\Delta t/N$. This merger probability only depends on the size of the components, not on the details of the edges, for example, the green component in Figure 4 could be given an extra edge making it into a triangle without changing the number of possible edges that would connect it to the blue component. Thus, the list of connected component sizes for a graph with N vertices behaves in exactly the same way as the list of the sizes of a set of particles coagulating according to the following rules:

- There are exactly N particles of size 1 at time 0.
- Each unordered pair of particles (sizes m and n) coagulates at rate mn/N.

We have proved [4] a large deviations principle in the $N \to \infty$ limit for the entire distribution of the sizes of particles coagulating according to the above rules, which is at the same time a large deviations principle for the connected component sizes in the (Erdős-Rényi) family of random graphs at a fixed time. For these two problems we looked at microscopic sizes, which do not grow as N increases, and macroscopic sizes, which grow linearly with N. We verified a known result that with high probability a unique macroscopic size appears at a critical time ($t = 1$) and proved new results about rare events such as seeing several macroscopic sizes or a non-trivial number of particles with sizes on intermediate scales.

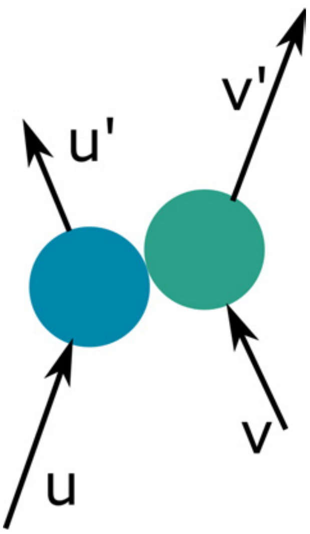

Fig. 5: Energy and momentum preserving collision between two molecules: $u^2 + v^2 = u'^2 + v'^2$ *and* $u + v = u' + v'$

Coagulation and collision clusters

The collision clusters introduced in Figure 2 arise from a model of a low density gas made up of N gas molecules. Each molecule is supposed to be a small sphere that moves in a straight line until colliding with another molecule (or possibly some kind of boundary). Collisions are modeled as happening instantaneously upon contact and as conserving kinetic energy and momentum as sketched in Figure 5. Two molecules are said to be connected if they have collided; this defines a partition of the molecules into collision clusters analogous to the connected components of a graph. For graphs it was the connected components that "coagulated" by merging; here, it is the collision clusters that "coagulate" as molecules from previously separate clusters collide (and rebound).

These clusters cannot be observed physically, because gas molecules are indistinguishable. However, it is possible to track the clusters while simulating the dynamics described above for a moderate value of N. From such simulations, we extracted the distribution of cluster sizes at a sequence of times; the results are shown in Figure 6 on log–log scales with time expressed in units of the mean free time. One sees that the cluster size distribution drops off faster than a power law distribution except for a very short period of time around $t = 1$ when it is aligned with a $-5/2$ power law.

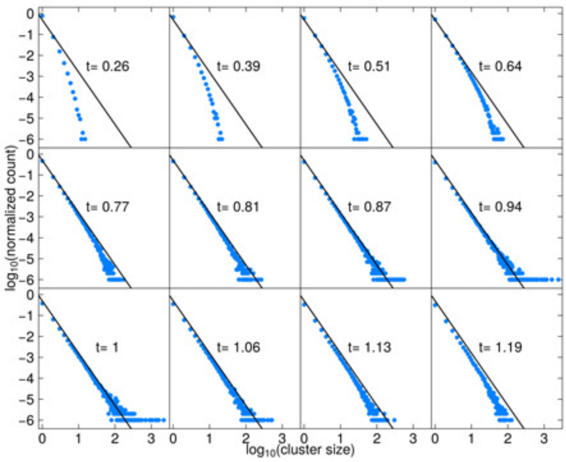

Fig. 6: *Fraction of clusters as a function of cluster size. The black line shows a* $-5/2$ *power law distribution.*

This transient $-5/2$ power law behavior is known from the coagulation model discussed in the previous sections, where it occurs at the same time as the formation of a macroscopic particle. One can confirm this interpretation by looking at Figure 7 where time is again expressed in multiples of the mean free time and one sees that just before $t = 1$ one cluster escapes from the main cloud and becomes several hundred times larger than every other cluster.

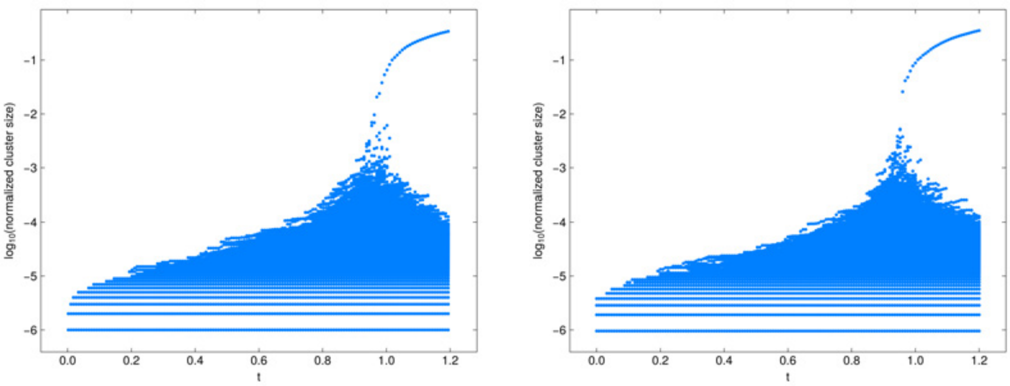

Fig. 7: *Cluster sizes present at different times. Left: Deterministic model. Right: Stochastic (Kac) model.*

Simulating this deterministic model of a gas is very slow, because of the need to check for collisions between every pair of molecules. The full deterministic model is rather hard to analyze mathematically, which is why the collision clusters are also studied. In simple situations where the properties of the gas are not expected to vary significantly in space, there is a simplified stochastic model where molecule positions are ignored and collisions can no longer be detected but are performed randomly at the same rate as would have been expected in the deterministic model.

This stochastic model (generally known as the Kac model) and the related numerical methods have been found to reproduce the properties of a gas with great accuracy and reliability. A necessary condition for this accuracy is correctly reproducing the correlations between molecules, and one can observe this successful reproduction by comparing the collision cluster size distribution for the stochastic model with the deterministic model in Figure 7.

One can approach these collision clusters by regarding the molecules as the vertices of a graph and putting an edge between two molecules when they collide. Arguing as in the previous section, one sees a kind of coagulation dynamics for the cluster sizes [3]. However, the situation is a little more complex than in the previous section since each molecule has a velocity, which changes due to collisions. In [6], we show that with some small modifications the Kac process interaction clusters can be identified with the connected components of a random graph where each vertex is labelled with a (time-invariant) velocity and where the clusters are characterized by the triple of their size, momentum and kinetic energy (the momentum and kinetic energy of a cluster is the sum of these quantities for the constituent vertices). This enabled us to find a closed-form expression for the time at which the macroscopic cluster appears.

Conclusions and outlook

- Expertise in stochastic coagulation processes was developed in order to understand and improve engineering calculations.
- Further development of this expertise led to new large deviations results that also apply to the connected component sizes of an important family of random graphs.
- The connection between coagulation and graphs enabled us to find the time when a macroscopic collision cluster emerges in a stochastic model for an ideal gas.

The interplay between coagulating particles and connected components in random graphs remains a fruitful topic of research. It is being exploited as a key tool in a project to analyze spatial models of particle coagulation, which are more sophisticated and realistic than those currently known.

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1.3 Leibniz Research Network “Mathematical Modeling and Simulation”

Alfonso Caiazzo, Torsten Köhler, Alexander Linke, and Matthias Wolfrum

One of the hallmarks of mathematics is its universality. The same mathematical concepts and methods can be fundamental for the understanding of very different phenomena in nature, technology, economy, and many other aspects of human life. This universality also relates to modern methods of applied mathematics, which include the development of algorithms for simulation and optimization of complex problems, or the handling of large sets of data.

Fig. 1: *Member institutions of the Leibniz MMS network*

In the light of this cross-sectional and transdisciplinary character of mathematics, it was a natural step for WIAS to take the initiative for a research network on Mathematical Modeling and Simulation (MMS) around 2013, in line with the continuous efforts of the Leibniz Association to further strengthen cooperation between its institutions. The MMS network has by now 34 member institutes from all sections of the Leibniz Association. Indeed, these are not only institutes from *Section*

D: Natural Sciences, Engineering, having in some cases large departments devoted to simulation-based research with an outstanding expertise in their respective fields, but also institutes with only a small group of scientists working on MMS, where the cooperation within the network can be particularly important to open new opportunities.

A major activity within the network was the organization of an annual series of workshops, the *Leibniz MMS Days*, which so far have taken place at five different Leibniz institutions. Identifying scientific fields of common interest among the network members and putting a specific emphasis on the specialization of the hosting institute, each workshop comprised several topical sessions in various fields, such as

- computational and geophysical fluid dynamics (CFD & GFD),
- systems biology and genetics,
- statistical data analysis,
- condensed matter.

Another purpose of these meetings is to address general topics concerning basic requirements and conditions, which are of interest for researchers doing MMS, independent of their specific field. This included talks and discussions on the development and management of research software as well as questions related to the handling of research data, or scholary research communication (open science, software citation). The intensive work on the above-mentioned topics made it possible to substantially support the Mathematical Research Data Initiative (MaRDI) within the German National Research Data Infrastructure program (NFDI). The Leibniz Association has also appointed experts from the network, Georg Feulner (PIK) and Jürgen Fuhrmann (WIAS), for an ad-hoc group on research software within the framework of the priority initiative *Digital Information* of the Alliance of German Science Organisations.

Since 2018, the network has also been organizing annual summer schools for Ph.D. students whose topics were *Statistical Modeling and Data Analysis* and *Modern Programming Languages for Science and Statistics: R and Julia*. These schools took place at Oberwolfach Research Institute for Mathematics, which is also a member of the MMS network.

Fig. 2: *Participants of the MMS summer school 2019*

The role of computational and geophysical fluid dynamics in MMS

Dynamics of gases and liquids are relevant for a large number of Leibniz institutes and, hence, establish the most prominent common research topic within the MMS network. It is essential for the transport of nutrients and metabolites in animals and humans, as well as for weather forecasts and the prediction of climate change, for the quality of modern semiconductor wafers grown from crystal melts, or for the development of magnetic fields on the earth or on other celestial bodies. The basic physical laws describing the motion of fluids, the Euler and Navier–Stokes equations, form today the root of a huge, diverse, and sometimes confusing family of related mathematical models. Similarly diverse are the approaches in the research of the members of the MMS network. Some of them mainly apply commercial or non-commercial simulation tools to address specific questions from their field of research. For other research institutes, which develop their own software, scientific computing and implementation issues play a major role. Finally, WIAS as a mathematical institute performs also basic mathematical research and rigorous numerical convergence analysis, in order to get a theoretical understanding about the advantages and disadvantages of various competing simulation algorithms and to improve today's powerful simulation tools even further.

Turbulence simulation with open source CFD solvers

During the MMS Days 2017, a collaboration between WIAS, the Leibniz Institute of Agricultural Engineering and Bio-economy (ATB), and the Leibniz Institute for Tropospheric Research (TROPOS) was initiated, with the purpose of exchanging experiences in the context of turbulence modeling, and, eventually, of assessing the performance of open source CFD solvers [3].

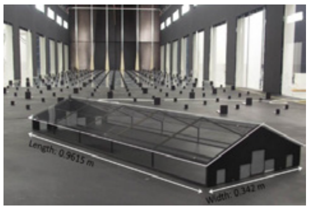

Fig. 3: *Scaled barn model in the wind tunnel*

The first goal was to demonstrate that these codes are able to provide reliable simulations in agricultural applications, reducing existing reservations towards the use of open source tools in this community. The second goal was to compare – in a realistic scenario – two solvers based on different meshes, discretization schemes, and turbulence models: OpenFOAM, a well-established free and open source solver and ParMooN (Parallel Mathematics and object-oriented Numerics), a finite element library developed at WIAS. The benchmark problem consisted in the simulation of the cross flow in a typical naturally ventilated barn. Experimental data were obtained via measurement campaigns in a 1:100 scaled wind tunnel model of the barn at the ATB (Figure 3). The turbulent flow was simulated solving numerically the time-dependent Navier–Stokes equations on a computational domain of 3 m length and 1 m height, including the floor and roof geometry of the wind tunnel model (see Figure 4).

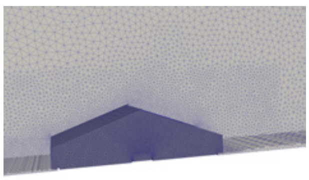

Fig. 4: *Section of one spatial discretization (mesh) used in ParMooN*

The results showed that both solvers achieve a good agreement with experimental data for time-averaged stream-wise and vertical-wise velocities. In particular, the air exchange was predicted with relative errors less than 5% compared to the experimental results. With respect to the turbulent quantities, good agreements at the second (downwind) half of the barn inside and especially outside the barn could be achieved. Hence, he solvers proved to be promising tools for the accurate prediction of time-dependent phenomena in an agricultural context, such as the transport of particulate matter or pathogen-laden aerosols in and around agricultural buildings.

Modeling, simulation, and optimization of geothermal energy production

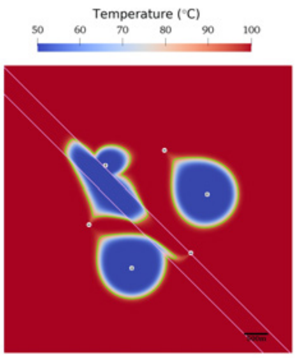

Fig. 5: *Temperature field in a hexagonal multi-well configuration with a thin damage region with lower permeability*

Geothermal energy, i.e., the energy stored as heat in the subsurface, constitutes a renewable resource that can be sustainably recovered using diverse concepts, such as district heating in urban environments. Geothermal plants operate through multiple *wells*, from which hot water is extracted (production wells) and colder water is injected (injection wells). The collaboration between WIAS and the Leibniz Institute for Applied Geophysics (LIAG), initiated during the MMS Days 2018, aimed at applying advanced finite element methods for porous media flows, combined with an open source optimization framework (NLopt), for the modeling, simulation, and optimization of the geothermal energy production.

The considered problem consisted in optimizing the installation – given a particular topological structure – in order to maximize the extracted energy and delaying the so-called *thermal breakthrough*, i.e., the time when the cold water front reaches the production well. In [4], we simulated the energy production process considering a Brinkman problem for the groundwater flow in a saturated aquifer and an advection-diffusion model for the temperature distribution. We investigated numerically the optimal positioning and spacing of multi-well arrays in the form of a lattice and a hexagonal structure, considering structural heterogeneities as well as varying reservoir temperatures. In particular, the results demonstrated that the proposed numerical framework is able to efficiently handle generic geometrical and geological configurations, and can be thus flexibly used in the context of multi-variable optimization problems.

Novel well-balanced schemes for the compressible Navier–Stokes equations

The annual "MMS Mini Workshop on CFD & GFD" triggered a collaboration between the Leibniz-Institute of Atmospheric Physics (IAP) and WIAS. Typical challenges of flow simulations are certain kinds of *extreme force balances* that can develop during the time evolution of the fluid motion. Many kinds of different physical forces determine the fluid motion simultaneously, e.g., the pressure gradient, the inertial force, the friction force, the Coriolis force, or the centrifugal force. But often only a few forces are dominant at a certain point in time. The starting point for the collaboration was substantial progress at WIAS on the question how to handle certain extreme force balances like *hydrostatics, geostrophic flows, high Reynolds number flows* in incompressible flows, i.e., in liquids [1], providing a novel approach how to implement a basic mathematical law, namely "gradient fields are irrotational", in the simulation algorithms. Since in meteorology, such extreme force balances in the atmosphere play a similar role, the question arised whether the WIAS results could be extended from incompressible to the mathematically much more challenging compressible flows, i.e., from liquids to gases. As a result, a novel kind of so-called *well-balanced schemes for compressible flows* was constructed that are able to handle certain kinds of extreme force balances in low Mach number and stratified flows, which are typical for meteorological applications [2]. Furthermore, the notion of a *gradient-robust scheme* was introduced.

A network dynamics model for the auditory cortex

Another cooperation within the MMS network was established between the Leibniz Institute for Neurobiology (LIN) in Magdeburg and WIAS. The subject of research here is a dynamical network model for the auditory cortex in the brain, which was developed at LIN together with colleagues from the Lancaster University, UK. This model is based on a detailed knowledge of anatomical and physiological structures (see Figure 6) and should contribute to a deeper understanding of the experimental findings in the *Non-Invasive Brain Imaging* lab at LIN.

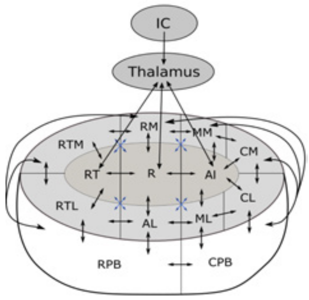

Fig. 6: *Network structure in the auditory cortex: connectivity between different core, belt, and parabelt regions*

The purpose of the ongoing cooperation is a mathematical analysis of the dynamics of this model using advanced tools from dynamical network theory. In particular, we are using multiple time-scale methods to analyze the adaptation to multiple external stimuli. In this way, the adaptation of the cortical response to repetitive stimulation could be understood as a result of the short-term synaptic depression that was included in the model by a dynamical adaptation of the connectivity weights with a recovery on a slow time scale, see Figure 7. Moreover, a hierarchical network approach was used to describe the connectivity structure on different levels of complexity and, in this way, to understand the role of the physiological complexity on a functional level.

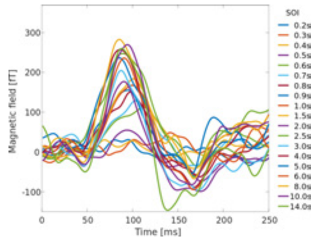

Fig. 7: *Simulated response of the auditory cortex for repetitive stimulation at different rates*

Conclusions and outlook

With the increasing importance of interdisciplinary research and cooperation, the Leibniz MMS network establishes a unique tool to strengthen the role of mathematical research within the Leibniz Association and to raise synergies among the member institutes. For WIAS it provides the opportunity to identify new important fields for its own research and to initiate collaborations with the prospect of launching joint, third-party funded projects.

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1.4 Mathematical Modeling of Lithium-ion Batteries

Manuel Landstorfer

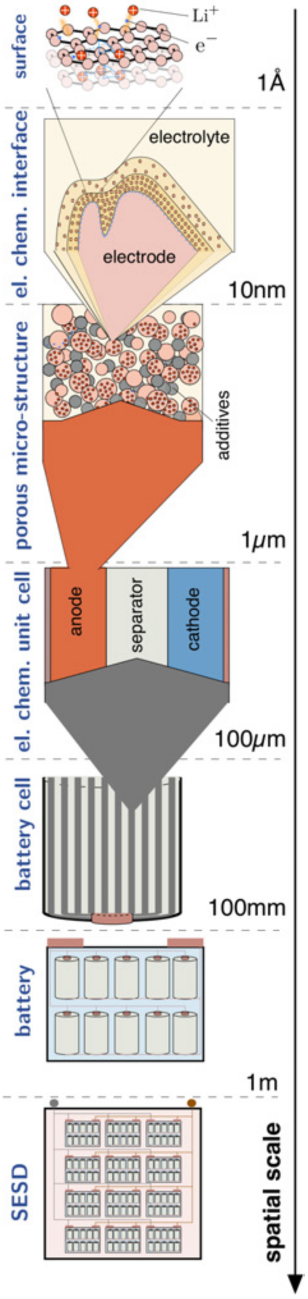

Fig. 1: *Sketch of the different scales within a battery*

Rechargeable lithium batteries[1] are of ultimate importance for the transition towards a fossil-free and socio-ecologically sustainable economy within this century. Especially for the exit from nuclear and fossil-fuel energy, batteries are crucial for a variety of applications, but mostly for (i) storing excess wind and sun electricity with a high efficiency and (ii) enabling full electric vehicles. The "2nd-life" concept combines these two main application areas in a sophisticated way.

Batteries can store an amount Q (mAh) of electricity due to electro-chemical reactions occurring within the cell. Q is commonly called the *capacity* of a battery, and modern standard cells have a capacity > 4000 mAh. However, due to charging and discharging, commonly called *cycling*, batteries degrade and loose capacity. Weight and volume restrictions of an electric vehicle require that the battery is retired at 80% of its initial capacity Q^0. But these batteries are by no means unusable. They simply no longer meet the weight-specific requirements of an electric vehicle. For stationary applications, however, weight is almost unimportant. Hence, retired batteries from electric vehicles can start a *2nd life* as a stationary energy storage device (SESD). Estimations of one million electric vehicles in 2020 could *produce* a storage capacity of about 25 GWh in 2025. A single SESD is built by an interconnection of various batteries of different degradation degrees. The control engineering of this circuit requires reliable information on the *future* behavior of each battery in order to meet safety, quality, and quantity standards. *Opening* and experimentally investigating each individual battery cell is far too tedious, and other strategies become necessary.

To overcome this problem, mathematical modeling, simulation and optimization (MSO) techniques are used to develop reliable prediction tools for lithium-ion batteries. These are of special importance for the 2nd-life application to estimate the further cycle number, the capacity evolution, safety aspects, and also pricing. But this requires a profound understanding and quantification of the complex degradation process occurring in lithium-ion batteries. Various effects contribute to the overall degradation, for example, the cycling rate, and they are diverse for various materials used nowadays. Two batteries of an electric vehicle, each ran 20,000 km, can have very different capacities if one battery was charged rather slowly while the other one was always charged quickly.

Since 2018, the BMBF has funded the joint project MALLi[2] *Model-based Assessment of the Life Span of Aged Li Batteries for 2nd-Life Use for Stationary Energy Storage* within the funding line *Mathematics for Innovation*. The project consortium consists of AG 1 (Kai Peter Birke, Universität Stuttgart, Institut für Photovoltaik), AG 2 (Sven Simon (Universität Stuttgart, Institut für Parallele und Verteilte Systeme), AG 3 (Volker Schmidt, Universität Ulm, Institut für Stochastik), AG 4 (WIAS, Manuel Landstorfer, project coordinator), AG 5 (Mario Ohlberger, Universität Münster, Institut für Numerische und Angewandte Mathematik), and AG 6 (VARTA Microbatteries). MALLi[2] aims to develop a model framework that can be used to estimate the further life span of a lithium-ion battery. This is achieved by a combination of mathematical modeling (AG 4 – multi-scale electrochemical modeling, AG 3 – porous micro-structure modeling), numerical simulations (AG 4 – validation studies, AG 5 – reduced basis methods for degradation), electrochemical experiments (AG 1 – cell

[1] also known as secondary batteries or "accumulators" and abbreviated as "battery" throughout this article.

production and cycling, AG 6 – deployment of cells with industry quality), and imaging procedures (AG 1 – three-dimensional micro-computed tomography investigations of lab cells, synchrotron experiments).

The central goal of MALLi[2] is a mathematical model framework of battery cell (see Figure 1), developed by RG 7 at WIAS, that is capable to predict the cycling behavior, i.e., the cell voltage E a battery delivers as a function of its capacity Q, its cycle rate C and cycle number n. The cycle rate C defines how fast a battery is charged and discharged, e.g., for $C = 1$ a battery is completely charged within one hour, while for $C = 0.5$ it is charged in two hours, and so forth. The model framework relies on various parameters such as reaction energies, diffusion coefficients, conductivities, surface reaction rates, and more, which are compactly written as $\vec{p}$. Once the model framework is validated for a battery without degradation effects, ageing is subsequently incorporated in the framework by cycle number n dependent parameters $\vec{p} = \vec{p}(n)$. The functional dependency is initially assumed to be unknown. Specific electrochemical unit cells (see Figure 1) are produced within the project and cycled under well-defined laboratory conditions yielding the necessary data to determine $\vec{p} = \vec{p}(n)$. Note that emulating the 1st-life cycle of an electric vehicle in laboratory conditions is a very time-consuming task. 4 000 cycles at a rate of $C = 1$ require 333 days of continuous charging and discharging. In AG 1 (Birke), 10 (equal) cells are cycled at rates of $C = 0.5, 1$ to capacities of 90%, 80%, 60%, and 40% of their initial capacity Q^0, where the electrochemical data is continuously recorded. The parametrization $\vec{p} = \vec{p}(n)$ is carried out by AG 5 (Ohlberger) with reduced basis methods. In addition, three-dimensional imaging techniques of AG 2 (Simon) are used to capture the evolution of geometries due to degradation on the different scales (c.f. in Figure 2). Specifically for the porous micro-structure, this data is used by AG 3 (Schmidt) to parametrize a stochastic model of the micro-structure evolution upon cycling. In the following, we focus on three aspects of the project carried out at WIAS, (i) the electrochemical model development, (ii) multi-scale expansions and homogenization, and (iii) numerical computations of the cell problem arising in homogenization for realistic micro-structures.

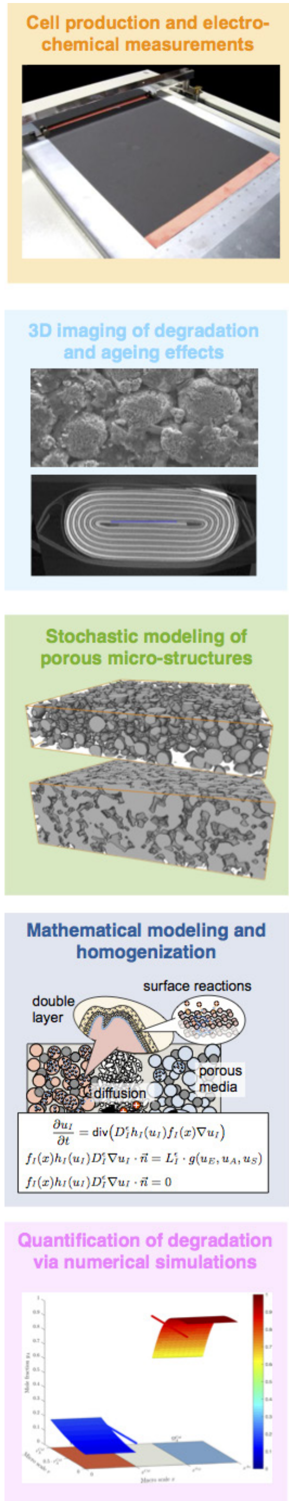

Fig. 2: *Tasks within the MALLi[2] consortium*

Electrochemical model development

The inherent multi-scale nature of a battery requires a structured and systematic approach to account for all major effects on the relevant spatial scales (c.f. Figure 1). This is of additional importance since materials, material compositions, and reaction principles continuously change in the development of lithium-ion batteries, and we seek a model framework that is also applicable to future batteries. In order to separate the impact of the porous microstructure from the electrochemical modeling, we considered for the model development a thin-film half-cell battery consisting of a dense, non-porous intercalation cathode Ω_C, an electrolyte Ω_E, and a metallic lithium anode Ω_A. The system is modeled within the framework of continuum non-equilibrium thermodynamics describing the space and time evolution of the desired variables in terms of partial differential equations. The main variables are the mole fraction y_C of intercalated lithium ions in the cathode, the electrostatic potential φ_C in the cathode, the mole fraction y_E of lithium ions in the electrolyte, the electrostatic potential φ_E in the electrolyte, and the electrostatic potential φ_A in the anode. A central quantity of the thermodynamic framework is the chemical potential μ, which quantifies the material-specific behavior. For example, intercalated lithium ions *in* a specific host material have a chemical potential μ_C that is quantified as $\mu_C = \mu_C(y_C)$. Different host mate-

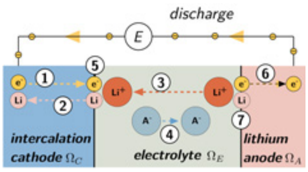

Fig. 3: *Sketch of the thin-film battery with the major transport phenomena*

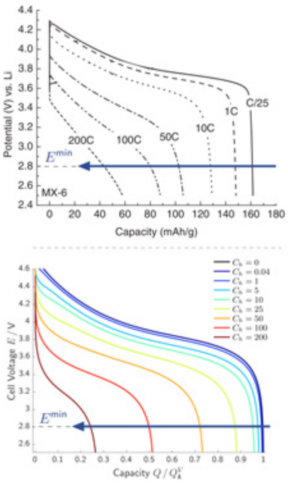

Fig. 4: *Top: Experimental data of a NMC-Li thin-film battery. Bottom: Computed discharge curves of a NMC-Li thin-film battery [2].*

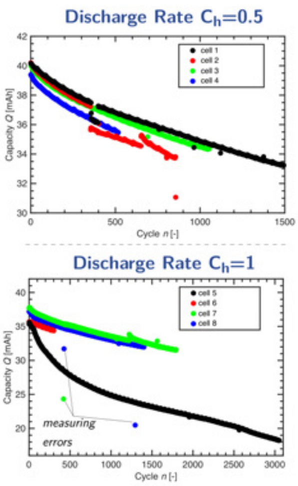

Fig. 5: *Experimental data of* Q^0 *with respect to the cycle number* n *for two discharge rates* $C = 0.5, 1$

rials, e.g., graphite or NMC (which is the most frequently used cathode material right now), have different *functional* relationships $\mu_C(y_C)$, while metallic lithium has a constant chemical potential μ_{Li}. At the interface between the cathode and the electrolyte, the intercalation reaction (6) $Li^+ + e^- \leftrightharpoons Li$ occurs [1], which determines how much lithium ions from electrolyte react with electrons from the cathode to intercalated lithium. A thin-film battery as shown in Figure 3 can be modeled [2] with five partial differential equations (PDEs) describing the (1) electron transport in the cathode determining φ_C, (2) the solid-state diffusion of intercalated Li determining y_C, (3) cation Li^+ and (4) anion A^- transport [3] in the electrolyte determining y_E and φ_E, and (5) electron transport in the anode determining φ_C. Vice versa, at the anode a similar reaction (7) occurs, where metallic lithium dissolves into lithium ions and electrons. During *discharge* of such a battery, lithium ions as well as electrons flow from the anode to the cathode, where the lithium ions flow *through* the cell, while the electrons pass through an outer circuit driving an electric engine, for example.

The voltage E that such a battery delivers is mainly dependent on two quantities: (i) the capacity

$$Q = Q^0 \cdot \bar{y}_C \quad \text{with} \quad \bar{y}_C = \frac{1}{\mathrm{vol}(\Omega_C)} \int_{\Omega_C} y_C \, dV \,, \tag{1}$$

and (ii) the rate C at which the battery is discharged. For the so-called *galvanostatic* cycling rate C is related to the discharge current I via $I = C \cdot \frac{Q^0}{[\mathrm{h}]}$. Based on the mathematical model, we seek to determine the cell voltage E as a function of the capacity Q and the rate C. A very special case is the *infinite* slow discharge $C \to 0$, which determines the so-called *open circuit voltage*

$$E = \frac{1}{e_0}(\mu_{Li} - \mu_C(y_C)) \,, \quad \text{together with} \quad \bar{y}_C = y_C \,. \tag{2}$$

This is a very important quantity of a lithium-ion battery and depends in a half cell, i.e., with metallic lithium as the anode, solely on the *status of charge* $y_C = Q/Q^0$, since μ_{Li} is constant. However, for cycle rates $C > 0$, the cell voltage E has to be determined *a posteriori* from numerical solutions of the above described equation system, which was carried out at WIAS and is summarized in [2]. Figure 5 shows experimental data (top) as well as numerical simulations (bottom) of the cell voltage E as a function of the capacity Q/Q^0 for discharge rates from $C = 0$ to $C = 200$. The first important aspect is the circumstance that the voltage of a lithium-ion battery decreases with its *status of charge* Q/Q^0 and, additionally, with respect to the discharge rate C in a nonlinear fashion. This has to be taken into account, for example, in the planning of integrated circuits. Another important characteristic feature is the decrease in maximum capacity at some *cut-off* voltage E^{min}. These aspects can be exploited to determine systematically the model parameters $\vec{p}$.

Based on the broad accordance between experiment and our theory (Figure 5 (top) and (bottom)), we are now able to investigate the origins of this complex behavior on the basis of our PDE model. This is of importance because ageing effects propagate in a similar characteristic manner to the cell voltage E, and the capacity Q^0, which become additionally dependent on the cycle number n. Figure 5 shows, for example, experimental data obtained within the project MALLi [2] of the capacity decline $Q^0 = Q^0(n)$ for two discharge rates C. A large electrochemical data set is generated within MALLi [2] used to quantify on its basis the parameter evolution $\vec{p} = \vec{p}(n)$ and thus to trace back individual ageing mechanisms.

Homogenization

In order to *apply* the validated model of a thin-film cell to a porous intercalation electrode, we require (periodic) homogenization techniques. A porous electrode consists of (at least) three phases, an active phase Ω_A, an electrolyte phase Ω_E, and the conductive additive phase Ω_C. The solid phase $\Omega_S = \Omega_A \cup \Omega_C$ and the electrolyte Ω_E are connected, while Ω_A is disconnected. In an abstract setting, we can write the model described above for a porous electrode as ($I = A, E, C$)

$$\frac{\partial u_I}{\partial t} = \mathrm{div}\big(D_I^\epsilon \nabla u_I\big) \qquad \text{in } \Omega_I\,, \tag{3}$$

$$D_I^\epsilon \nabla u_I \cdot \vec{n} = L_I^\epsilon \cdot g(u_E, u_C, u_S) \qquad \text{on } \Sigma_{A,E}\,, \tag{4}$$

where u_I can be ($I = A$) the intercalated Li mole fraction, ($I = E$), the electrolyte mole fraction, or the electrostatic potential in the electrolyte, and ($I = S$) the electrostatic potential in the solid phase. The boundary conditions (4) describe the intercalation reaction at the interface $\Sigma_{A,E}$. The quantities D_I^ϵ and L_I^ϵ depend on the small parameter $\epsilon = \frac{w}{W}$, where w encodes the spatial dimension of the unit cell and W the *large* scale of the whole porous electrode. A scale analysis shows that $D_S^\epsilon = \epsilon^0 D_S$ and $D_E^\epsilon = \epsilon^0 D_E$, while $D_A^\epsilon = \epsilon^2 D_A$ and $L_I^\epsilon = \epsilon^1 L_I$.

For spherical particles ω_A, we obtain via a multi-scale expansion in leading order ($I = E, S$)

$$\psi_I \frac{\partial u_I(x,t)}{\partial t} = \partial_x\big(\psi_I \pi_I \cdot D_I \partial_x u_I\big) + \theta_{A,E}\, L_I \cdot g\,, \tag{5}$$

$$\frac{\partial u_A(x,r,t)}{\partial t} = \frac{1}{r^2}\partial_r\big(r^2 D_A \partial_r u_A\big)\,, \qquad D_A \partial_r u_A\Big|_{r=r_A} = L_A\, g\,. \tag{6}$$

with $g = g\big(u_E, u_S, u_A|_{r=r_A}\big)$. The porous media parameters $\vec{p}_{\mathrm{PM}} = (\psi_I, \pi_I, \theta_{A,E})$ are determined from the actual unit cell ω, more precisely, for $I = A, S$, we have

$$\psi_I = \frac{\mathrm{vol}(\omega_I)}{\mathrm{vol}(\omega)}\,,\ \pi_I := 1 - \frac{1}{\mathrm{vol}(\omega_I)}\int_{\omega_I} \nabla_y \vec{\chi}_I dV(y)\,,\ \theta_{A,E} = \frac{\mathrm{area}(\sigma_{A,E})}{\mathrm{vol}(\omega)}\,, \tag{7}$$

where $\vec{\chi}_I = \vec{\chi}_I = (\chi_I^1, \chi_I^2, \chi_I^3)$ is determined from the **cell problem** ($k = 1, 2, 3$)

$$(\mathbf{CP}_I) \qquad \begin{cases} \mathrm{div}_y\Big(\big(\vec{e}^{\,k} - \nabla_y \chi_I^k\big)\Big) = 0 & y \in \omega_I, \\ \big(\vec{e}^{\,k} - \nabla_y \chi_I^k\big)\cdot \vec{n} = 0 & \text{on } \sigma_{A,E} \\ \chi_I^k & \text{is periodic}\ . \end{cases} \tag{8}$$

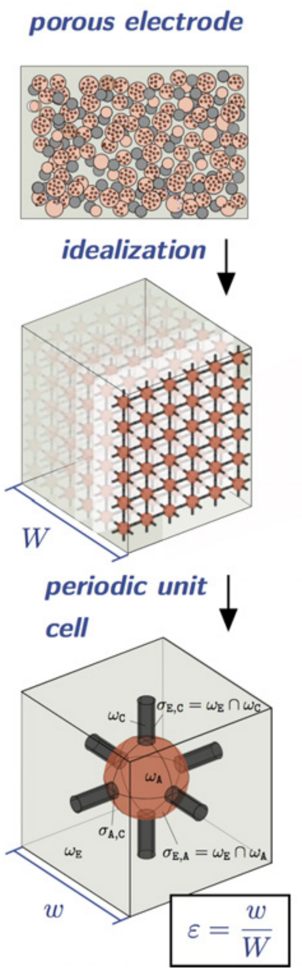

Fig. 6: *Sketch of a porous electrode and its idealization as periodic repetition of unit cells* ω

Numerical computations of the cell problem

The unit cell ω of Figure 6 can be considered as the most simple example of a porous intercalation electrode. However, the methodology of homogenization is not restricted to such *simple* geometries. Within MALLi2 [2], the AG 3 (Schmidt) produces characteristic micro-structures of porous battery electrodes on the basis of stochastic process. A micro-structure M of L particles is then described as $M = (\vec{y}_\ell, r_\ell(\theta,\varphi))_{\ell=1}^L$, where $\vec{y}_\ell$ is the mass center of each particle and $r_\ell(\theta,\varphi)$ the angle-dependent radius function. This allows to prescribe, for example, a distribution function of the average particle radii (see Figure 7), yielding an explicit realization of a (periodic) micro-structure M (see Figure 8, left). In order to compute the micro-structure parameters, i.e., numeri-

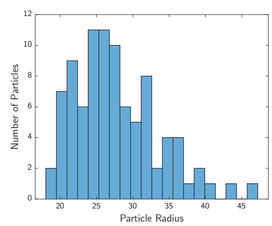

Fig. 7: *Distribution function of particle radii for a porous electrode micro-structure*

cally solve the cell problem $(\mathbf{CP}_I)$, a proper volumetric *mesh* of M is required. Within RG 7 at WIAS, a method was developed that produces a *high-quality* periodic surface mesh on the basis of the representation $M = (\vec{y}_\ell, r_\ell(\theta,\varphi))_{\ell=1}^L$. This surface mesh serves as input to the WIAS software TetGen, producing high-quality volume meshes, which can be used in any modern finite element code. Numerical solutions in the electrolyte phase of the cell problem (8) are shown in Figure 8 (right).

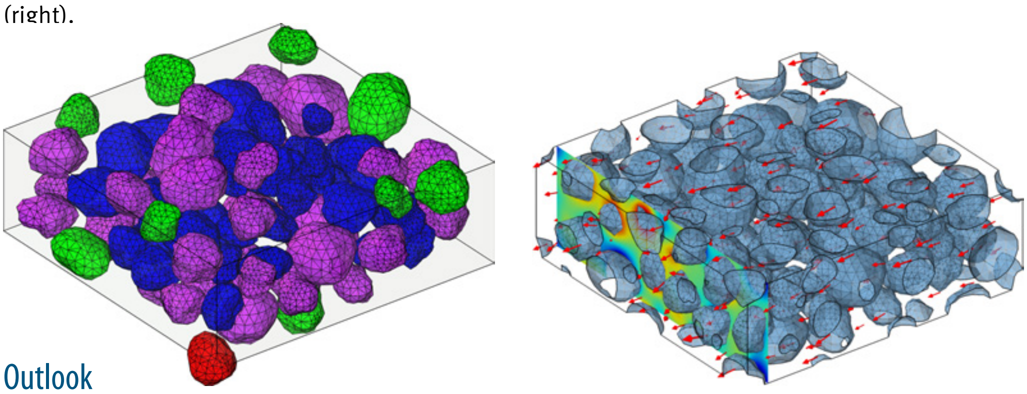

Fig. 8: *Left: Realistic micro-structure of a porous battery electrode described with L=91 particles. The colors encode the number of periodic repetitions, red: 4, green: 2, magenta: 1, blue: 0. Right: Periodic surface mesh and numerical solution of the cell problem* $(\mathbf{CP}_I)$ *on the volume mesh of the electrolyte phase. The arrows indicate* $\nabla\chi_E^1(\vec{y})$.

Outlook

With the sketched homogenization procedure, an entire model of an electrochemical unit cell (see Figure 1) was recently derived. This model is currently validated by using experimental data obtained within the MALLi[2] consortium on the basis of a numerical implementation of AG 4 (WIAS). Simultaneously, reduced basis methods of AG 5 (Ohlberger) are currently developed for this model to quantify the degradation mechanisms of the underlying parameters $\vec{p} = \vec{p}(n)$. Furthermore, three-dimensional synchrotron investigations of the micro-structure evolution upon cycling will be carried out at Helmholtz-Zentrum Berlin für Materialien und Energie (HZB – BESSY II) in 2020. The very same cells for which the electrochemical data was recorded will be investigated. We obtain thus a parametrization of the micro-structure M with respect to the cycle number n, whereby the micro-scale geometries become $\omega_I = \omega_I(n)$. Hence, we can determine the evolution of the porous media parameters $\vec{p}_{\mathrm{PM}}(n)$ from the cell problem $(\mathbf{CP}_I)$ to separate the degradation of the micro-structure from the remaining parameters ($\vec{p}_{\mathrm{PM}} \subset \vec{p}$). This yields the *toolbox* to trace back the variation of individual model parameters with respect to the cycle number and, therefore, allows us to quantify individual ageing mechanisms which are associated to certain parameters.

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1.5 Non-smooth and Complementarity-based Systems

Amal Alphonse and Michael Hintermüller

Introduction

In this article, we present a survey of the main research aims and achievements of the DFG Priority Programme SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* and detail, in particular, the contributions of WIAS in the SPP. Many challenging problems in biology, chemistry, physics and economics (and, more generally, in the applied sciences) can be described through mathematical objects, and many of these mathematical descriptors necessarily involve some form of **non-smoothness**, which is a property of a class of mathematical problems where the underlying structure describing the problem is somehow "rough" or fuzzy or contains such components. This non-smoothness creates considerable difficulties in the ensuing analysis of the problem at hand and also the numerical simulation and computational realization thereof. Some particular physical applications that such problems encompass include those related to magnetic superconductivity, multi-physics problems, optimal system design in robotics and biomechanics and motion optimization, among others. The aims of the SPP 1962 are to establish a mathematically rigorous theoretical and numerical foundation, as well as new techniques and tools to handle the inherent non-smooth phenomena encountered in the context of the various mathematical models/problems that fall into the described category. The results of the SPP 1962 will be of benefit not only to applied mathematicians but also to computational scientists and engineers. With foundations in applied mathematics, the SPP 1962 has an interdisciplinary outreach since its findings will be of benefit to computational scientists and engineers who face challenging applications involving non-smooth components. Structurally, research in the SPP 1962 is carried out in individual projects spread throughout Germany (see Figure 1) while for the synthesis and fostering of ideas and techniques the networking of research groups is done. In the same vein, each project belongs to one or more *communicating research areas* which helps to broadly classify the type of work that will be done in the project (see Figure 2). Moreover, categorizing research projects around prototypical applications is crucial to achieve landmark results and to succeed in addressing challenging applications.

Fig. 1: *Location of projects*

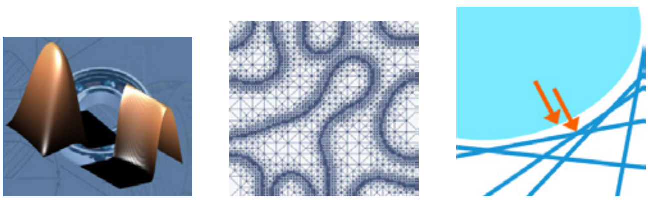


Fig. 2: *Three communicating research areas: (1) analysis, modeling, algorithm design; (2) realization of algorithms and discretization; (3) incorporation of parameter dependencies*

Non-smoothness

In the context of the SPP 1962, the above-mentioned problems involve partial differential operators and optimization problems with non-differentiable structures. Non-smoothness can arise in three ways:

1. **Directly in the formulation of the problem**, for example, applications in frictional contact problems or non-smooth constitutive laws for underlying physical processes in models describing magnetization of superconductors,
2. **Through inequality constraints, nonlinear complementarity systems or switching systems**, for example, non-penetration conditions in contact/obstacle problems, which upon reformulation can be seen as complementarity problems,
3. **As a result of competition and hierarchy**, for example, in modeling competition with generalized Nash equilibrium problems or partial differential games.

These types of problems tend to be highly nonlinear and typically lead to the presence of variational inequalities (VIs) and quasi-variational inequalities (a quasi-variational inequality or QVI is a VI where the solution is sought in a set that itself depends on the solution) and represent novel mathematical structures. A major emphasis of the SPP 1962 is the transition from smoothing/regularization or simulation-based approaches to the development of genuinely non-smooth techniques. As alluded to, the SPP 1962 is motivated by important applications but also by recent developments in the theory and numerics for non-smooth distributed parameter systems (for example, semi-smoothness in infinite dimensional spaces) and their optimization as well as the beginning of the interaction of non-smooth systems with problems that require robust solutions.

Achievements

Below, we list some exemplary findings from the SPP 1962 projects:

- Progress on designing and analyzing fast solvers for dissipative and non-dissipative QVIs
- Optimal control of type-II superconductors
- Progress on better analytical and numerical understanding of mathematical programs with equilibrium constraints (MPECs) in function spaces
- Stability/sensitivity of solutions for VIs of second kind with non-smooth structures
- Characterizations of normal cones in Sobolev and Lebesgue spaces
- Specific applications involving MPECs: rate independent systems, multiphase fluids, etc.
- Generalized Nash equilibrium problems in Banach spaces
- Adaptive methods and model reduction for VI problems
- Directional differentiability for parabolic VIs

The last of these contributions will be detailed below.

Contributions of WIAS to the SPP 1962

The contributions of WIAS to the SPP 1962 are manifold, not least since the coordination of the SPP 1962 is based at WIAS. On the research level, we highlight a few of our contributions here.

Directional differentiability

A major focus of the authors' (along with Carlos N. Rautenberg, George Mason University, Fairfax) work in the SPP 1962 has been the sensitivity analysis related to QVIs.

Directional differentiability for elliptic QVIs. We studied in [1] the directional differentiability associated to the elliptic QVI

$$\begin{aligned} y \in & \mathbf{K}(y): \quad \langle Ay - f, v - y\rangle \geq 0 \quad \forall v \in \mathbf{K}(y), \\ & \mathbf{K}(y) := \{v \in V : v \leq \Phi(y)\}, \end{aligned} \tag{1}$$

in particular, the directional differentiability of the multi-valued (or set-valued) mapping $\mathbf{Q}$ taking the source term f into the set of solutions y. The non-smoothness in this case pertains to the map $\mathbf{Q}$ which in general is not differentiable in the classical sense, necessitating weaker concepts of differentiability and more advanced techniques. Here, V is a Hilbert space taken to be an appropriate subspace of an L^2-type space on a domain in $\mathbb{R}^n$, $\Phi\colon V \to V$ is increasing, $f \in V^*$ is a given source term, and $A\colon V \to V^*$ is an elliptic operator. Showing that the map $\mathbf{Q}$ is differentiable is an interesting analytical problem in its own right but it is also of significance for optimal control, numerics, and applications. This work provided the first result for the directional differentiability for QVIs in the infinite-dimensional setting (the corresponding theory for VIs has been thoroughly investigated; see, e.g., [4]).

The idea in [1] is as following. We take a source term $f \in V^*$, a direction $d \in V^*$, and a small perturbation parameter $t \in \mathbb{R}$, $t > 0$, and approximate an element $q(t) \in \mathbf{Q}(f + td)$ (that is, $q(t)$ solves the QVI (1) with source term $f + td$) by a sequence $q_n(t)$ of solutions of VIs, obtain suitable differential formulae for those VI solutions, and then pass to the limit in those formulae to obtain an expansion formula relating elements of $\mathbf{Q}(f + td)$ to elements of $\mathbf{Q}(f)$. There are some complications in this procedure:

1. **Derivation of the expansion formulae** for the above-mentioned $q_n(t)$; they must relate $q(t)$ to some $y \in \mathbf{Q}(f)$, and recursion plays a highly nonlinear role in the relationship between the iterates.
2. **Obtaining uniform bounds on the directional derivatives associated to the iterates**; even though the derivatives satisfy a VI, one has to handle a recurrence inequality in order to obtain uniform estimates.
3. **Identifying the limit of the higher-order terms as a higher-order term**; this procedure involves two limits: one as $t \to 0^+$ and one as $n \to \infty$, and commutation of limits in general requires an additional uniform convergence.

The main difficulty is the final point above. This iteration scheme requires some further restrictions on the data f and the direction d, namely we require them to be non-negative. Since we study the differentiability of implicit obstacle problems defined through the obstacle mapping Φ, it is clear that we need some differentiability of Φ.

The main result of [1] essentially states that under some assumptions, given $y \in \mathbf{Q}(f)$, there exists $q(t) \in \mathbf{Q}(f+td)$ and $\alpha = \alpha(d)$ such that

$$q(t) = y + t\alpha + o(t), \qquad t \to 0^+ \text{ in } V$$

holds where $t^{-1}o(t) \to 0$ as $t \to 0^+$ in V and α satisfies the QVI

$$\alpha \in \mathcal{K}_{\mathbf{K}(y)}(y,\alpha) : \langle A\alpha - d, v - \alpha \rangle \geq 0 \quad \forall v \in \mathcal{K}_{\mathbf{K}(y)}(y,\alpha),$$

where the constraint set appearing above is the critical cone defined by

$$\mathcal{K}_{\mathbf{K}(y)}(y,\alpha) := \{\varphi \in V : \varphi \leq \Phi'(y)(\alpha) \text{ q.e. on } \{y = \Phi(y)\} \text{ and } \langle Ay - f, \varphi - \Phi'(y)(\alpha)\rangle = 0\}.$$

Directional differentiability for parabolic QVIs. The authors have also recently extended the study of the above issues for the case of parabolic QVIs in [2]. There, we considered time-dependent QVIs of the form

$$\text{find } z : z \leq \Phi(z) : \int_0^T \langle z'(t) + Az(t) - f(t), z(t) - v(t)\rangle \,\mathrm{d}t \leq 0 \quad \forall v : v \leq \Phi(z),$$

and show that solutions exist in appropriate Bochner spaces under certain assumptions. These solutions have been shown to be given as a limit related to elliptic QVIs arising from the time discretization of the problem [2, Theorem 2.9] and as a limit of solutions of parabolic VIs [2, Theorems 3.8 and 3.10]. Directional differentiability is also proved [2, Theorem 5.15] in much the same way as in the elliptic case using the recently obtained results in [3] on the directional differentiability of parabolic VIs.

Application to thermoforming

We present an application of QVIs to thermoforming that was initially proposed by the authors in [1]. The aim of thermoforming is to manufacture products by heating a membrane or plastic sheet to its pliable temperature and then forcing the membrane onto a mould, which deforms the membrane and enables it to take on the shape of the mould. The process is applied to create both large structures like car panels and microscopic products such as microfluidic structures.

The contact problem associated with the heated membrane and the mould can be described as a VI problem. However, a non-trivial physical phenomenon occurs when the heated sheet is forced into contact with the mould: The mould is not at the same temperature as the plastic sheet, and this triggers heat transfer with hard-to-predict consequences.

A common mould material is aluminum, and its size is highly sensitive to heat fluctuations; aluminum has a relatively high thermal expansion volumetric coefficient, and this implies that there is a dynamic change in the mould (the obstacle) as the polymer sheet is forced in contact with it. This determines a compliant obstacle-type problem and, hence, the overall process is a QVI with underlying nonlinear PDEs determining the heat transfer and the volume change in the obstacle. In what follows, we consider this compliant obstacle behavior whilst making simplifying assumptions in order to study a basic but meaningful model.

The model. Let $\Phi_0 \colon [0,1] \to \mathbb{R}^+$ be the parametrized mould shape to be reproduced through a membrane. The membrane lies below the mould and is pushed upwards through some process f. We assume that

1. the temperature for the membrane is a prescribed constant,
2. the mould grows affinely with respect to changes in its temperature,
3. the temperature of the mould is subject to diffusion, convection, and boundary conditions arising from the insulated boundary, and it depends on its vertical distance to the membrane.

The thermoforming process is a time evolution system, but the setting described by the previous assumptions is appropriate for one time step in the time semi-discretization. We denote the position of the mould and membrane by $\Phi(u)$ and u, respectively, and T will stand for the temperature of the mould. The system we consider is the following:

$$u \in V : u \leq \Phi(u), \quad \langle -\Delta u - f, u - v \rangle \leq 0 \quad \forall v \in V : v \leq \Phi(u), \tag{2}$$

$$kT - \Delta T = g(\Phi(u) - u) \qquad \text{on } [0,1], \tag{3}$$

$$\partial_\nu T = 0 \qquad \text{on } \{0,1\}, \tag{4}$$

$$\Phi(u) = \Phi_0 + LT \qquad \text{on } [0,1], \tag{5}$$

where f is given, L is some linear increasing operator, $k > 0$ is a constant, $\Phi_0 \in V$, and $g \colon \mathbb{R} \to \mathbb{R}$ is decreasing and with $g(0) > 0$ and $0 \leq g \leq M$. Thus, when the membrane and mould are in contact or are close to each other, there is a maximum level of heat transfer onto the mould, whilst when they are sufficiently separated, there is no heat exchange.

Numerical implementation details. We approximate the QVI (2) by a penalized equation and numerically solve

$$\begin{aligned} Au + \alpha \max(0, u - y) - f &= 0, \\ kT - \Delta T - g(y - u) &= 0, \\ \partial_\nu T &= 0, \\ y - \Phi_0 - LT &= 0, \end{aligned} \tag{6}$$

for a large parameter α (as $\alpha \to \infty$, the solution of (6) converges to the solution of (2)–(5)). We use a finite difference scheme with N^2 uniformly distributed nodes with $N = 256$. The system (6) is discretized and solved via a semismooth Newton method applied to the mapping

$$(u, T, y) \mapsto \mathcal{F}(u, T, y)$$

defined by the left-hand side of (6). An approximation to the directional derivative of the QVI solution mapping was computed by first smoothing the nonlinearity in the first equation of (6) by a function $\max_g$ and differentiating it with respect to f in a direction d:

$$Au'(f)(d) + \alpha \max_g'(0, u - y)u'(f)(d) - d = 0.$$

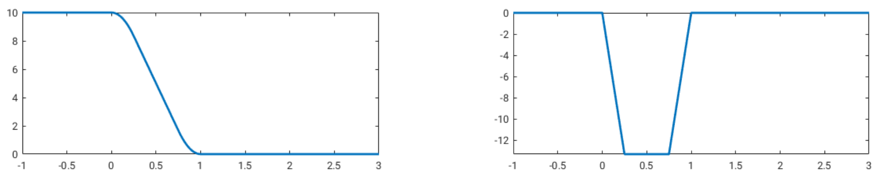


Fig. 3: Plot of the function g and its derivative

We take the source term $f \equiv 10^2$. The nonlinearity g appearing in the source term for the T equation is selected as a piecewise smooth function, see Figure 3.

The directional derivative is taken in the direction χ_A, the characteristic function of the set $A = \{(x,y) : x > 1/2\}$. The remaining parameters appearing in the physical model are $k = 1$ and $\alpha = 10^8$.

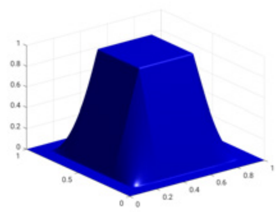
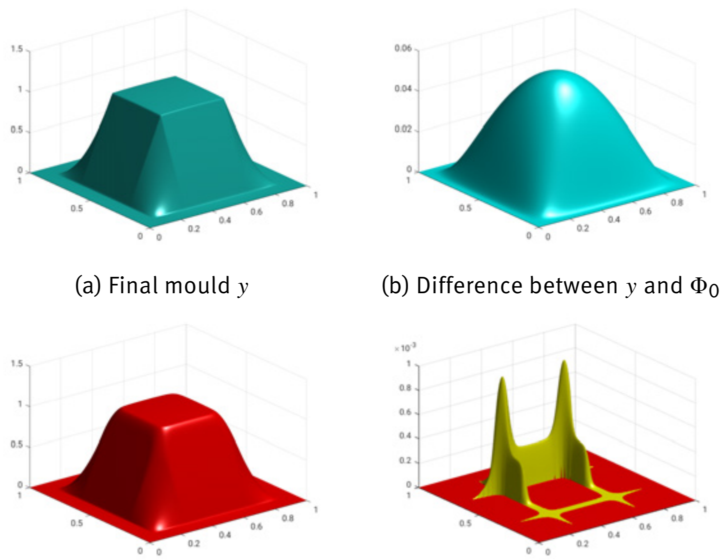


Fig. 4: The initial mould Φ_0

Numerical results. The results of the numerical simulation are shown in Figure 5.

- The effect of the temperature interplay between the membrane and mould can be immediately seen: Φ_0 (Figure 4) grows and becomes more curved and smoothed out, which is natural given that the membrane is initially placed below the mould and is pushed upwards.
- The model produces a membrane u that appears to be a good fit for the thermoforming process; it can be observed to be similar to the final mould.
- The directional derivative is colored yellow and red; red refers to the parts of the domain corresponding to the coincidence set $\{u = y\}$. It can be seen that the derivative is non-zero on the non-coincidence set (since the membrane has freedom to move there), but one also sees non-zero contributions on the coincidence set: a feature of the underlying *compliant* obstacle behavior.



(a) Final mould y (b) Difference between y and Φ_0

(c) Membrane u (d) The directional derivative

Fig. 5: *Computational results*

Outlook. In the direction of the work elucidated above, the authors intend to continue by studying optimal control problems with QVI constraints. In particular, the derivation of stationarity or optimality conditions and the intermediary techniques required for those derivations (such as theory for approximating solutions to QVIs via penalization techniques, for example) are of fundamental importance to advance the field. Furthermore, a more complicated thermoforming model will also be studied.

References

[1] A. Alphonse, M. Hintermüller, C.N. Rautenberg, *Directional differentiability for elliptic quasi-variational inequalities of obstacle type*, Calc. Var., **58** (2019), pp. 39/1–39/47.

[2] A. Alphonse, M. Hintermüller, C.N. Rautenberg, *Existence, iteration procedures and directional differentiability for parabolic QVIs*, to appear in: Calc. Var., 2020.

[3] C. Christof, *Sensitivity analysis and optimal control of obstacle-type evolution variational inequalities*, SIAM J. Control Optim., **57**:1 (2019), pp. 192–218.

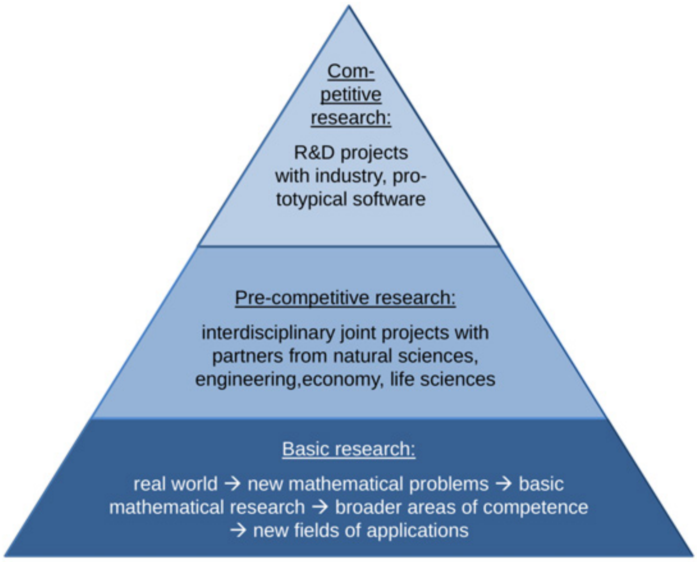
[4] F. Mignot, *Contrôle dans les inéquations variationelles elliptiques*, J. Funct. Anal., **22**:2 (1976), pp. 130–185.

2 WIAS in 2019

- 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-four 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 "4th Leibniz MMS Days" took place from March 20 to 22, 2019, in Kühlungsborn; see page 116.

WIAS has a number of cooperation agreements with universities. The main joint project with the Berlin universities is 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), which has been funded since January 2019. The WIAS Director, Michael Hintermüller, is a founding member (PI) of MATH+, one of three co-speakers of the center, and a Scientist-In-Charge of MATH+' Emerging Field *Model-based Imaging*. The structure of MATH+ 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.

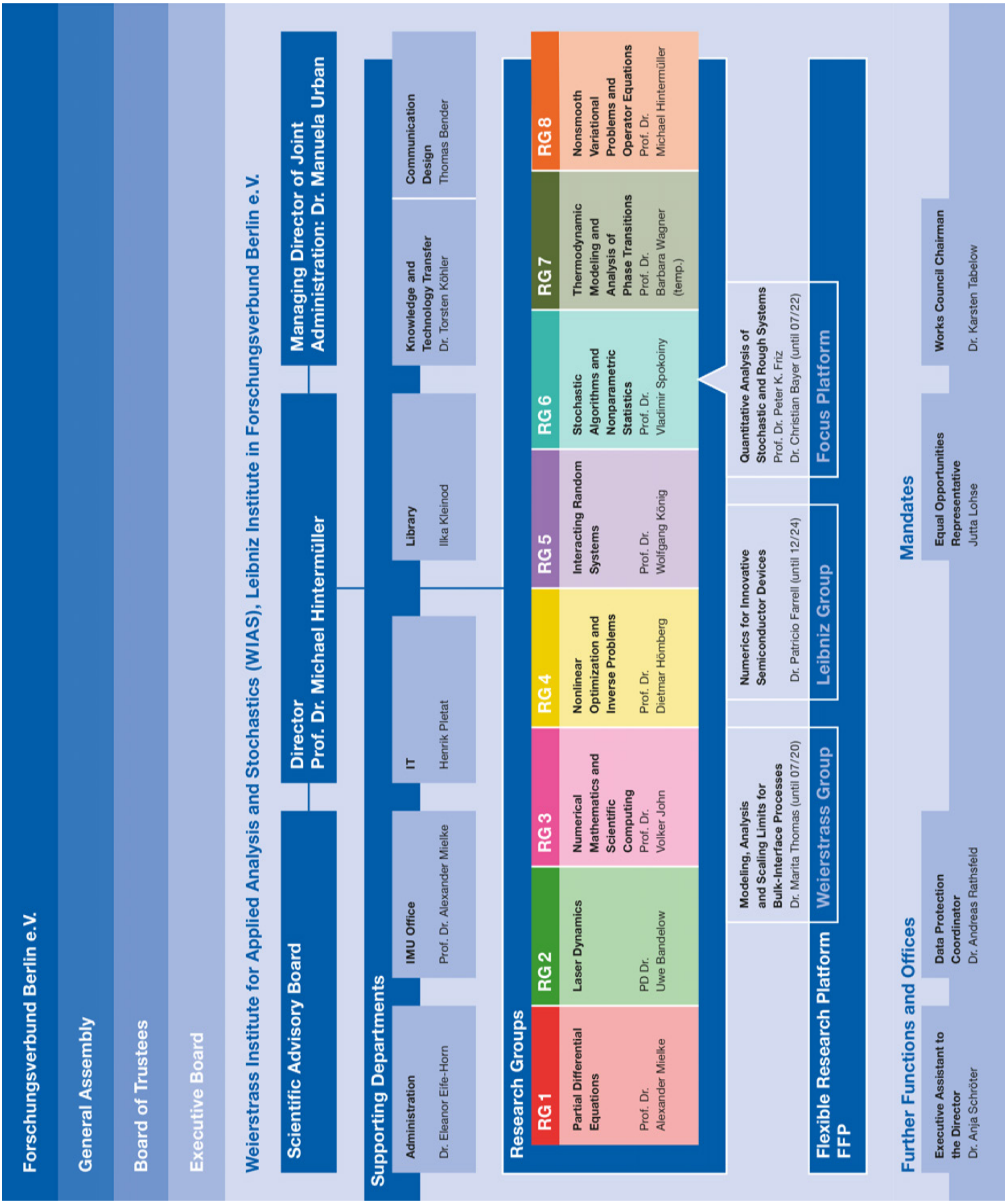
MATH+

2.2 Structure and Scientific Organization

2.2.1 Structure

In 2019, WIAS was organized into the following divisions for fulfilling its mission: Eight research groups, 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.

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


Forschungsverbund Berlin e.V.
General Assembly
Board of Trustees
Executive Board
Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Leibniz Institute in Forschungsverbund Berlin e.V.
Scientific Advisory Board
Director Prof. Dr. Michael Hintermüller
Managing Director of Joint Administration: Dr. Manuela Urban
Supporting Departments
Administration Dr. Eleanor Eife-Horn
IMU Office Prof. Dr. Alexander Mielke
IT Henrik Pletat
Library Ilka Kleinod
Knowledge and Technology Transfer Dr. Torsten Köhler
Communication Design Thomas Bender
Research Groups
RG 1 Partial Differential Equations Prof. Dr. Alexander Mielke
RG 2 Laser Dynamics PD Dr. Uwe Bandelow
RG 3 Numerical Mathematics and Scientific Computing Prof. Dr. Volker John
RG 4 Nonlinear Optimization and Inverse Problems Prof. Dr. Dietmar Hömberg
RG 5 Interacting Random Systems Prof. Dr. Wolfgang König
RG 6 Stochastic Algorithms and Nonparametric Statistics Prof. Dr. Vladimir Spokoiny
RG 7 Thermodynamic Modeling and Analysis of Phase Transitions Prof. Dr. Barbara Wagner (temp.)
RG 8 Nonsmooth Variational Problems and Operator Equations Prof. Dr. Michael Hintermüller
Flexible Research Platform FFP
Weierstrass Group
Modeling, Analysis and Scaling Limits for Bulk-Interface Processes Dr. Marita Thomas (until 07/20)
Leibniz Group
Numerics for Innovative Semiconductor Devices Dr. Patricio Farrell (until 12/24)
Focus Platform
Quantitative Analysis of Stochastic and Rough Systems Prof. Dr. Peter K. Friz Dr. Christian Bayer (until 07/22)
Further Functions and Offices
Executive Assistant to the Director Dr. Anja Schröter
Data Protection Coordinator Dr. Andreas Rathsfeld
Mandates
Equal Opportunities Representative Jutta Lohse
Works Council Chairman Dr. Karsten Tabelow

The Secretariat of the International Mathematical Union (IMU, see page 52), 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:

WG 1. Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes
FP 1. Quantitative Analysis of Stochastic and Rough Systems

The organization chart on page 42 gives an overview of the organizational structure of WIAS in 2019.

2.2.2 Main Application Areas

The research at WIAS focused in 2019 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 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 2019 in the interdisciplinary solution process described above (dark color: over 20% of the group's working time, light color: up to 20% of the group's working time, blue: no contribution).

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

In the following, special research topics are listed that were addressed in 2019 within the general framework of the main application areas.

Conversion, Storage and Distribution of Energy

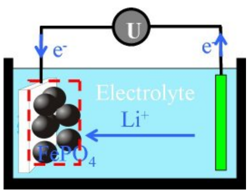


Fig. 1: *Sketch of a lithium-ion battery (LiFePO4)*

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, for which mathematical models are developed in RG 7. Modern mathematical methods such as homogenization techniques enable a sound description of porous battery electrodes. With this, some key aspects are the prediction of the cell voltage, the incorporation of ageing phenomena, and validation with experimental data. 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.

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.

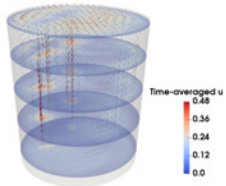


Fig. 2: *Time-averaged turbulent flow through a laddle*

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)
- Description of random message trajectories in spatial telecommunication models (in RG 5)
- Modeling, analysis, and simulation of multiphase flows (variational modeling/thermodynamics and free boundaries; in RG 7 and WG 1)

Materials Modeling

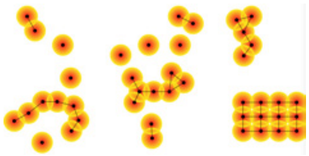


Fig. 3: *A realisation of a many-body system showing a small crystal in the lower right corner*

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 (in RG 3, RG 5, and RG 6)
- 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 WG 1, RG 1, RG 6, and RG 7)
- Material models with stochastic coefficients (in RG 1, RG 4, RG 5, and RG 7)
- Modeling and analysis of complex fluids (suspensions, hydrogels, polyelectrolytes; in RG 7 and WG 1)
- 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, WG 1, and RG 7)
- Modeling of elastoplastic and phase-separating materials (including damage and fracture processes; in RG 1, RG 7, and WG 1)
- Derivation and analysis of local and nonlocal phase field models and their sharp-interface limits (in RG 1, RG 7, and WG 1)

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 and WG 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)

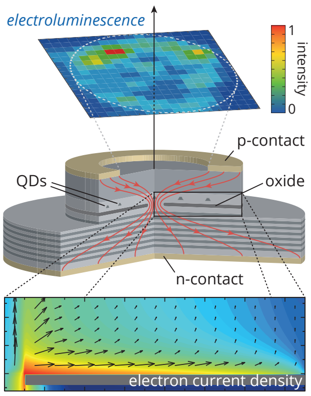


Fig. 4: *Simulated spreading of injection current density in a quantum-dot based single photon emitter with Al-oxide aperture. An improved design was proposed on that base in:* M. KANTNER, U. BANDELOW, T. KOPRUCKI, J.-H. SCHULZE, A. STRITTMATTER, H.-J. WÜNSCHE, Efficient current injection into single 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.

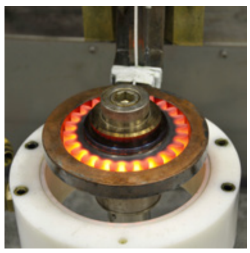


Fig. 5: *Induction heat treatment of a gear*

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

Core areas:

- Simulation and control in process engineering (in RG 3, RG 4, and RG 6)
- Problems of optimal shape and topology design (in RG 4 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)

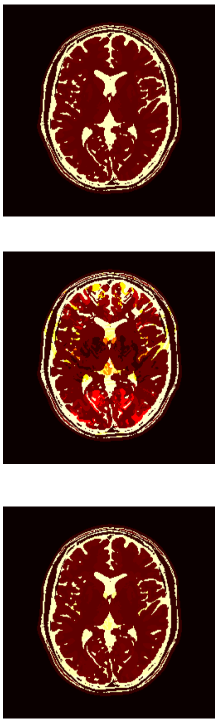


Fig. 6: *Quantitative MRI: Estimation of the T_2 relaxation times of matter leading to characterization of different types of tissue. (1) Ground truth, (2) State-of-the-art dictionary-based method (improved variant of Magnetic Resonance Fingerprinting-MRF), (3) Integrated physics-based approach where 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, problems from image and signal processing with applications especially in the neurosciences are considered. They include classical tasks like registration, denoising, equalization, and segmentation. Moreover, (low-rank/sparse) data decomposition and functional correlations, e.g., in neurological processes, are also studied. These processes typically lead to complex, nonlinear, or nonsmooth inverse problems where often also statistical aspects play a central part for data modeling and analysis methods. The current focus of research is the consideration of (bio)-physics-based models for data and image analysis. Furthermore, 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.

Core areas:

- Numerical methods for biofluids and biological tissues (in RG 3 and RG 8)
- Image processing (in RG 6 and RG 8)
- Modeling of high-resolution magnetic resonance experiments (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)
- (Bio-)physics-based quantitative imaging (in RG 6 and RG 8)

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 engage the services of benefit@work, a family service agency whose offers are optimized to meet the needs of WIAS's staff.

Zertifikat seit 2013
audit berufundfamilie
www.berufundfamilie.de

In every year, another member of the direction of WIAS is appointed to take the responsibility for equality affairs in the institute. In 2019, this was Wolfgang König, the head of Research Group 5 "Interacting Random Systems". Since September 1, 2018, Jutta Lohse has been the new equal opportunities officer of WIAS. Both are part of the team "Work and Family" that also comprises the project head of the berufundfamilie audit, Olaf Klein, and Laura Wartenberg. The most important activities of this team in 2019 were on the one hand the implementation and evaluation of an employee attitude survey, and on the other hand the preparation of the final report and several intensive discussion meetings on the three-years period of the *audit berufundfamilie*, jointly with the application for the certificate for the consolidation phase, April 2020 – March 2023. The formulation of the new Target Agreement for the said period of time was another very demanding task. Furthermore, new measures with respect to conflict management have been installed in September 2019, and a management coaching took place in June 2019.

On March 28, 2019, 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. Eleven 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 lectures with workshops by external experts on March 3, 2019, on "Balance of work, family and private life", and another one on August 22, 2019, on "Stress- und Konfliktmanagement", which were again well attended. Furthermore, the administration organized a couple of opportunities for individual massage units at the institute for sustaining the employees' general health. On December 9, 2019, the "Work and Family" team of WIAS organized the second Christmas party for the children of the collaborators. Eleven 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 2019, having raised a total of 3.6 million euros, from which 41 additional researchers [2] (plus 8 outside WIAS; Dec. 31, 2019) were financed. In total in 2019, 25.19 percent of the total budget of WIAS and 42.27 percent[2] of its scientific staff originated from grants.

For a detailed account of projects funded by third parties, the reader is referred to the appendix, Section A.2 Grants below on pages 106ff.

[2] Including scholarship holders.

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.

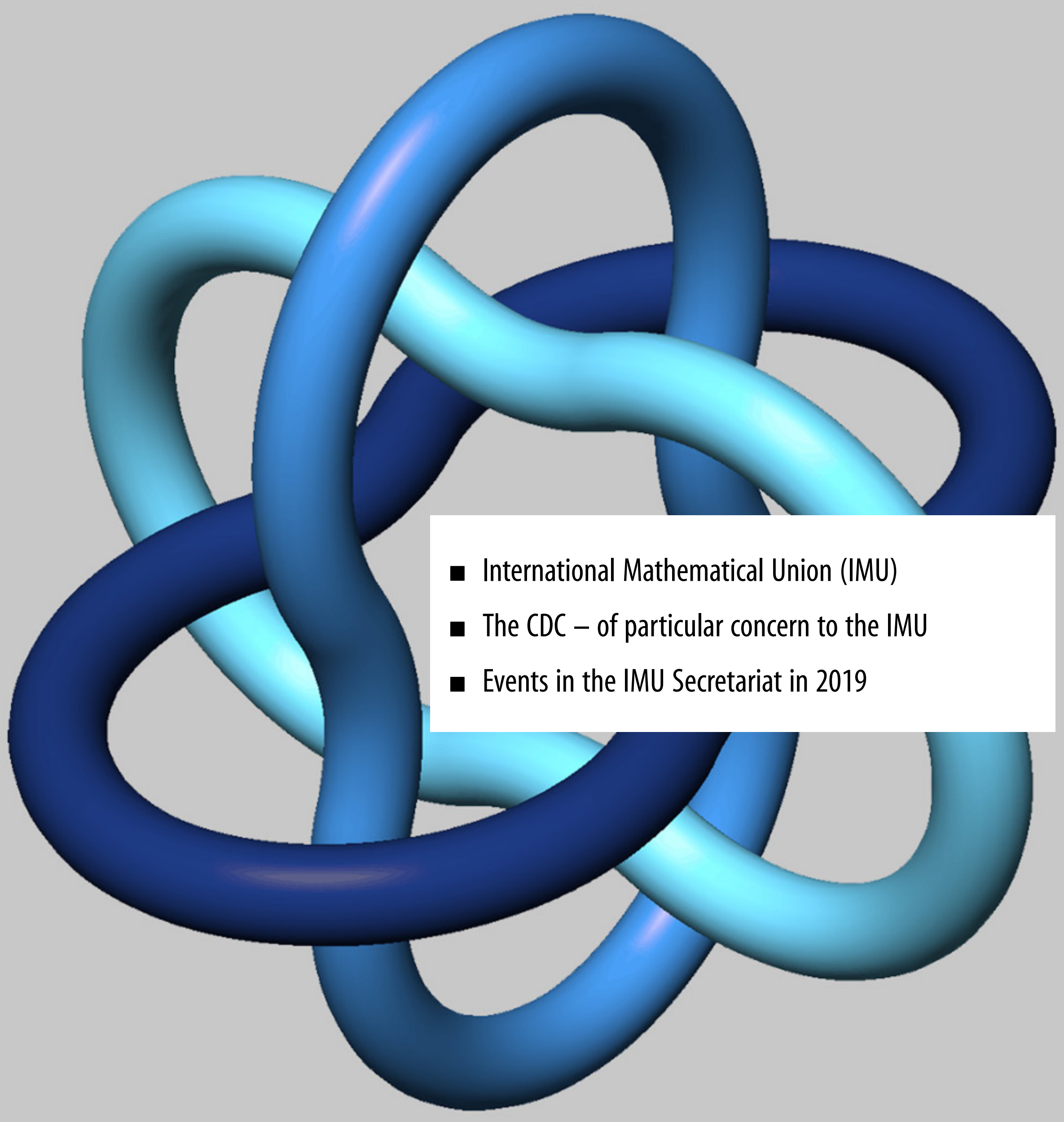
International Research Training Group (IRTG) 1792 *High Dimensional Non Stationary Time Series Analysis* of the DFG

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 177ff. 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



- International Mathematical Union (IMU)
- The CDC – of particular concern to the IMU
- Events in the IMU Secretariat in 2019

3.1 International Mathematical Union (IMU)

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

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 during the period 2011–2018, the IMU General Assembly 2018 passed a resolution to make enter into a new and unlimited Cooperation Agreement, which was signed immediately after this General Assembly meeting was closed.

Since April 2018, the IMU Secretariat has its headquarters on the 4th floor of Hausvogteiplatz 11A, close to the main building of WIAS.

Staff members

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

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

Lena Koch, *ICMI and CDC Administrative Manager*. L. Koch was on leave. Her responsibilities include to support administratively the activities of the Commission for Developing Countries and the International Commission on Mathematical Instruction. This refers, in particular, to 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, *ICMI and CDC Administration*. R. Fischer was handling CDC and ICMI activities during the ICMI and CDC Administrative Manager's leave.

Imren Karci, *Project Assistant*. I. Karci's task is to support the administrative work of the IMU Secretariat, in particular, to assist in the organizational handling of CDC programs and general IMU activities.

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 CDC – of particular concern to the IMU

Olga Gil Medrano (CDC)

The Commission for Developing Countries (CDC) aims to design and carry out IMU activities focused on the development of mathematics in those countries with the greatest difficulties, either due to the lack of adequate structures or the shortage of economic resources. The Commission, created in the General Assembly (GA) that took place in Bangalore (India) in 2010, has existed since January 2011 and is the heir of other previous IMU structures, since international solidarity with mathematicians who are in less favoured situations has been a constant of the IMU in its one hundred years of existence.

Fig. 1: *First meeting of the new CDC, Feb. 2019, Photo K. Herschelmann*

The work of the CDC follows the four-year cycle pattern set by the International Congresses of Mathematicians. Thus, at the beginning of the year 2019, a significant proportion of the ten members of the Commission have been renewed.

The first meeting of the new CDC took place on February 27–28, 2019, at the IMU headquarters in Berlin. This is the most important meeting in the four-year period and not only because of the content of the agenda. It also allows personal contact that will later facilitate communication between members, which is essentially done electronically.

On this occasion, all the activities underway were studied to decide those that would continue with small reviews and those that will need to be evaluated in greater depth. Responsibilities were distributed among the members and, in particular, the composition of the evaluation committees of the different programs was decided, which also include mathematicians external to the CDC. A framework budget was also decided on for the entire period. The good work, kindness, and effort of the IMU staff, together with the suitability of the new facilities in Hausvogteiplatz, made this crucial meeting very beneficial, thus facilitating the operation of the Commission throughout the year and probably during the entire period.

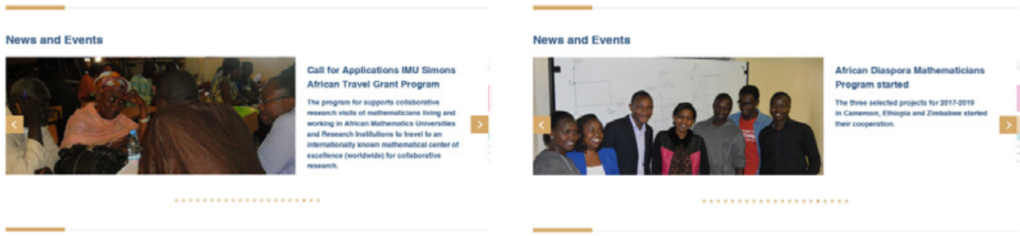


Fig. 2: *From CDC News and Events: Call for Applications IMU Simons African Travel Grant Program, African Diaspora Mathematicians Program started*

An informal meeting with the Executive Committee (EC) took place on February 28 and, on March 1, the President and the two Secretaries of the CDC were invited to report during the EC meeting. The CDC was commissioned by the EC to submit a proposal to revise the definition of a developing country that IMU will apply during the four-year period in all its activities, including financial assistance for participation in ICM2022.

The subject is delicate and far from trivial. After a few months of study and deliberations of the different possibilities, the CDC reached the proposal to include in the list of developing countries all those who are not classified as *High Income countries* by the World Bank (WB) in its July 2019 update. These countries are those that, according to the WB data for the year 2018, have a gross national income per capita of less than USD 12,375. The CDC also proposed a division into five priority groups, based on the above-mentioned WB data. The list, approved by the IMU EC, is in effect since the last quarter of 2019.

Fig. 3: *From CDC News and Events: Mentoring African Research in Mathematics (MARM), IMU 2019 Breakout Graduate Fellowships Awarded*

Annual calls for programs have been carried out in parallel to this reflection on definitions and programs, its set-up to adapt them to the circumstances of a world that changes so quickly, the implementation on the CDC website and dissemination of these updates; as for instance, the *Conference Support Grants Program* that gives partial support to 30–40 conferences and research schools every year.

Research Travel Grants support mathematicians professionally based in developing countries to visit an international research collaborator for a period of one month. The travel costs of up to 3–4 mathematicians are supported within the *Individual Travel Support Program*. All travel and living expenses of the grantees are covered by the 7–8 fellowships offered within the *IMU-Simons African Fellowship Program* and the 3–4 fellowships, restricted to young mathematicians, awarded by the *Abel Visiting Scholar Program*, that are financed by the Simons Foundation (USA) and the Niels Henrik Abel Board (Norway), respectively.

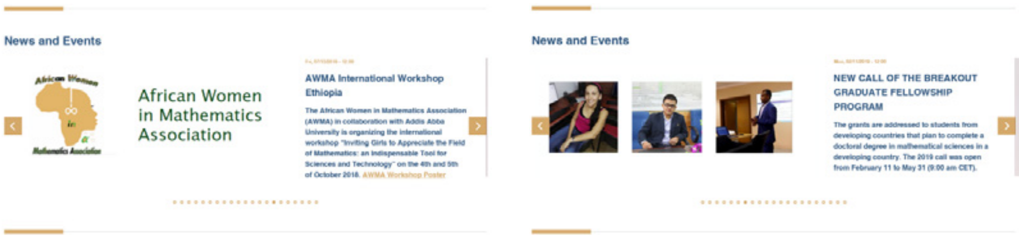


Fig. 4: *From CDC News and Events: AWMA International Workshop Ethiopia, New Call of the Breakout Graduate Fellowship Program*

The goal of the *Volunteer Lecturer Program* is to foster research and international cooperation between mathematicians in developing countries and the international mathematical community, offering to the universities in the developing countries the economic support to host volunteer lecturers for intensive 3–4-week courses in mathematics. The American Mathematical Society and the Niels Henrik Abel Board fund this program that supports about ten visits every year.

Thanks to a generous donation by all the winners of the Breakthrough Prizes in Mathematics, the *IMU Breakout Graduate Fellowships Program* offers full-time research grants for excellent students from developing countries following studies leading to a Ph.D. degree, in a developing country. Three students were awarded in 2019. Another scheme, the *GRAID (Graduate Assistantships in Developing Countries) Program*, provides modest support for emerging research groups, working in a developing country listed in Priority 1 or 2 of the IMU definition, making it possible for them to fund their most talented students to study full-time and pursue a Master or Ph.D. graduate degree in mathematics. The GRAID Program, funded by voluntary donations from mathematicians or mathematical institutions worldwide, has awarded two groups with a total of five students in 2019.

The necessary financial contribution for these programs comes from the stable allocation that the IMU General Assembly grants to the CDC in the IMU budgets, to which are added the generous contributions mentioned above and those from Mathematical Society of Japan, London Mathematical Society, Swiss Mathematical Society, and about one thousand individual mathematicians. On average, the activities of the CDC obtain two thirds of their total funding from these external sources.

Fig. 5: *From CDC News and Events: New Call of the IMU-CDC Graduate Assistantships in Developing Countries Program (GRAID), IMU Mathematics Library Assistance Scheme for Developing Countries*

Still, when observing the great difficulties that mathematical research and doctoral training suffer in many countries, in some of them they are endemic and in others, such as the so-called *emerging countries*, due to the economic slowdown, it is easy to conclude that the efforts of IMU through the CDC are a drop in the ocean. But, within the economic and administrative limits of an international union, these efforts are a reflection of—and we expect, a stimulus for—the solidarity work of the international mathematical community in helping mathematical development in countries in difficulty, through very different initiatives and especially the work of many volunteers.

3.3 Events in the IMU Secretariat in 2019

Meeting of the ICMI IPC for ICMI Study 25, February 11–13, 2019. The International Program Committee of the ICMI Study 25 met in order to prepare the study conference on "Teachers of Mathematics Working and Learning in Collaborative Groups", taking place in Lisbon, Portugal, February 3–7, 2020. The conference addresses mathematics education researchers, teachers, teacher educators, mathematicians, educational policy makers, and other stakeholders who offer diverse perspectives from various contexts.

Participants: Jill Adler, Abraham Arcavi, Kelly Boles, Hilda Borko, Shelley Dole, Cristina Esteley, Rongjin Huang, Ronny Karsenty, Takeshi Miyakawa, Joao Pedro da Ponte, Despina Potari, Ornella Robutti, Luc Trouche.

Meeting of the Commission for Developing Countries (CDC), February 27–28, 2019. The newly elected CDC had its first physical meeting in its four-year term. On February 28, there was a one-hour joint meeting of the CDC and IMU EC members.

Participants: Dipendra Prasad, Olga Gil Medrano, Alf Onshuus, José Maria P. Balmaceda, Jean-Luc Dorier, Mama Foupouagnigni, Galina Rusu, Andrea Solotar, Michel Waldschmidt, Carlos E. Kenig, Luigi Ambrosio.

Fig. 1: *Gathering of the participants of the meeting of the CDC, the IMU EC, and guests*

Meeting of the IMU Executive Committee (IMU EC), March 1–3, 2019. The newly elected IMU EC held its first annual meeting in its four-year term. A. Mielke, as the Head of the IMU Secretariat, introduced the IMU Secretariat staff to the new EC. The Director of Weierstrass Institute (WIAS), M. Hintermüller, welcomed the EC and made a brief presentation of the WIAS.

Participants: Carlos E. Kenig, Helge Holden, Nalini Joshi, Loyiso G. Nongxa, Luigi Ambrosio, Andrei Okounkov, Paolo Piccione, R.T. Ramadas, Gang Tian, Günter M. Ziegler, Shigefumi Mori, Ulrike Tillmann, Martin Hairer. Via Skype: Terence Tao, Patrick Ion.

Meeting of the Committee on Electronic Information and Communication (CEIC), October 26–27, 2019. The newly appointed CEIC held its first annual meeting in the premises of the IMU Secretariat.

Participants: Henry Cohn, Marie Farge, Patrick Ion, Alf Onshuus, Mila Runnwerth, Nalini Joshi, Helge Holden. Via Skype: Tim Cole, Rajeeva Karandikar, Victoria Stodden.

Visit of the Berliner Wissenschaftliche Gesellschaft (BWG), July 9, 2019. Members of the BWG were taken on a guided tour through the IMU Secretariat on the occasion of the BWG annual meeting that was hosted by the WIAS.

Participants: Günter Bärwolff, Detlef Bartsch, Hans-Peter Berlien, Ulrich Bommer, Hans-Jörg Buhk, Aljoscha Burchardt, Ralf Einspanier, Heinz Fortak, Elke Frommann, Rolf Großklaus, Dieter Großklaus, Martin Heger, Andreas Herrmann, Constanze Hoffmann, Hannelore Horn, Hans Lechner, Michael Linscheid, Friedrich Meuser, Sophia Meuser, Katrina Meyer, Karin Mölling, Eberhard Müller, Ulrike Nikutta-Wasmuht, Helmut Pucher, Ingrid Reisinger, Petra Roloff, Jakob Schirrmacher, Eckehard Schöll, Peter Scholz, Bernd Sösemann, Julia von Thienen, Peter Theodor Wilrich, Birgit Wilrich.

Other guests. Historian Antina Scholz did research in the IMU Archive (March 20–21 and July 8–9); CWM Chair Marie-Françoise Roy paid an individual visit to the office; Historian Nobert Schappacher did research in the IMU Archive (October 22–25, November 12–13, and December 4); ICMI Archive Curator Bernard Hodgson did research in the ICMI Archive (November 28–December 5).

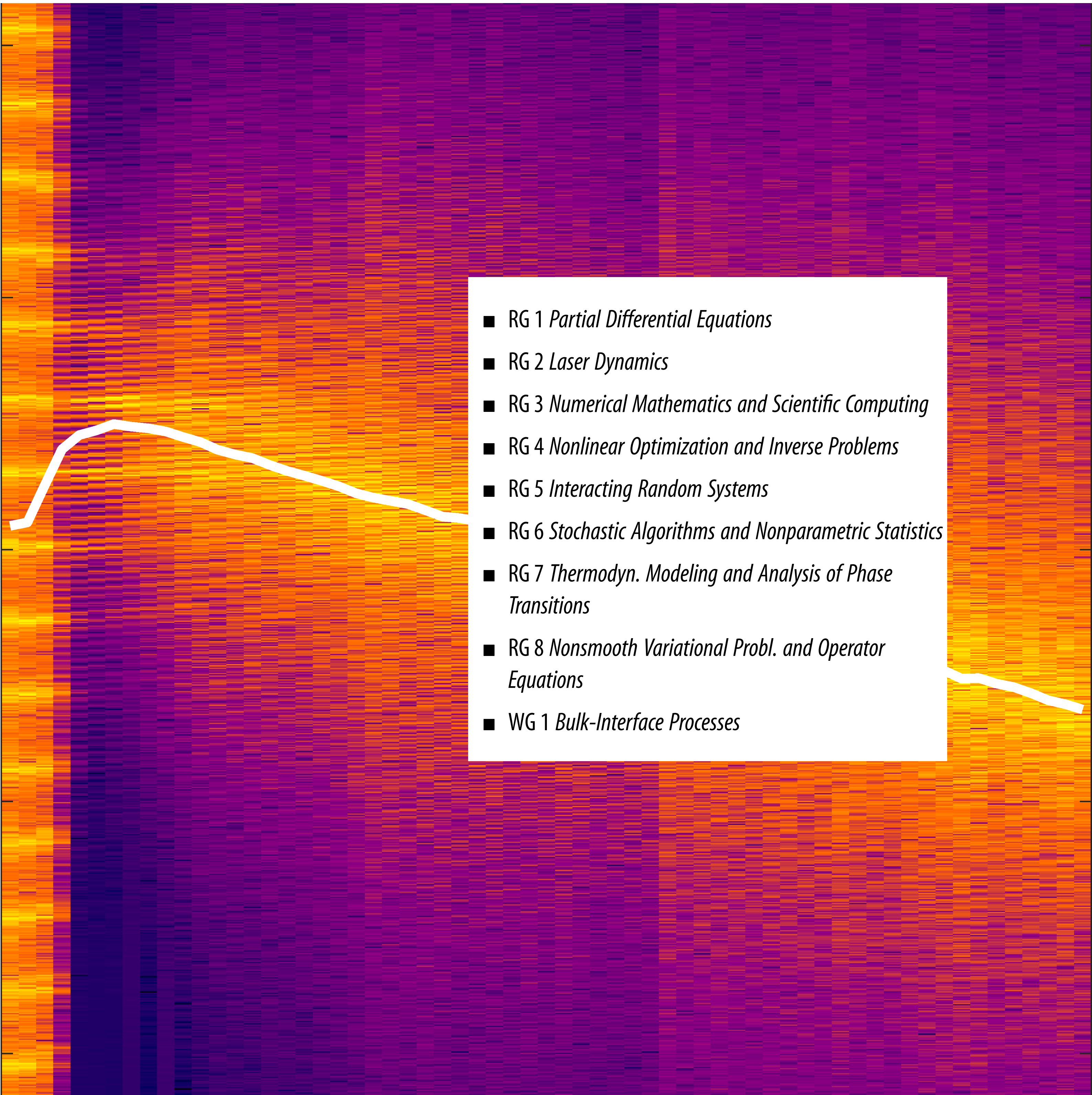
Announcement of the IMU

March 14 – The International Day of Mathematics

On the initiative of the IMU, the 40th General Conference of UNESCO in Paris approved the Proclamation of March 14 (Pi Day) as the **International Day of Mathematics (IDM)**. The international launch of the IDM will take place in Paris and Nairobi in 2020.

"Mathematics is everywhere” is the theme for IDM in 2020.

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*
- WG 1 *Bulk-Interface Processes*

4.1 Research Group 1 "Partial Differential Equations"

Head:	Prof. Dr. Alexander Mielke
Deputy Head:	Priv.-Doz. Dr. Annegret Glitzky
Team:	Dr. Duy Hai Doan Thomas Frenzel Dr. Martin Heida Dr. Katharina Hopf Dr. Hans-Christoph Kaiser Dr. Thomas Koprucki Dr. Matthias Liero Anieza Maltsi Dr. Oliver Marquardt Dr. Grigor Nika Dr. Joachim Rehberg Dr. Nella Rotundo Artur Stephan
Secretary:	Andrea Eismann
Nonresident Members:	Prof. Dr. Herbert Gajewski Prof. Dr. Konrad Gröger Prof. Dr. Jürgen Sprekels

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
- Nonlinear material models, in particular, 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 fields of applications, e.g., in natural sciences, technology, economy, and life science. 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.

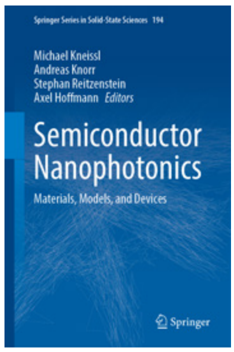
PDE 2019: Partial Differential Equations in Fluids and Solids. This international workshop took place at Weierstrass Institute Berlin, September 9–13, 2019. It fused expertise on the analysis of PDEs in solids, fluid dynamics, complex fluids, and interaction of fluids with solid structures and advanced analytical methods in current research related to systems with bulk-interface interaction, geometrically nonlinear materials, and fluid-structure interaction. This concerns, e.g., Lagrangian and Eulerian descriptions, free boundaries and moving domains, and variational approaches via energy/entropy methods. In addition, PDE 2019 hosted a meeting of the GAMM Activity Group Analysis of Partial Differential Equations on Thursday, September 12, 2019.

Fig. 1: *The participants of the workshop organized by RG 1 (Alexander Mielke, Hans-Christoph Kaiser), WG 1 (Marita Thomas), Helmut Abels (U Regensburg), and Karoline Disser (TU Darmstadt)*

L^p-theory for second-order elliptic operators in divergence form with complex coefficients. For second-order elliptic operators with *real* coefficients, far reaching results up to holomorphic calculi and maximal parabolic regularity are available even in the case of nonsmooth data. Unfortunately, in the case of *complex* coefficients, one is confronted with the following obstructions: (i) even if there is a consistent semigroup on L^∞, this needs not be a contraction semigroup – and not even quasicontractive, (ii) the "parabolic maximum principle" does not hold. The main result of the paper [4] was to construct – in terms of the data, the domain, and the coefficient function – a large interval I, such that, for $p \in I$, the semigroup still exists on L^p. Furthermore, it is proved that these semigroups are even analytic and admit a bounded holomorphic calculus. The Dore–Venni theorem ensures that the operator even satisfies maximal parabolic regularity. By perturbation arguments, it is shown that Gaussian estimates are maintained for small perturbations of *real* coefficient functions.

Semiconductors

In this field, RG 1 benefits from a strong cooperation with RG 2 *Laser Dynamics* and RG 3 *Numerical Mathematics and Scientific Computing*. The group was involved in the successful conclusion of the DFG Collaborative Research Center CRC 787 *Semiconductor Nanophotonics: Materials, Models, Devices* (2008–2019) via the subproject B4 "Multi-dimensional modeling and simulation of electrically pumped semiconductor-based emitters" (jointly with RG 2 and Zuse Institute Berlin),



see [5]. RG 1 acquired three subprojects within the Cluster of Excellence *Berlin Mathematics Research Center* MATH+ starting January 2019, namely AA2-1, "Hybrid models for the electrothermal behavior of organic semiconductor devices", AA2-5, "Data driven electronic structure calculations for nanostructures (DESCANT)", and EF3-1 "Model-based geometry reconstruction from TEM images" (together with RG 6 *Stochastic Algorithms and Nonparametric Statistics*), see the report of RG 6 on page 84. Additionally, the transition project SE18 "Models for heat and charge-carrier flow in organic electronics" was funded by MATH+ for nine months.

Electronic properties of graded-composition quantum dots. Within the MATH+ subproject AA2-5, electronic properties of $InAs_{1-x-y}Sb_xP_y$ quantum dots (QDs) were determined mathematically. These QDs are grown using liquid phase epitaxy by Prof. Gambaryan (Yerevan State University, Armenia) and characterized by different microscopic and spectroscopic techniques of the Paul Drude Institute and the Institute for Crystal Growth, Berlin. A side-view obtained by scanning transmission electron microscopy (STEM) of such a typical, cone-shaped QD is shown in Figure 2 a), and the QDs furthermore exhibit a composition gradient along their growth axis, having a maximum Sb (P) contents of 20 (15)% at the QDs top (bottom). Figure 2 b) shows the diameter distribution within the QD ensemble, typical QD heights are 8 ± 1 nm. Based on these data, the hole ground state energies and charge densities for the observed systems were computed by an eight-band $\mathbf{k}\cdot\mathbf{p}$ model (cf. Figure 2 c)). The simulated absorption spectrum predicted a maximum at 3.829 μm, which perfectly matches the experimentally observed peak at 3.83 μm [3].

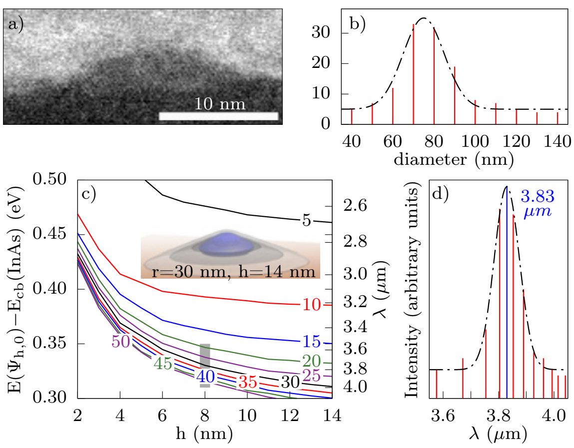


Fig. 2: *a) Side view STEM image of a typical QD. b) Diameter distribution in an ensemble. c) Transition energy as a function of QD height and diameter. QD diameters are indicated directly at the respective curves in nm. The inset shows an example hole ground state (blue) inside a graded-composition QD. d) Simulated ensemble spectrum obtained by combining Figs. b) and c). The experimentally observed peak emission energy is indicated in blue. [3].*

Electrothermal models for organic semiconductor devices. The MATH+ subprojects SE18 and AA2-1 investigated the interplay of Joule heating, heat flow, and temperature-activated hopping transport in organic semiconductor materials with Gaussian disorder. Possible effects are, in the worst case, the thermal destruction of the material, but more interesting phenomena are S-shaped current-voltage relations with regions of negative differential resistance, or inhomogeneous luminance of large-area organic LEDs. The drift-diffusion-based electrothermal models for organic semiconductors take into account Gauss–Fermi statistics and mobility functions depending on temperature, charge carrier density, and electrical field strength with positive feedback. In 3D, the solvability of the problem (weak solutions for the quasi-Fermi potentials and the electrostatic potential, entropy solution for the heat equation) was established by Schauder's fixed point theorem. The system with Gauss–Fermi statistics, positive temperature feedback in the mobilities, and with temperature-dependent Ohmic contact boundary conditions was discretized by a finite volume-based generalized Scharfetter–Gummel scheme. Using path-following techniques, it was demonstrated in [2] that the model exhibits S-shaped current-voltage curves with regions of negative differential resistance (see Figure 3), as observed experimentally by the cooperation partners of the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP).

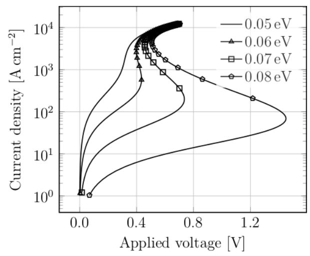


Fig. 3: *Simulated current-voltage relations for different values of Gaussian disorder parameters of organic materials*

Material modeling

The research in this topic is done in cooperation with RG 5 *Interacting Random Systems* and the WG 1 *Modeling, Analysis and Scaling Limits for Bulk-Interface Processes* and was driven by subprojects of the DFG Collaborative Research Center CRC 1114 *Scaling Cascades in Complex Systems*. In the second period of the CRC 1114, the group participates with three subprojects: B01 (together with FU Berlin and GFZ Potsdam), C02 (with FU Berlin), and C05 (WIAS only).

Stochastic homogenization. Within the subproject C05 "Effective models for materials and interfaces with multiple scales", an important gap in the theory of stochastic homogenization was closed. Within the theory of homogenization on perforated domains, it has been shown that even very irregularly perforated domains possess a family of uniformly bounded extension operators. For a random geometry of balls as indicated in Figure 4, functions defined on the white area need to be extended to the grey area in such a way that the gradient of the extended functions can be controlled uniformly by the original gradient. Such extension operators are the prerequisite for a theory of homogenization of nonlinear partial differential equations and were known in the periodic theory for a long time, but not in the more general stochastic setting. Accordingly, this work is relevant for multiscale modeling beyond the CRC 1114.

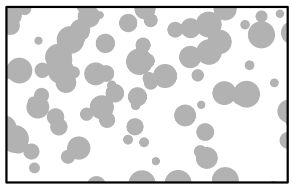
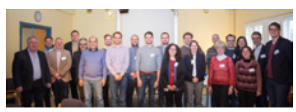


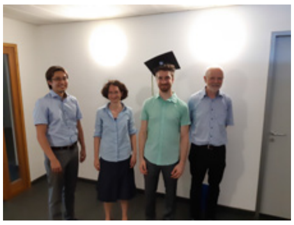
Fig. 4: *A random geometry of balls with random sizes*

Thermoviscoelasticity in Kelvin–Voigt rheology. Using the concept of the second-grade nonsimple materials, the frame-indifferent thermodynamically-consistent model of thermoviscoelasticity at large strain is formulated in the reference configuration. The focus is on physically correct viscous stresses that are frame indifferent under time-dependent rotations. Also elastic stresses are frame indifferent under rotations and respect positivity of the determinant of the deformation gradient. The heat transfer is governed by the Fourier law in the actual deformed configuration, which leads to a nontrivial description when pulled back into the reference configuration. In the quasistatic setting, the existence of weak solutions is shown by time discretization in [1].

Further highlights of 2019

ECMI SIG. Patricio Farrell (RG 3), Dirk Peschka (WG 1), and Nella Rotundo (RG 1) hosted the first meeting of the Special Interest Group "Modeling, Simulation and Optimization in Electrical Engineering (MSOEE)" of the European Consortium for Mathematics in Industry (ECMI) at the Weierstrass Institute in Berlin (January 31 – February 1, 2019).





Dissertation. Thomas Frenzel (RG 1) successfully defended his Ph.D. thesis "On the derivation of effective gradient systems via EDP-convergence" at HU Berlin (June 26, 2019).

Visit of Prof. Karen M. Gambaryan. Prof. Dr. Karen M. Gambaryan, head of the Faculty of Radiophysics and Chair of the Semiconductor and Microelectronics Department at Yerevan State University, Armenia, visited RG 1 in July and August. The visit was financed by the German Academic Exchange Service (DAAD). Using the Sphinx software, he computed elastic and electronic properties of semiconductor nanostructures in collaboration with Oliver Marquardt.

Conferences. Alexander Mielke gave a plenary talk on "Gradient systems and Gamma-convergence" at the Conference 2019 of the Deutsche Mathematiker-Vereinigung DMV in Karlsruhe. Several members of RG 1 and WG 1 participated in the "International Congress on Industrial and Applied Mathematics" (July 15–19, Valencia, Spain); Nella Rotundo co-organized there the two minisymposia "Modeling, Simulation and Optimization in Electrical Engineering" and "Simulation, Modeling, and Analysis of Semiconductors".

GAMM Seminar on Microstructures. Carsten Carstensen (HU Berlin) and RG 1 organized the 18th Seminar on Microstructures of the International Association of Applied Mathematics and Mechanics (GAMM, WIAS Berlin, January 18–19, 2019). It focussed on various aspects of microstructures in solid mechanics, material science, and applied mathematics.

Colloquium in honor of the 80th birthday of Prof. Dr. Herbert Gajewski. On October 23, 2019, the Berliner Oberseminar "Nonlinear Partial Differential Equations" (Langenbach Seminar) hosted a colloquium in honor of Prof. Dr. Herbert Gajewski's 80th birthday. Ansgar Jüngel (TU Vienna) gave a special lecture titled "Cross-diffusion systems: From spin semiconductors to biological populations with stochastic forcing", which touched several of Herbert Gajewski's scientific research fields.

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4.2 Research Group 2 “Laser Dynamics”

Head: Priv.-Doz. Dr. Uwe Bandelow

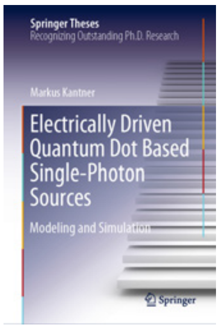
Deputy Head: Dr. Matthias Wolfrum

Team: Dr. Shalva Amiranashvili
Dr. Carsten Brée
Dr. Sebastian Eydam
Alexander Gerdes
Dr. Markus Kantner
Dr. Alexander Pimenov
Dr. Mindaugas Radziunas
Mina Stöhr
Dr. Andrei G. Vladimirov
Dr. Hans-Jürgen Wünsche

Secretary: Laura Wartenberg

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*.

In 2019, external funding was received 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*, Zuse Institute Berlin, and B5 “Effective models, simulation and analysis of the dynamics in quantum-dot devices”), which ended after twelve successful years in 12/2019. Further funded projects are the subproject A3 “Self-organization and control in coupled networks and time-delayed systems” within the DFG Collaborative Research Center 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application* and the project AA2-3 “Quantum-classical simulation of quantum dot nanolasers” within the Cluster of Excellence MATH+. Moreover, 2019 was the final year of the group’s work on the (externally funded) EU framework Eurostars project E!10524 “High Power Composites of Edge Emitting Semiconductor Lasers” (HIP-Lasers) in collaboration with Universitat Politécnica de Catalunya (Barcelona, Spain) and the companies Monocrom (Vilanova, Spain), Femtika (Vilnius, Lithuania), and Raab-Photonik GmbH (Potsdam), as well as subcontracts from the Ferdinand Braun Institute for High-Frequency Technology (FBH) within the projects HoTLas (on high-performance efficient and brilliant broad-area diode lasers for high ambient temperatures) and PLUS (on pulse lasers and scanners for LiDAR applications – automotive, consumer, robotic), 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 the WIAS RGs 1 *Partial Differential Equations* and 3 *Numerical Mathematics and Scientific Computing* as well as the companies Jenoptic Diode Lab GmbH (Berlin) and Coherent | DILAS (Mainz).



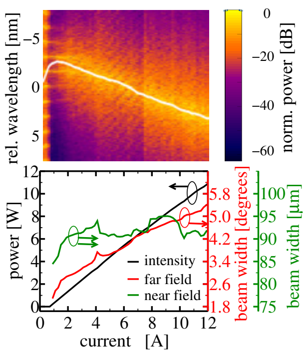


Fig. 1: Basic simulated characteristics of a typical broad-area laser as functions of the bias

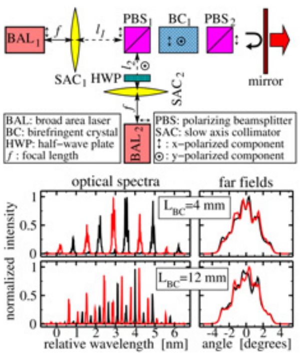


Fig. 2: Coupling of a pair of BALs within the EC and simulated characteristics of these BALs

Important events in 2019 were the International Workshop *"Optical Solitons and Frequency Comb Generation"*, organized at WIAS on September 18–20 (organizers: Shalva Amiranashvili, Uwe Bandelow, Andrei G. Vladimirov), and the Ph.D. thesis of Markus Kantner that was nominated by the Technische Universität Berlin for the Springer Theses Award and will be published by Springer as a monograph in early 2020. Moreover, Andrei G. Vladimirov was a member of the International Advisory Committee of the International Symposium on Physics and Applications of Laser Dynamics 2019 (IS-PALD 2019), November 20–22, Metz, France, and Matthias Wolfrum was invited for a plenary talk at the 11th Colloquium on the Qualitative Theory of Differential Equations at the University of Szeged, Bolyai Institute, Hungary.

Dynamics of semiconductor lasers and single-photon emitters

In the frame of the HotLas project, the dynamic electro-optical (EO) and the static heat-flow (HF) models for broad area edge-emitting semiconductor lasers (BALs) were coupled within the software kit BALaser, see Figure 1. In the framework of the Eurostars HIP-Lasers project, a model for the spectral combining of beams emitted from 2^n BALs within a frequency-filtering external cavity (EC) was developed. The EC (top of Figure 2 showing the case of $n = 1$) implies different filtering of the feedback to each laser, such that the resulting emission of the individual BALs is preserved, whereas the power scales with the number of emitters, see lower part of Figure 2 and Ref. [1]. After implementation into BALaser, the dependence of the separate and coupled beam quality on parameters of the optical elements could be simulated and analyzed [1].

In collaboration with the Macquarie University in Sydney, the impact of optical feedback coherence on the (irregular) dynamics of a semiconductor laser with conventional optical feedback was studied. For this reason, a new model allowing random dephasing of optical feedback was implemented into the WIAS software `LDSL-tool`. It was found that by increasing the level of incoherence, the signature of the cavity modes is smeared, the typical feedback-induced reduction of lasing threshold and red-shift of the lasing wavelengths is diminished, whereas the radiofrequency spectrum is flattened [2].

Quantum-classical modeling of single-photon emitters. Within the project AA2-3 of the Cluster of Excellence MATH+, efforts on the modeling and simulation of quantum light-emitting diodes were continued. The previously developed hybrid quantum-classical modeling approach for the simulation of quantum dot-based single-photon sources and nanolasers was extended towards a refined description of the quantum dot states. The new model includes a stationary Schrödinger equation for the energy levels and carrier wave functions that depend self-consistently on the diode's internal electostatic field. The population dynamics of these states is described by a Lindblad-type quantum master equation, which allows to accurately describe the quantum confined Stark effect. This effect is important for the tuning of quantum dot energy levels into resonance with cavity modes.

Next to the Stark effect, also a temperature tuning of the quantum dot states is possible. The research group investigated the non-isothermal drift-diffusion system using a novel model for the Seebeck coefficient. The new model yields an interesting special case of the coupled system with an appealing structure of the thermoelectric cross-effects. Moreover, a novel non-isothermal generalization of the finite volume Scharfetter–Gummel method for degenerate semiconductors that preserves practically all important structural features of the continuous system was derived.

Mode-locked pulses and temporally localized structures of light. Ultrafast lasers play an important role in the development of photonic science and technology and also provide an ideal experimental test-bed for the investigation of nonlinear wave dynamics. Especially interesting is the formation of short optical pulses, also known as *temporal localized structures (TLS)*, which present an ideal example of optical coherent structures and correspond (in the spectral domain) to the so-called *optical frequency combs* having numerous practical applications. An investigation of the formation of TLS in laser systems was performed in collaboration with colleagues from the Institut de Physique de Nice, the University of Balearic Islands, the University of Münster, and the ITMO University in St. Petersburg. The operation regimes in a class-A ring laser with a nonlinear amplifying loop mirror (see Figure 3), were studied numerically and analytically [3]. It was shown that these regimes can be destabilized via a modulational and a Turing-type instability, as well as by an instability leading to the appearance of square waves. It was demonstrated that mode-locked pulses are very asymmetric with an exponential decay of the trailing edge in positive time and a faster-than-exponential (superexponential) decay of the leading edge in negative time and that such a type of asymmetry strongly affects the interaction of the pulses. The formation of harmonic mode-locked regimes resulting from the interaction of TLS is illustrated in Figure 4. Another possible optical setup for this generation of TLS and frequency combs consisting of a nonlinear micro-cavity, operated in the Gires–Tournois regime and coupled to a long cavity with coherent injection, was investigated theoretically.

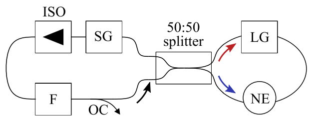


Fig. 3: *Schematic view of a ring mode-locked laser with a saturable gain (SG), bandpass filter (F), optical isolator (ISO), output coupler (OC), and linear gain (LG) together with a nonlinear element (NE) in a Sagnac interferometer forming a nonlinear mirror*

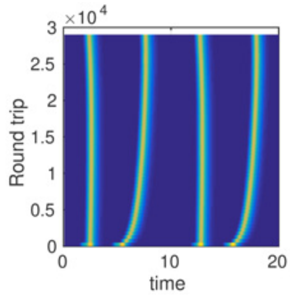


Fig. 4: *Interaction of two mode-locked pulses leading to a harmonic mode-locked regime with two pulses per cavity round trip. A common drift of the pulses is eliminated. The time axis spans the interval of two round trip times.*

Pulses in nonlinear optical media

Few-cycle optical pulses, as opposed to their "not too short" partners with well-defined envelope, require a sophisticated mathematical description. An important problem is to translate the standard concepts and results of wave- and fiber-optics to the field of extremely short electromagnetic perturbations governed by the non-envelope equations. The research group addressed both numerical and analytical aspects of this problem. From the analytical side, the influence of short perturbations on the stability of a continuous pump wave was discussed and a generalized Lighthill criterion to cover the classical and novel regimes of the modulation instability was developed [4]. From the numerical side the research group extended the numerical methods, as initially developed for the envelope equations, to solve the so-called *forward Maxwell equation* [5]; see Figure 5.

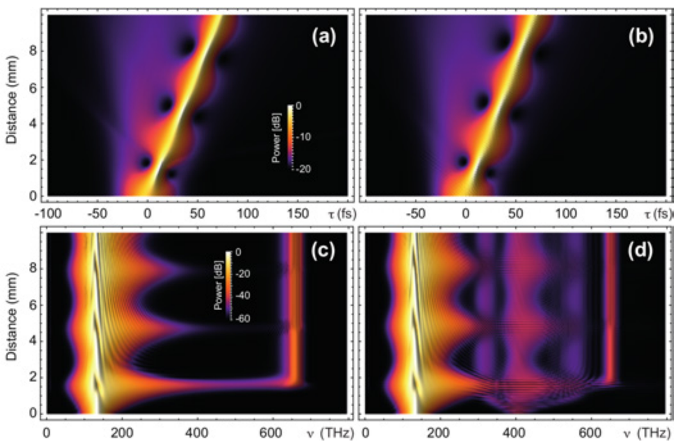


Fig. 5: *(a,c) Evolution of the second-order optical soliton and the induced Cherenkov radiation along the fiber. The calculation presented in (a,c) employs the standard envelope equation, in (a) space-time and (c) frequency domains. In (b) and (d), we use the forward Maxwell equation for which one observes the generation of the higher harmonics. See Ref. [5] for more details.*

Theory of dynamical systems

In the field of the theory of nonlinear dynamical systems, an important result for delay-differential equations (DDEs) with large delay was obtained. Such equations play an important role in the modeling of various types of optoelectronic systems. Of particular interest in optics are situations, where the delay time is much larger than the internal time scale. In such cases, a temporal self-localization of the light can be observed leading to soliton-like solutions of the DDE system, as, e.g., in the mode-locked lasers mentioned above. Due to the large delay and the resulting multiple time scales, such DDE systems have to be studied within the context of singular perturbations, and their numerical treatment with standard tools becomes infeasible. An asymptotic theory for the existence and stability of such temporal dissipative solitons (TDS) was developed. This provides a complete classification of the spectrum of TDS into interface and pseudo-continuous spectrum. Moreover, desingularized problems for the singular limit of infinite delay provide a robust approximation for the spectral problem, see Figure 6

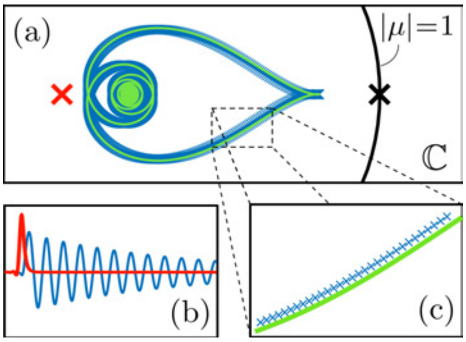


Fig. 6: *Floquet spectrum of a temporal dissipative soliton of a phase oscillator with delay. Panel (a) with zoomed part in (c) shows numerically computed multipliers (crosses) and approximating curves of pseudo-continuous spectrum. The interface spectrum (red and black crosses) can be computed from an Evans function. Panel (b) shows corresponding eigenfunctions (red mode from isolated interface spectrum, non-localized blue mode from pseudo-continuous spectrum). See Ref. [6] for more details.*

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

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Deputy Head: Dr. Jürgen Fuhrmann

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Priv.-Doz. Dr. Alfonso Caiazzo
Prof. Dr. Wolfgang Dreyer
Dr. Patricio Farrell
Derk Frerichs
Marko Jahn
Abhinav Jha
René Kehl
Dr. Zahra Lakdawala
Priv.-Doz. Dr. Alexander Linke
Dr. Christian Merdon
Dr. Baptiste Moreau
Dr. Rainer Schlundt
Dr. Hang Si
Dr. Holger Stephan
Timo Streckenbach
Dr. Petr Vagner
Dr. Ulrich Wilbrandt

Secretary: Marion Lawrenz

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, e.g., see the Scientific Highlights article on page 21. Below, a selection of research topics of the group will be described briefly. Further topics include tetrahedral mesh generation, physically consistent discretizations for equations from fluid dynamics, numerical methods for population balance systems with applications in chemical engineering (in collaboration with RG 5 *Interacting Random Systems*), and the simulation and control of flows modeling ladle stirring (in collaboration with RG 4 *Nonlinear Optimization and Inverse Problems*).

Modeling of biological flows and tissues

The dynamics of biological tissues results from the complex interaction of different physical processes, involving several spatial and temporal scales. Treating computationally the whole spectrum of these dynamics, from cellular biology to organ mechanics, is practically infeasible, such that multiscale and reduced-order models are needed.

Multiscale immersed methods for vascularized tissues. In [2], a model was proposed for a biological tissue composed of a three-dimensional elastic structure and a one-dimensional vascular

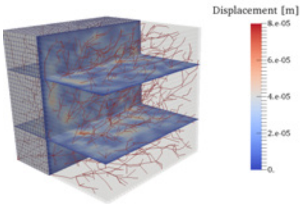

Fig. 1: *Solid displacement field in an elastic tissue with an immersed vasculature at constant pressure [2]*

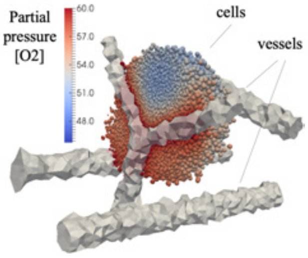

Fig. 2: *Simulation of a cancer cell population growing around an arbitrary vascular structure [5]*

network. In particular, the fluid vessels are modeled using an immersed method. In practice, each vessel is described by a hypersingular forcing term defined on a one-dimensional manifold, whose magnitude depends on the fluid pressure and on the geometry of the vasculature. The main advantage of this approach is that the vasculature network does not need to be explicitly discretized within the three-dimensional computational mesh and, thus, vessels can be arbitrarily placed in the domain.

The model was validated at examples with a known solution and then tested for the simulation of a synthetic tissue sample with a randomly generated vascular network, see Figure 1. Moreover, using the immersed formulation, an equivalent homogenized problem was derived, in which the singular force given by the fluid pressure is approximated by a bulk force and can be directly related to mechanical parameters of the effective (biphasic) material.

Hybrid modeling of cancer growth. The modeling of cell populations requires the coupling of biophysical processes happening at the level of single cells (cell-cell interaction, cell cycle, mutations, mitosis) with the dynamics of the surrounding environment, e.g., with the availability of nutrients, which are necessary for the activity of the cells, or the presence of structures such as vessels or fibers. In order to efficiently handle these phenomena numerically, a multiscale model was proposed in [5] that couples an individual-based method for the cells with a finite element method to describe the oxygen diffusion within the tissue.

Vessels are treated as one-dimensional sources of nutrients in the novel method. At the same time, they represent impenetrable boundaries for the cells. In order to deal with this constraint, the vessels are described by pseudo-cells that do not undergo any dynamics but exert repulsion forces on neighboring cells. Similarly, fibers are treated as cylindrical-shaped cells that can pull cancer cells (adhesion) along specific directions. It was shown that the computational model is capable of simulating a high number of cells and fibers, as well as dealing with arbitrary vascular networks without increasing the overall complexity, see Figure 2. Ongoing research includes analyzing quantitatively the link between individual-based methods and statistical PDEs describing cellular phenomena at the continuous level, as well as extending the existing model to enable the development of vasculature (angiogenesis) depending on tumor growth.

Modeling of semiconductor devices and electrochemical systems

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 the electroneutral limit of large sizes of the computational domain, as it is, e.g., the case during the simulation of electrochemical experiments, the Poisson equation for the electric potential can be reduced to an algebraic constraint.

In close cooperation with other groups at WIAS and external partners, numerical methods and simulation tools are developed that aim at accurately reflecting the qualitative and quantitative behavior of these systems. A particular focus is the consistency of the discretized models to fundamental thermodynamical principles, and the coupling of these drift-diffusion-type models with various other physical processes like fluid flow, atomistic simulations, heat transport and elastic deformation. In the framework of the joint German-Czech research project "Investigation of electrochemical double layers in solid oxide cells (EDLSOC)", a detailed thermodynamic description of the interface processes occurring in electrodes of solid oxide cells shall be developed and experimentally verified; for first results, see [7] and Figure 3. Together with RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, the group supports experimental investigations by continuum-based mathematical and numerical modeling in the framework of the project "Continuum-based modeling" within the network "Paths to secondary Mg/Ca – Air Batteries (LuCaMag)" funded by the German Ministry of Education and Research, and the development of novel mathematical models of polycrystalline electrodes in the project "Multi-Material Electrocatalysis" (MultECat) within the Excellence Cluster MATH+. In cooperation with RG 1 *Partial Differential Equations* and the Tyndall National Institute (Cork, Ireland), a multi-scale model of electronic, optical, and transport properties of III-nitride alloys and heterostructures is developed; see Figure 4. The contributions of the group are based on the prototype drift-diffusion simulator DDFERMI and the PDE solution tool box PDELIB [6]. A novel mathematical model and a tool chain for the numerical simulation of transmission electron microscopy images of semiconductor quantum dots was developed in cooperation with RG 1, RG 6 *Stochastic Algorithms and Nonparametric Statistics* and the MATH+ project "Model-based geometry reconstruction from TEM". Nonlinear temperature feedback in drift-diffusion calculations coupled with Joule heating and heat transport manifesting itself in S-shaped current-voltage curves was observed in numerical simulations.

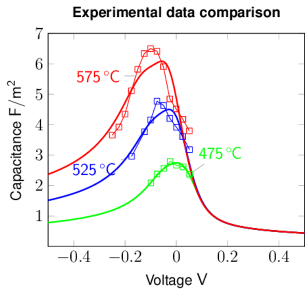

Fig. 3: *Double layer capacitance of a blocking electrode (experimental data from literature) [7]*

The efforts of the group in this field resulted in two new projects starting in 2020. Patricio Farrell successfully applied in the Leibniz Competition for a junior research group "Numerics for Innovative Semiconductor Devices" which starts as LG 5. In addition, together with Nella Rotundo (RG 1) and Natascha Dropka from the Leibniz Institute of Crystal Growth, he obtained funding for the MATH+ incubator project "Understanding doping variations in semiconductor crystals". These projects allow to start new cooperations on perovskites, nanowires, accurate lasers and measurement of impurities in semiconductor crystals with several German and international academic partners.

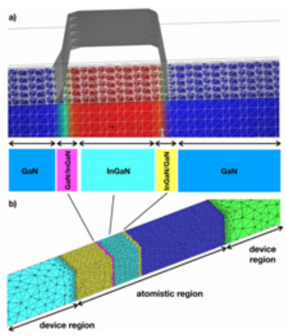

Fig. 4: *(a) Atomistic finite element mesh along with the valence band edge profile on a cross section (gray). Material domains and interface regions are indicated in the lower part. (b) Finite volume mesh generated for device simulations attached to the atomistic region [6]*

Algebraic stabilizations for convection-diffusion equations

Scalar convection-diffusion equations are utilized for modeling conservation laws, e.g., energy conservation via an equation for the temperature, or the conservation of concentrations of solved species in fluids. Such equations can be found in many systems that model processes in applications. Usually, the (numerical) solution of a convection-diffusion equation is an input parameter for other equations in such systems. Hence, it should be accurate and it must not possess non-physical values (spurious oscillations), i.e., it has to satisfy the discrete maximum principle (DMP). In applications, convection often dominates diffusion by several orders of magnitude. It is well known that in this situation a stabilization mechanism has to be introduced in the discretization, since the solution of the equation possesses layers that cannot be resolved on affordable meshes. There are only very few stabilized discretizations that satisfy both properties mentioned above. Among them are algebraic stabilizations, which have been studied in RG 3 in recent years

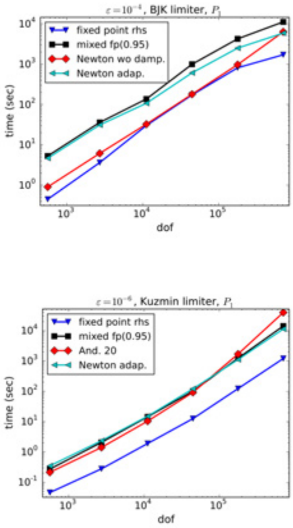

Fig. 5: *Two-dimensional problem, efficiency of some methods for solving the nonlinear problem [4]*

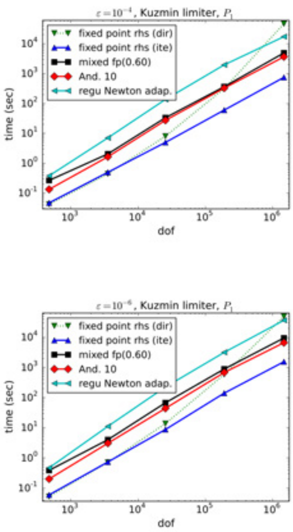

Fig. 6: *Three-dimensional problem, efficiency of some methods for solving the nonlinear problem [4]*

for steady-state equations, where they are called *algebraic flux correction (AFC) schemes*. The first convergence analysis for such schemes was presented and an AFC scheme was developed that satisfies the DMP on arbitrary simplicial meshes, the AFC scheme with BJK limiter (by **B**arrenechea, **J**ohn and **K**nobloch). The appropriate choice of the limiters in AFC schemes depends on the numerical solution. Hence, these discretizations are nonlinear, and solving the nonlinear problem becomes an issue. A recent review of the state of the art and connections to a different stabilization technique is provided in [1].

A comprehensive study of solvers for the nonlinear problem in AFC methods is presented in [4]. Different fixed point iterations and formal Newton methods were included. The formal Newton methods used some special treatment of the situations where the limiters are not differentiable. Besides the BJK limiter, also the Kuzmin limiter was studied. In the case that the nonlinear problems could be solved, the solutions obtained with the BJK limiter were somewhat more accurate. But for very small diffusion coefficients, there was sometimes no approach that was able to solve these problems for the BJK limiter. Among the studied methods, the simplest one, a fixed point iteration with fixed matrix in all steps and coupled with an adaptive damping algorithm, turned out to be most efficient in terms of computing times, see Figures 5 and 6. For two-dimensional problems (fixed point rhs), a sparse direct solver was applied where only in the first iteration the factorization of the matrix is required and all other steps can be performed very fast with the available factorization. In three dimensions (fixed point rhs(ite)), the utilized iterative solver for linear systems performed most efficiently since the constant matrix is by construction an M-matrix.

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4.4 Research Group 4 "Nonlinear Optimization and Inverse Problems"

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Deputy Head:	Priv.-Doz. Dr. René Henrion
Team:	Manuel J. Arenas Jaén Dr. Ingo Bremer Luigino Capone Moritz Ebeling-Rump Dr. Martin Eigel Robert Gruhlke Dr. Holger Heitsch Dr. Robert Lasarzik Manuel Marschall Dr. Andreas Rathsfeld
Secretary:	Anke Giese

The research group investigates optimization and inverse problems occurring in current engineering and economic applications. A specific focus of research in optimization and optimal control is the investigation of special structures resulting from the presence of uncertain and nonsmooth data. Together with RG 3 *Numerical Mathematics and Scientific Computing* and RG 6 *Stochastic Algorithms and Nonparametric Statistics*, the group investigates direct and inverse problems for partial differential equations (PDEs) with uncertain coefficients.

Last year has seen the end of the European Industrial Doctorate (EID) project MIMESIS – *Mathematics and Material Science for Steel Production and Manufacturing*. Three students already defended their Ph.D. theses ahead of time, and four further students are expected to finalize their respective theses soon. Up to now, 33 publications emerged from this project, and the knowledge gained helped to improve manufacturing processes of the companies involved in terms of efficiency, sustainability, and resulting materials properties. Several successful cooperations with industrial partners were initiated and will hopefully outlast the end of this project.

Fig. 1: *Participants of* MIMESIS *workshop, Skien, Norway*

The final consortium meeting was embedded in an international "Workshop on Mathematics and Materials Science for Steel Production and Manufacturing" and took place on June 4 to 5 in Skien, Norway, at the production site of the industrial partner EFD Induction.

The group successfully applied for the second phase (2021–2023) of DFG SPP 1886 *Polymorphic Uncertainty Modelling for the Numerical Design of Structures*. Moreover, the participation in the Gaspard Monge Programme for Optimization (PGMO) funded by the Fondation Mathématique Jacques Hadamard (FMJH) could be renewed for another year.

In the following, selected scientific achievements of the research group in 2019 are detailed.

Stochastic and nonsmooth optimization

The group continued its research in the areas of stochastic and nonsmooth optimization. Last year's work was mainly motivated by the participation in DFG Transregio (TRR) 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks* whose second phase (2018–2022) is devoted to the modeling of market equilibria in gas networks. The joint presence of uncertainty and of a hierarchic decision structure leads to new classes of optimization problems (e.g., probabilistic MPECs) on the interface of the two domains of continuous optimization mentioned above. Another source for this same object of investigation is the inherent nonsmoothness of probability functions even with smooth initial data. This motivated a detailed analysis of constraint qualifications in a stationary gas network model, followed by the numerical solution of the capacity maximization problem under random demands [6].

The effect of nonsmoothness on the probability function is even more pronounced in the case of infinite systems of underlying random inequalities. Using tools from generalized differentiation (Mordukhovich subdifferential, coderivative, etc.), (sub-) gradient formulae for probability functions could be found for the general situation where the random inequality system is continuously indexed by a moving set [5]. The algorithmic solution of this kind of problems along with applications in water reservoir and gas network management will be focused on in a cooperation with ITWM Kaiserslautern in the framework of a co-supervised Ph.D. thesis. An additional contribution to the algorithmic solution of optimization problems subject to probabilistic constraints was devoted to the derivation of confidence intervals for optimal values as a means for defining a stopping rule of sequential quadratic programming (SQP)-based solvers in such environment. Another topic of research was on the structural analysis of dynamic probabilistic constraints that led to the successful defense of a Ph.D. thesis (Tatiana Gonzalez–Grandon). The strategic direction of the mentioned research activities is the incorporation of probabilistic constraints in the context of PDE-constrained optimization. Cooperation has been initiated here with Martin Gugat (Erlangen), Georg Stadler (New York), and Boris Mordukhovich (Detroit).

Inverse problems for stochastic data and reconstruction of stochastic surfaces

A novel method for the accurate functional approximation of possibly highly concentrated probability densities was developed [4]. It is based on the combination of several modern techniques such as transport maps and low-rank approximations via a nonintrusive tensor train reconstruction. The central idea is to carry out computations for statistical quantities of interest such as moments based on a convenient reference density for which accurate numerical methods can be employed. Since the exact transport from target to reference can usually not be determined exactly (as illustrated in Figure 2), one has to cope with a perturbed reference density due to a numerically approximated transport map.

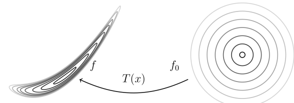

Fig. 2: *Transport of a Gaussian reference density by a nonlinear (quadratic) transport map for Bayesian inverse problems*

In scatterometric measurements, a surface is illuminated by an inspecting wave, and the surface, or at least some properties of the surface, are to be reconstructed from measurements of the scattered wave. Already the simplest stochastic example of rough surface measurements is of great importance. A model for the detection of the statistical parameters characterizing such a surface was developed and applied to stochastic periodic interfaces. If the surface is generated as a stochastic field with a single normal distribution for the height corrugations and with Gaussian correlation function, then the corresponding parameters can be identified by an algorithm based on Karhunen–Loève expansion for the surface together with a Bayesian approach for the inverse problem using Markov Chain Monte Carlo methods.

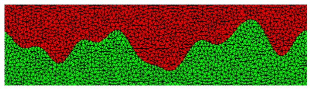

Fig. 3: *Typical rough interface simulated over a period $p = 8\,\mu m$ used for the computation of density functions*

A further aim was to generalize the results to an infinite rough surface, i.e., to a bounded but nonlocal perturbation of a half space. In order to enable the approximation of such a surface by periodic ones (cf. Figure 3) and to apply the code for periodic structures, the radiation condition for the rough surfaces were analyzed in [8].

Another application is the modeling of porous adhesive bonds for rotor blade simulations within the DFG SPP 1886 project. Here, a novel domain decomposition method was developed for random domains, in particular, for materials with randomly shaped perforations (see Figure 4). A central idea is to obtain quantities of interest associated with local properties in a neighborhood of the perforations using local information only. Under the assumption of isolation of the perforations, local parametric (physically discretized) Poincaré–Steklov operators are approximated via neural network surrogates. Polymorphic uncertainties determining the shapes of the perforations are modeled parametrically. Hence, the considered multiple perforations introduce a very high-dimensional parametric dependence in the underlying quantities of interest, which becomes accessible by employing local surrogates. This consequently results in a highly efficient sampling scheme in an online phase: Given a sample set of perforations, the pathwise contribution to the underlying quantity of interest can be determined without the requirement of a full meshing or computation including the meso-scale inclusion structures.

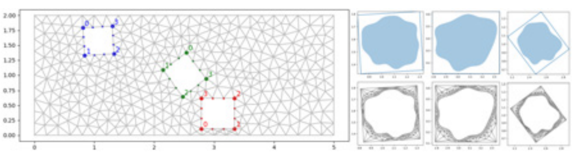

Fig. 4: *Inclusion of complicated randomly parametric geometrical shapes into a macroscopic domain by means of domain decomposition and local high-dimensional surrogates*

Optimal control of multifield and multiscale problems

Last year's work in this area was ranging from generalized solution concepts to nonlinear partial differential equations to optimization problems in steel industry and topology optimization for additive manufacturing. Even though weak solutions are well accepted in the mathematical community, recent approaches showed that weak solutions may develop non physically non-uniqueness, if they exceed certain regularity assumptions. For a given energy profile, it is known that there exist an infinite number of weak solutions to the Euler equations and to the Navier–Stokes equations. To circumvent these issues, a new solution concept is introduced in [7], the so-called *maximal dissipative solutions* using the example of incompressible fluid dynamics. Compared to weak solutions, their solution set has more desirable properties, i.e., it is closed and convex. This helps to define selection criteria, implying uniqueness of solutions.

Steel manufacturing processes are a long-standing topic in the research group, and we revised the theoretical grounds for this work. Introducing the concept of weak entropy solutions to systems modeling the induction hardening process, we were able to show existence and weak-strong uniqueness for these solutions. This work provides the framework to consider convergence of implemented numerical schemes for applications involving multiple time scales or the singular limit analysis for high frequencies. This work thematically falls into the framework of the EID project MIMESIS, coordinated by the research group.

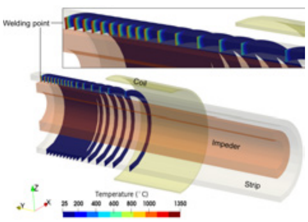

Fig. 5: *Evolution of temperature profile in the strip edge towards welding point*

The group's subprojects 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 to inductive pre-heating for the thermal cutting of steel plates. The heating is caused by eddy currents induced by a varying magnetic flux. In [2], the high-frequency induction (HFI) welding process is studied numerically. A numerical stabilization approach for the finite element discretization allows to consider realistic weld-line speeds and thus a fairly comprehensive three-dimensional simulation of the tube welding process. The resultant temperature field provides information near the welding point relevant to understand the process in detail (see Figure 5).

Another project studies a prototype set-up for inductive pre-heating in the thermal cutting of steel plates. A flame cutting model was developed and presented in [1]. Starting from this model, an optimization scheme for induction pre-heating of steel plates is introduced in order to achieve an optimal temperature distribution to avoid cold cracks arising after the thermal cutting.

Components with micro-structure have become important construction materials. Additive manufacturing offers the capability of creating those high-complexity structures. However, additive manufacturing comes with its own set of difficulties. For example, overhangs lead to instabilities during the printing process. This problem was successfully tackled by considering the compliances with intermediate building steps, see [3].

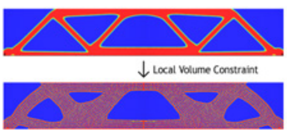

Fig. 6: *Influence of the local volume constraint*

Additionally, a way to enforce microstructure via a local volume constraint was developed (Figure 6). It was shown that the resulting topologies are better equipped to deal with buckling.

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4.5 Research Group 5 "Interacting Random Systems"

Head:	Prof. Dr. Wolfgang König
Deputy Head:	Dr. Robert Patterson
Team:	Dr. Benedikt Jahnel Dr. Luisa Andreis Dr. Lorenzo Taggi Dr. Michiel Renger Dr. Willem van Zuijlen Dr. Tal Orenshtein Alexander Hinsen Charles Kwofie Dr. Franziska Flegel
Secretary:	Christina van de Sand

In 2019, the RG 5 *Interacting Random Systems* 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 most important highlight, which will have a long-lasting impact on the group, was the award of a DFG Priority Programme on *Random Geometric Systems (SPP 2265)* with the head of the group as the coordinator. This SPP lies precisely in the main part of the scientific interests of the group and will hopefully fund several projects of the group in the periods 2020–23 and 2023–26. Therefore, group members devoted much time during the fall of 2019 to writing applications for projects in this SPP on subjects like random loop models and condensation effects, spatial telecommunication models and emergence of global pictures, spatial particle models with coagulation and formation of gels, and statistical mechanics of interlacement processes and Bose–Einstein condensation. All these topics are currently important for the RG 5 *Interacting Random Systems*, and their importance will even increase. The common theme of these topics (and more) is the investigation of the interplay between randomness and geometry and space in many situations where many microscopic interacting random entities let macroscopic effects emerge, like phase transitions or laws of large numbers.

Another big field of activity, as already since a few years, is the fruitful contact with our prominent partner Orange S.A. (Paris) on applied questions in telecommunication (related to new 5G technologies). In 2019, the group was delivering scientific work for two contracts at the same time, and Orange expressed constant interest to go on. Since this subject is expected to be increasingly attractive for many young scientists on various levels, the head of the group and group member *Benedikt Jahnel* finished an introductory book on probabilistic methods in this field in fall 2019.

Another highlight of the year 2019 was a three-week stay by *Wolfgang König* and *Benedikt Jahnel* in Accra, the capital of Ghana, to deliver a concentrated introductory probability course and to establish and foster contacts to the African Institute for Mathematical Sciences *AIMS Ghana* and its Masters students and the associated Ghanaian professors. This is part of the programme of the Deutscher Akademischer Austauschdienst *DAAD* for exchange between *AIMS Ghana* and Berlin in

Stochastics. Embedded in this three-week stay, the group members also organized a joint workshop with Germans and Africans, and they delivered some soft-skill talks on how to apply to European Ph.D. programs and the like. The head of the RG 5 *Interacting Random Systems* thinks that it is a noble and important European goal to invest time and effort in the development of advanced mathematical training and research in Africa by means of personal scientific contact.

Apart from the scientific topics related to the interplay of randomness and geometry (see above), a number of further topics were under investigation by members of the group in 2019, like the behavior of the eigenvalues of the Laplace operator with random white-noise potential in large boxes in the plane (funded by the DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*), large deviations for reaction fluxes (funded by the DFG Collaboration Research Center SFB 1114 *Scaling Cascades in Physical Systems*), the weakly self-avoiding walk in random potential and the standard random walk in random potential on random graphs, and crystallization in many-body systems at positive temperature, see below.

Apart from the workshop at Accra, the group also organized a workshop on Phase Transitions and Particle Systems on the premises of the WIAS, see also page 117.

In teaching, the head of RG 5 *Interacting Random Systems*, 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 *Interacting Random Systems*.

Please find below a more detailed description of some of the group's achievements in 2019.

Crystallization in many-body systems at positive temperature

A many-body system is a random N-particle system in a box in the Euclidean space whose probabilistic structure is given in terms of a Gibbs measure that assigns the exponential of a negative energy term to the configuration. The prefactor in the exponent is called the *inverse temperature*, β. The energy is a pair-interaction with a Lennard–Jones-type interaction functional, i.e., there is a strong repulsive force between each pair of particles and a preference to assume a certain fixed positive distance. In the two-dimensional situation, the minimal configuration of this energy approaches, for large N, a triangular grid, and in dimension one, a regularly spaced deterministic scaling of $\mathbb{Z}$. Certainly, for fixed N and large β, one expects that the system approaches this energy-minimizing state as well.

The purpose of the preprint [1] is to understand in which way the thermodynamic limit ($N \to \infty$ in a box with volume of order N) approaches this deterministic structure if $\beta > 0$ is kept fixed and very large (i.e., at very low temperature). This is enormously difficult in two or more dimensions since there may be regions in which the configuration approaches a grid, but also those in which symmetry is broken or another type of deficiency occurs, and it is currently not possible to control the co-existence of many such areas of various shapes and types.

Therefore, the authors of [1] decided to turn to dimension one. Here, it has been known for many years that there is no phase transition, i.e., for finite β, there will be no macroscopic substructure (cluster) to be found in the configuration. However, in the thermodynamic limit, as β gets large, the finite-size clusters indeed display a highly interesting spatial structure: indeed, it turned out that, if the ambient box is large enough, all the clusters show the same internal and boundary structure: the optimal grid internally, and a certain deterministic boundary layer at the ends of the clusters. The authors of [1] characterized these limiting deterministic structures, including the fluctuations around them.

Exponential moments for planar tessellations

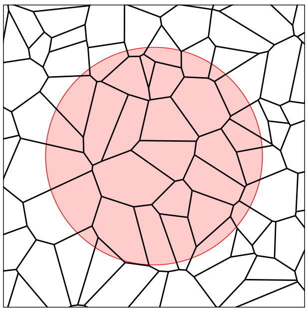

Fig. 1: *Poisson–Voronoi tessellation in a box. We measure characteristics such as the total edge length in a unit ball, indicated in red.*

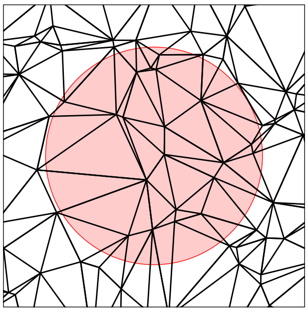

Fig. 2: *Poisson–Delaunay tessellation in a box. We measure characteristics such as the total edge length in a unit ball, indicated in red.*

The study of random tessellation processes is one of the corner stones of *stochastic geometry*, the subfield of probability theory that investigates random geometric objects in space. The prototypical example of such a tiling is the famous *Poisson–Voronoi tessellation*, which is constructed as follows. We first take a realization of a random cloud of points in space, drawn from a *Poisson point process*. Then, we associate to every point in the point cloud its *Voronoi cell*, which is given by the set of locations in space that are closer to the point than to any other point in the point cloud. The different cells or tiles then give rise to a tessellation of space; see the black lines in Figure 1. Drawing an edge between all the points in the point cloud, which have neighboring Voronoi cells, yet gives rise to another famous tessellation, the *Poisson–Delaunay tessellation*; see Figure 2.

The motivation to investigate random tessellations is manifold, and ranges from the study of crystal growth, numerical analysis of partial differential equations, geo sciences, to the material sciences and astro physics. In our group the main motivation, for the last years, has come from the similarity of random tessellations with urban street systems, as well as cellular telecommunication systems.

Very often, as in the case of the Poisson–Voronoi tessellation, the construction rule for the tessellation is rather simple, and the system has only a few natural parameters. For example, if the underlying Poisson point process is shift invariant, there is really just one relevant parameter, the scalar *intensity* of the process. However, the distribution of the random tessellation is a highly complex object and typically cannot be described in any simple way. In order to cope with this fact, instead of describing the distribution as a whole, we limit our attention to certain characteristics of the tessellation. For example, we can consider the tessellation in a unit ball, as indicated in red in Figure 1 and Figure 2, and count the number of cells intersecting the ball, or measure the total edge length in the ball, or count the number of triangles, etc. Unfortunately, even the distributions of these simpler quantities are often hard to describe, and that is why we start with further characteristics of the distributions, such as the expected value, variance and moments, which can hopefully be described as functions of the system parameters.

Our contributions to the field in 2019 are presented in two papers, see [2], [3]. In [2], we show that, under rather general conditions, the total edge length as well as the number of cells in a unit ball have a distribution whose exponential moments all exist. In simple words, this means that events in which we see a very large total length are extremely unlikely. In [3], we show that a large class of tessellations that are based on Poisson point processes satisfy a lower large-deviation principle. That is, the probability to see certain characteristics to be smaller than their average behavior in large boxes is exponentially small with semi-explicit exponential rate.

Random loop models

We consider the model of lattice permutations, whose configurations are permutations of the vertices of a torus, $\mathbb{Z}^d/L\mathbb{Z}^d$, such that each vertex is mapped to a nearest neighbor. We conceive each such map as a graph by putting a directed edge from each vertex to its image. Since by definition of permutation each vertex has precisely one input and precisely one output, it follows that we can view each such graph as a collection of mutually-disjoint self-avoiding loops (see, for example, Figure 3). What is the "typical" length of the loops in the limit as the size of the torus goes to infinity when such permutations are drawn uniformly at random? This is one of the central questions about this model and it is not only interesting on its own from a purely mathematical perspective, but also very important in statistical physics. This question is challenging since lattice permutations belong to a class of models which was not studied before, whose rigorous analysis requires the introduction of new mathematical methods. One of the major difficulties is the presence of hard-core constraints and long-range correlations.

The study of lattice permutations has been proposed by Betz, Biskup, Gandolfo, Grosskinsky, Ueltschi in view of their connections to the *quantum Bose gas*. As was shown by Feynman [4], the quantum Bose gas can be "represented" as a system of random interacting Brownian loops, which is heuristically related to lattice permutations. The central question for the quantum Bose gas is whether *Bose–Einstein condensation* takes place, which is an important unsolved mathematical problem. It was shown that the two-point function, namely the ratio of the partition functions of one system with a forced "open" loop and one without, can be used to detect Bose–Einstein condensation: If this ratio stays uniformly positive in the volume and in the spatial separation of the two endpoints of the forced open loop, then Bose–Einstein condensation occurs [5]. Our research work [6] provides a rigorous proof of this fact in the model of lattice permutations.

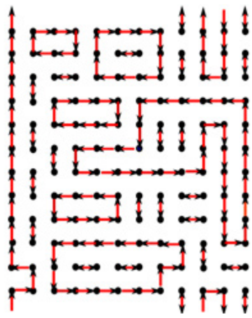

Fig. 3: *Representation of a permutation of the vertices of a box such that each vertex is mapped to a nearest neighbor*

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

Head: Prof. Dr. Vladimir Spokoiny

Deputy Head: Priv.-Doz. Dr. John Schoenmakers

Team:
Dr. Valeriy Avanesov
Priv.-Doz. Dr. Christian Bayer
Franz Besold
Dr. Oleg Butkovsky
Darina Dvinskikh
Dr. Pavel Dvurechensky
Prof. Dr. Peter Friz
Priv.-Doz. Dr. Peter Mathé
Dr. Paolo Pigato
Dr. Jörg Polzehl
Dr. Martin Redmann
Massimo Secci
Dr. Karsten Tabelow
Dr. Nikolas Esteban Tapia Muñoz

Secretary: Christine Schneider

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 the DFG Collaborative Research Center SFB 1294 *Data Assimilation*, the DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, the DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics* and the Cluster of Excellence *Berlin Mathematics Research Center MATH+*.

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 2019:

- The paper "Optimal tensor methods in smooth convex and uniformly convex optimization" by Alexander Gasnikov, Pavel Dvurechensky (RG 6), Eduard Gorbunov, Evgeniya A. Vorontsova, Daniil Selikhanovych, César A. Uribe was presented at the Conference on Learning Theory 2019.
- The paper "On the complexity of approximating Wasserstein barycenter" by Alexey Kroshnin, Nazarii Tupitsa, Darina Dvinskikh (RG 6), Pavel Dvurechensky (RG 6), Alexander Gasnikov, César A. Uribe was presented at the International Conference on Machine Learning 2019.
- Larisa Adamyan successfully defended her dissertation "Adaptive weights community detection" at Humboldt-Universität zu Berlin (under supervison of Vladimir Spokoiny, RG 6).
- The monograph [2] on "Magnetic Resonance Brain Imaging with R" by Jörg Polzehl and Karsten Tabelow (both RG 6) was published at Springer.

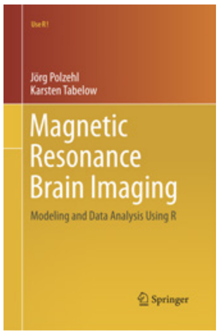
In 2019, the members of the group made some significant contributions to statistical literature.

A new bootstrap-based procedure for the estimation of a spectral projector of a high-dimensional covariance matrix was developed. The proof of bootstrap validity relies on recent advances in high-dimensional probability.

In [3], we developed a new data-projection-based algorithm for structure-adaptive manifold estimation, yielding nearly optimal recovery of the manifold under Hausdorff loss, allowing for noise of larger magnitude than previous contributions, as well as the application for a preliminary denoising step for any machine-learning task. Motivated by high-dimensional data analysis applications, e.g., image processing, we extend the adaptive weight clustering algorithm [4] for data concentrating on a low-dimensional manifold. Surprisingly, a slight adjustment to the curvature of the manifold is enough for the algorithm to recover the cluster structure at a nearly optimal rate.

We investigated the issues concerning statistical inference in 2-Wasserstein space related to the construction of nonasymptotic confidence sets centered at the empirical 2-Wasserstein barycenter. We continue the line of research on the convergence and concentration properties of the empirical barycenters and extend the setting to the Bures–Wasserstein distance. The obtained theoretical results are used for the introduction of Gaussian processes indexed by multidimensional distributions: Positive definite kernels between multivariate distributions are constructed via Hilbert space embedding relying on optimal transport maps.

We provide new upper complexity bounds for approximating Wasserstein barycenters of a set of discrete measures by an analysis of two algorithms, the first one being Iterative Bregman Projections (a generalization of the Sinkhorn's algorithm for optimal transport distances), and the second one is based on Nesterov's accelerated gradient method. We also discuss scaling up the algorithms using distributed optimization techniques. In 2019 within the project "Optimal transport for imaging" (together with RG 8) funded by the Cluster of Excellence *Berlin Mathematics Research Center* MATH+, we focused on the compression of transmitted information and privacy in distributed algorithms for Wasserstein barycenter as well as modeling aspects of image segmentation via optimal transport distances.



In 2019, we published a monograph in the Springer UseR! series summarizing more than a decade of work within the research group on modeling and analysis problems of data from various magnetic resonance imaging (MRI) modalities. This has been accompanied by a major update of the

WIAS Software Collection for Neuroscience largely extending their functionality while ensuring and enhancing their usability. In cooperation with RG 8, recent progress on structural adaptive smoothing algorithms was made using patchwise local comparisons in feature space. This improvement is able to deal with local image gradients and smooth discontinuity manifolds, a much more realistic situation often found in MRI. An emerging application of this new adaptive noise reduction method is quantitative MRI, see also the Scientific Highlights article "Modeling and Analysis of Quantitative Magnetic Resonance Imaging" on page 10.

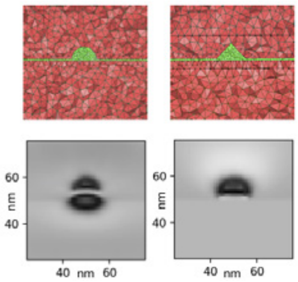


Fig. 1: *Quantum dot geometry and FEM mesh (top) and simulated TEM image (bottom)*

In 2019, the project EF3-1 "Model-based geometry reconstruction from TEM images" (together with RG 1) funded by the Cluster of Excellence *Berlin Mathematics Research Center* MATH+ has started. Within the project and in cooperation with RG 3 and Technische Universität Berlin, we developed a full modeling and simulation framework for transmission electron microscopy (TEM) images of semiconductor nanostructures such as quantum dots (QD). The software is able to create a database of simulated images for a very large set of geometric configurations and excitation conditions; see Figure 1. This is the basis for the solution of the inverse problem to infer on geometric properties of QDs. Furthermore, first steps towards a mathematical justification of the theoretical framework were made.

In recent years, the topic of research data has reached the mathematical discipline. RG 6 together with RG 1 has made large contributions to the Mathematical Research Data Inititive (MaRDI) (`http://www.mardi4nfdi.org/`) coordinated by WIAS as a leading institution within the National Research Data Initiative (NFDI).

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.

Highlights 2019:

- On March 14, 2019, Benjamin Stemper successfully defended his dissertation "Rough volatility models: Monte Carlo, asymptotics and deep calibration" at Technische Universität Berlin (under supervison of Peter Friz and Christian Bayer, both RG 6).
- The Research Unit 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics* was approved 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).

- Martin Redmann and Paolo Pigato received junior professorships in Halle and Rome, respectively.
- Christian Bayer obtained his habilitation from Technische Universität Berlin.
- The paper "A regularity structure for rough volatility" appeared in Mathematical Finance.

In the area of regression-based methods for optimal stopping and control in energy markets, the new approach towards solving numerically optimal stopping problems via reinforced regression-based Monte Carlo algorithms, started in the preceding year, was continued and culminated in paper [6]. The main idea of the method is a backward regression where in each backward induction step the regression basis is enhanced with new basis functions "learned" from the preceding backward induction step. As such, this method has a flavor of deep learning.

The research on nonlinear Markov or McKean–Vlasov processes, which are stochastic processes related to nonlinear Fokker–Planck equations whose dynamics at a certain time depend on the present distribution of the process at that time, was continued. Such processes arise in various applications, for example, lithium battery modeling, population dynamics, neuroscience, and financial mathematics. This year's focus was on the analysis of a regression-based estimator for solving McKean–Vlasov-related final value problems globally in space. This estimator involves the realization of an interacting particle system connected with the McKean–Vlasov equation. The main issue in this study is the fact that the particles are correlated due to their interaction, unlike the case of standard Monte Carlo regression. Subsequently, these estimators were incorporated in a backward dynamic program for the simulation-based solving of optimal stopping problems due to underlying McKean–Vlasov processes. The convergence analysis of the regression procedure and the convergence analysis of the algorithm for solving the optimal stopping problem were finalized. A further focus was and still is the study of related issues in the context of more general common noise mean-field processes, i.e., McKean–Vlasov processes with a common stochastic driver.

Focus Platform *Quantitative Analysis of Rough and Stochastic Systems*

The project AA4-2 "Optimal control in energy markets using rough analysis and deep networks" within MATH+ started. Work on randomized optimal control algorithms began, with the aim of applying such methods to energy and financial markets. From a theoretical point of view, rates of convergence of these algorithms were studied. Such methods were implemented for benchmark examples in the literature, and satisfying numerical results were obtained.

The investigation of rough volatility models continued. Our seminal paper [5], introducing a powerful and flexible framework for analysis and numerics of rough volatility models based on Hairer's theory of regularity structures was published. Starting from previous results on precise short-time and small noise asymptotics for option prices, based on Hairer's theory of regularity structures (FGP), consequent precise implied volatility expansions were derived.

In addition, the numerical approximation of rough volatility models was studied. In WIAS Preprint no. 2652, the applicability of efficient order numerical quadrature methods for rough volatility models was studied. It was found out that these methods work very well when coupled with extrapolation schemes to improve the weak order of convergence such as Richardson extrapolation.

A further topic in the focus platform was model order reduction (MOR) techniques for nonlinear stochastic and deterministic systems. An important application of MOR is the field of stochastic optimal control problems (SOCP). A large-scale SOCP was successfully reduced in its dimension and, subsequently, the optimal control was derived in the reduced system. MOR was extended to new classes of nonlinear systems, and error bounds were obtained for the reduction error in large-scale systems. As a highlight, a link between bilinear deterministic systems and linear stochastic systems was shown. With the help of this link, many open questions in the field of deterministic control theory could be answered using probabilistic arguments.

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

Head (acting):	Prof. Dr. Barbara Wagner
Deputy Head (acting):	Priv.-Doz. Dr. Olaf Klein
Team:	Dr. Sibylle Bergmann Dr. Pierre-Étienne Druet Dr. Clemens Guhlke Prof. Dr. Christiane Kraus Dr. Manuel Landstorfer Dr. Rüdiger Müller
Secretary:	Ina Hohn

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 focused 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.

Multiphase flow problems in complex liquids

Concentrated suspensions. The collaboration within the Cluster of Excellence *Berlin Mathematics Research Center* MATH+ joint project "Modeling and analysis of suspension flows", headed by Volker Mehrmann (TU Berlin), Dirk Peschka (WG 1), Matthias Rosenau (GFZ Potsdam), Marita Thomas (WG 1), and Barbara Wagner (RG 7), has led to a successful application of the PI's together with Alexander Mielke (RG 1) for a new Thematic Einstein Semester on "Energy-based mathematical methods for reactive multiphase flows" that will be carried out during the winter semester 2020/21.

Dewetting dynamics and morphology of liquid polymers. Dewetting is the hydrodynamic process where a uniform layer of liquid destabilizes and decays into distinct patterns of stationary droplets by virtue of interfacial and intermolecular energies. In collaboration with a group of experimental physicists at the University of Saarland and colleagues at the University of Oxford, the members of RG 7, Barbara Wagner, and WG 1, Dirk Peschka, developed a mathematical model and numerical algorithms to determine the underlying mechanisms for the emergence of the different droplet patterns, namely, Navier slip at the liquid-solid interface. This fundamental result appeared in one of the leading interdisciplinary journals, Proceedings of the National Academy of Sciences (PNAS) [4].

The successful collaboration with the University of Saarland will be continued after a new tandem project "Dynamic wetting and dewetting of viscous liquid droplets/films on viscoelastic substrates" (PIs: Barbara Wagner, Ralf Seemann) within the new DFG Priority Programme SPP 2171 *Dynamic Wetting* was granted. Within this project, fundamental open questions regarding morphology and dynamics of a liquid layer on soft, viscoelastic substrates are investigated, combining asymptotic analysis, numerical simulation, and experimental studies.

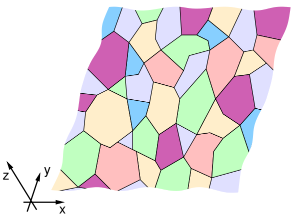

Fig. 1: *Sketch of the facet structure of a polycrystalline surface*

Multiphase problems in quantitative biomedicine. The Oxford-Berlin network for Quantitative Regenerative Medicine initiated by Sarah Waters, Andreas Münch (both U Oxford), Georg Duda (Charité), and Barbara Wagner (RG 7) led to the formation of interdisciplinary research teams that focused, in particular, on controlled tissue regeneration and led to another seed grant "Quantitative Modelling of Interstitial Fluid Pressure in Fibre Reinforced Hydrated Networks" funded by the UK Regenerative Medicine Platform with partners from Imperial College London, University of Nottingham, University of Oxford, and WIAS. Our theory on hydrogels was extended in several ways to accommodate the properties of fibre-reinforced networks as toy models for muscle tissue: (a) addition of a second network phase that accounts for anisotropic stretching, (b) extension to polyelectrolyte gels in salt solution that show a new type of phase transition in connection with gel collapse. Apart from these more applied results, a new asymptotic theory was developed, based on the self-consistent field theory (SCFT) that correctly captures the different stretching regimes of a polymer network; see [3] for the case of a polymer brush.

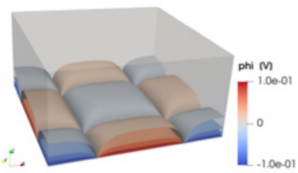

Fig. 2: *Isosurfaces of the electric potential in the electrolyte from 3D-FEM computation. The surface consists of a periodic checkerboard pattern of equally sized facets.*

Mathematical models and theory of electrochemical processes

MATH+ AA2-6:"Modeling and simulation of multi-material electrocatalysis". Multi-material electrodes play an important role in modern electrocatalysis applications. The project, headed by Manuel Landstorfer (RG 7) and Jürgen Fuhrmann (RG 3), aims at continuum models for electrocatalysis at the nm – μm scale, coupling reactions on catalytic interfaces, reactant transport in electrolytes, and charge transport in catalyst substrates. In a first step, an electrochemical characterization of the equilibrium properties of polycrystalline electrodes was obtained. While single crystal surfaces are rather well understood, most standard solid electrodes are polycrystalline, exhibiting many facets of differently oriented grains to the electrolyte. Therefore, the surface is non-homogeneous in its physical properties. A typical surface pattern is sketched in Figure 1. The differential capacitance and the potential of zero charge of patterned surfaces are calculated by a three-dimensional finite-element method (FEM) simulation of an improved Poisson–Boltzmann model developed in RG 7 during the recent years; see Figure 2. The numerical results [1] show already for moderately large facets that a polycrystalline electrode is well approximated by an ensemble of independent single crystal electrodes. The construction of the capacitance of a bi-crystal with equal surface fraction of both kinds of facets is sketched in Figure 3. The results show that one has to be careful when transferring well-known qualitative properties of single crystal electrodes to the polycrystalline case, the potential of zero charge is, in general, not located at the averaged potential of the contributing facets and is, in general, not found at a local capacitance minimum.

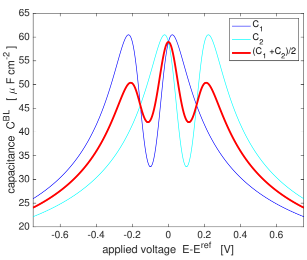

Fig. 3: *Construction of the differential capacitance of a symmetric bi-crystal electrode with* $s_1 = s_2 = \frac{1}{2}$

A precise measurement of all surface facets and their corresponding work functions is extremely expensive, if possible, and even measurements on very similar facets may contain some scatter. Hence, the input values for the mathematical model can only be determined to a certain precision, which has to be taken into account when realistic polycrystalline surfaces are to be described. The obtained results in [1] allow a stochastic description of the polycrystalline surface. To describe a non-ideal Ag polycrystal that is mainly covered by facets near to low index surfaces like (100), (110) and (111), different probability densities can be considered that consist of a superposition of non-overlapping scaled normal distributions around the potentials of the low index facets; see Figure 4. The resulting capacity curve remains close to the capacity of an ideal polycrystal with equal surface fractions $s_i = \frac{1}{3}$ for $i = 1, 2, 3$. Moreover, we perturb the configuration such that an equi-distribution in a 1 V potential range is superimposed in the probability density. As a result, we obtain a much more smooth capacity curve. The pure equi-distribution results in stronger smearing of the capacitance over the potential range such that the capacity minima actually disappear. In light of this result, the function of supercapacitors can be explained by the inhomogeneity of the fine faceted granular electrode surface.

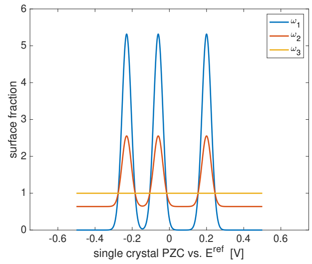

Fig. 4: *Different probability densities to describe the surface chemical potential of electrons on a non-ideal Ag polycrystal*

BMBF Project MALLi[2]. Manuel Landstorfer of RG 7 is the project coordinator of the BMBF compound project MALLi[2] [1] with Mario Ohlberger (WWU Münster), Volker Schmidt (U Ulm), Sven Simon (U Stuttgart) and Kai Birke (U Stuttgart) as scientific partners and VARTA Microbattery as industrial partners.

The project aims to improve the lifetime estimation of lithium ion batteries (LIBs) with mathematical modeling techniques. During the first life cycle, e.g., in electric vehicles, LIBs degrade and are decommissioned at 80% of their original capacity due to weight issues. However, these cells can be further used as stationary energy storage devices if proper and reliable lifetime estimations exist. Within MALLi[2], the ageing processes are systematically investigated with a batch of LIB cells (provided by VARTA Microbattery), which are cycled at well-defined laboratory conditions. The electrochemical characteristics, i.e., current-voltage relations and impedance spectra, are continuously recorded over the (1–2)-year charge-discharge cycles (U Stuttgart). Further, the microstructural degradations of the very same cells are investigated with X-ray computed tomography (Nano-CT, U Stuttgart, and Synchrotron-CT, Helmholtz-Zentrum Berlin), yielding three-dimensional datasets of the porous electrode structure evolution. In combination, we obtain a time series of structural and electrochemical data for various charge-discharge rates and cycle numbers, which serve to validate the mathematical models developed within MALLi[2].

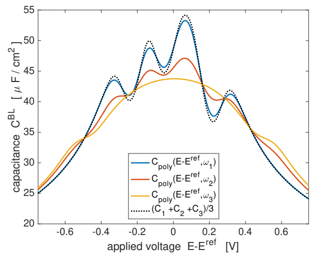

Fig. 5: *Capacity curves related to Figure 4 (solid lines). For comparison, the capacity of an ideal polycrystal of three low index facets with equal surface fraction. (dotted line).*

The mathematical modeling is based on non-equilibrium thermodynamics and the WIAS framework for electrochemical interfaces (WIAS Preprint no. 2560, WIAS Preprint no. 2563). This yields a PDE system that accounts for diffusion and conductivity in the electrolyte phase, lithium ion concentration in the active particles, and intercalation reactions at the electrode-electrolyte interface (WIAS Preprint no. 2563, [2]). The determination of the effective parameters requires a proper description of the three-dimensional microstructure (U Ulm) and a subsequent meshing as well as the numerical solution (WIAS). Homogenization techniques lead to a macroscopic PDE system with effective parameters, which are determined from the porous microstructure of the electrodes.

[1] Modellbasierte Abschätzung der Lebensdauer von gealterten Li-Batterien für die 2nd-Life Anwendung als stationärer Stromspeicher

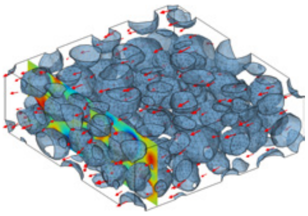

Fig. 6: *3D numerical solution of homogenization cell problem for a porous battery electrode. The blue particles are the solid intercalation particles, in which lithium ions are stored, whereas the complement phase corresponds to the electrolyte.*

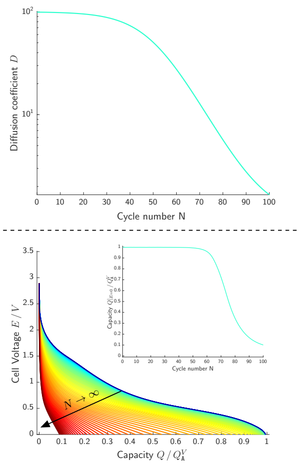

Fig. 7: *Top: Prescribed variation of the effective diffusion coefficient D with cycle number N, e.g., due to microscopic cracks within the battery electrode. Bottom: Consequence of the $D = D(N)$ variation on the electrochemical model determining the cell voltage E as function of the battery capacity Q (w.r.t the initial capacity Q_A^V) and the cycle number N.*

Figure 6 shows a three-dimensional microstructure as well as a numerical solution of the cell problem, which determines the effective diffusion coefficient in the electrolyte phase. The resulting homogenized model of a porous battery cell is then used in the first place to *reproduce* the electrochemical data of the un-aged battery cell, yielding the initial point for degradation modeling.

Within an LIB *in operando*, several ageing effects occur simultaneously, and a proper bottom-up modeling is very tedious. However, certain ageing effects leave specific traces in the electrochemical data. From a modeling perspective, we exploit this by assuming that the ageing effects propagate into time variations of the (effective) parameters of the battery model; see Figure 7. These time variations due to ageing are subsequently identified and quantified by reduced basis models (U Münster), which yields a powerful tool to investigate and estimate the impact of various parameters on the lifetime of an LIB.

DFG Project: Analysis of improved Nernst–Planck–Poisson models for incompressible electrolytic mixtures subject to chemical reactions

In this project, obtained by Pierre-Étienne Druet in the framework of the DFG module Temporary Positions for Principal Investigators ("Eigene Stelle"), 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 were developed. In the simplest case of a mixture of chemical substances $A_1, \ldots, A_N$, with $N \geq 2$, which is incompressible near the reference pressure of the system, the constraint is

$$\sum_{i=1}^{N} \frac{\rho_i}{\rho_i^{ref}} = 1,$$

where $\rho_1, \ldots, \rho_N$ are the mass densities of the species, and $\rho_1^{ref}, \ldots, \rho_N^{ref}$ are the bulk mass densities of the pure substances at the reference pressure. This condition is the correct generalization of the condition $\rho = \rho^{ref}$ well known in the context of single component fluids. In [5], a general solution theory for global-in-time weak solutions is developed for this problem. Two further essential and novel results were achieved in [6], where we prove that initial-boundary value problems for purely convective, multicomponent Darcy flows are well posed; and in [7], where we prove the well-posedness of the general equations of diffusion in multicomponent fluids both for Fick–Onsager and Maxwell–Stefan constitutive equations. It is worth noting that in the latter work, no restrictions are needed beyond the basic requirements of thermodynamical consistency for the Onsager operator and the Helmholtz free energy.

Hysteresis, electromagnetic-mechanical components, and uncertainty quantification

The investigations on uncertainty quantification for models involving hysteresis operators were continued. In the past, experimental data for Terfenol-D, provided by Daniele Davino (Benevento, Italy), had been used to compute appropriate values for the parameters in a model involving 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. In view of modeling issues, one should replace the generalized Prandtl–Ishlinskiĭ operator by a hysteresis operator being a corresponding admissible counter-clockwise potential. First identification results for the parameters for this updated model were obtained.

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

Head:	Prof. Dr. Michael Hintermüller
Deputy Head:	Dr. Carlos N. Rautenberg
Team:	Dr. Amal Alphonse Jo Andrea Brüggemann Dr. Guozhi Dong Tobias Keil Dr. Axel Kröner Dr. Caroline Löbhard Dr. Kostas Papafitsoros Dr. Ruchi Sandilya Steven-Marian Stengl
Guests:	Rafael Arndt Jonas Holley Dr. Olivier Huber Charles Emeka Onyi
Secretary:	Cecilia Bonetti
Nonresident Members:	Prof. Dr. Martin Brokate

The research expertise of the group lies in the area of optimization associated to nonsmooth energies in infinite-dimensional spaces as well as to partial differential equations (PDEs) with nonsmooth structure. The group focuses on the theoretical analysis and modeling of corresponding real-world problems as well as the development of efficient solution algorithms and their computational realization. Particular fields of interest involve nonsmooth energy functionals in image processing, generalized Nash equilibrium problems, modeling of gas networks, quasi-variational inequalities (QVIs) as well as modeling of multiphase flows. RG 8 actively contributes to the main application areas of WIAS *Quantitative Biomedicine*, *Optimization and Control in Technology and Economy*, *Flow and Transport*, as well as aspects of *Materials Modeling*.

RG 8 was founded in 2016 and has now achieved a well-established integration within WIAS. Two new members have started in the reported period: Ruchi Sandilya (postdoc) and Axel Kröner (postdoc).

General relevance of the scientific topics considered by the RG

The study of problems that are associated with a nonsmooth structure is the main research focus of RG 8. This is motivated by the plethora of ways in which nonsmoothness arises in real-world applications. Examples include constitutive laws (like friction), game theory (Nash equilibrium), nondifferentiable constraints, or objective functionals in optimization models.

Nonsmoothness is challenging since regularity is a classical assumptions for existing results to hold. To tackle such problems, there are two main approaches: The first approach is to regularize the nonsmoothness in order to use existing results and perform some limiting analysis. The second approach is to develop theories that can directly handle specific types of nonsmoothness. For instance, in the variational models in image processing, where nonsmooth objectives have a crucial role in preserving discontinuities (image edges), nonsmoothness can be tackled via convex duality theory. There, the nonsmooth image reconstruction problem (primal problem) can be linked to its dual problem, typically a smooth problem with box-type constraints, which can be handled more efficiently [5]. On the other hand, in the context of noncooperative games, the characterization of Nash equilibrium can be done by considering the collection of first-order conditions for all game participants. This leads to a (quasi-)variational inequality, for which existence results and numerical schemes are available.

Selected research results

Mathematical analysis of the gas markets. An ambitious energy agenda in Germany and Europe aims at improving the sustainability of the power generation as well as the diversification of the energy sources. This calls for important political decisions on the directions to follow. This has to be done in a context of a liberalized and decentralized energy markets. Hence, a particular attention is paid to formulate mathematical models with meaningful economic interpretations. RG 8 continues its participation in the DFG Collaborative Research Center SFB/TRR 154 *Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks* with the subproject B02 "Multicriteria optimization subject to equilibrium constraints at the example of gas markets". Paramount in this analysis are the optimal distribution of gas and the analysis of market inefficiencies. The gas transport over a large network is captured by the Euler equations, a system of hyperbolic PDEs, which can be approximated depending on the desired granularity of the physical model. The controls are acting through the Dirichlet boundary conditions, and finally, bilateral state constraints are present.

Mathematically, the market structure gives rise to a GNEP (Generalized Nash Equilibrium Problem), where the equations for gas transport through the network are shared among all market participants. In order to get economically meaningful results, we have to restrict the solution concept to be the one of variational equilibria. This ensures that all market participants have the same perception of the shared constraints. On the mathematical side, this changes the problem structure from a QVI into a nicer variational inequality (VI). The structure of this VI presents the following challenges: It is usually nonmonotone, and the system of PDEs is hyperbolic. For the latter part, we use a viscosity regularization to get parabolic PDEs. For the numerics, a Moreau–Yosida regularization of the state constraints is done. The research effort focuses on the existence of solutions to the GNEP and the numerical methods to solve such games.

Image processing. The group has been active in the field of image processing following the completion of the ECMath CH12 project on "Advanced magnetic resonance imaging: Fingerprinting and geometric quantification". Part of the group's research in this field is now carried out within the currently running project EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization" in the Center of Excellence MATH+. In this project, the following novel framework for quantitative imaging problems is considered:

$$A(u,\theta) = y, \quad \text{where } u = \mathcal{N}(\theta) \text{ and } \theta \in \mathcal{C}_{ad}. \tag{1}$$

The first equation denotes an image reconstruction task, typically an inverse problem, while the second one denotes a constraint involving a neural network $\mathcal{N}$ which aims to approximate a physical modeling process. This process involves some physical parameters θ that need to be quantified, and it is typically given in a form of (a system of) differential equations, e.g., the Bloch equations in the case of quantitative magnetic resonance imaging. This extends our previous work in [4] where the solution map of the Bloch equations was embedded into a single nonlinear equation with unknowns being $\theta = (T_1, T_2)$, the magnetization relaxation times of the imaged tissue. Our new extended work overcomes the obstacle of having to know this solution map explicitly as it can now be "learned" from data through the neural network $\mathcal{N}$ and be embedded into an analogous scheme to the one used in [4].

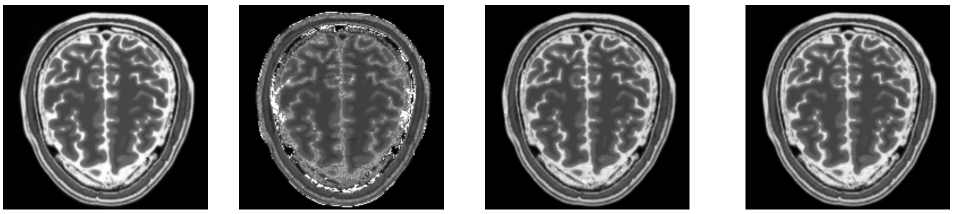

Fig. 1: *Improved reconstruction of the T_1 map using our proposed physics learning-based approach*

Furthermore, a bilevel optimization framework for the automatic selection of spatially dependent regularization parameters for total generalized variation (TGV) regularization was introduced. The computed regularization parameters not only result in preservation of fine scale image details, but also lead to elimination of the staircasing effect, a well-known artifact of total variation regularization. This general methodology for designing automated (monolithic) image reconstruction workflows using bilevel optimization was summarized in an extensive invited review article in the latest volume of the Handbook of Numerical Analysis [5].

Fig. 2: *Improved TGV-based denoising with automatically computed spatially distributed regularization parameters via bilevel minimization*

Generalized Nash Equilibrium Problems. The research group's activities with regard to this focus area have been broadened and intensified. Besides project B02 in the SFB/TRR 154 (see above), the following activities took place:

Research was initiated on the derivation of error estimators for finite element discretization schemes applied to the first-order system of Nash equilibrium problems. With an adaptive method at hand, a more efficient computation of Nash equilibria for problems related to PDE-constrained optimization is possible. The associated results are subsequently capable to synergize with other projects and research activities.

The project "Generalized Nash equilibrium problems with partial differential operators: Theory, algorithms, and risk aversion" within the DFG Priority Program SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* entered its final phase. An overview of the project's achievements can be found in [3]. This work includes results on stochastic aspects of the project done in collaboration with the Philipps-Universität Marburg.

In early March, the follow-up project "Constrained mean field games: Analysis and algorithms" within the second phase of the SPP 1962 was successfully defended in Bad Honnef. Its main objective is to supplement the existing efforts of the research: The situation of a high number of players makes the solution of the arising Karush–Kuhn–Tucker system numerically infeasible. Under the use of symmetries in the players' objectives, one passes the number of players to infinity deriving a system allowing a numerical treatment. The interplay of this paradigm and the presence of a state constraint, as conceptionally arising in the previous research, will be the subject of future investigation.

Multiphase fluids. The research of RG 8 in this area is motivated by recent developments in the construction of microfluidic devices, e.g., lab-on-a-chip devices and photovoltaic cells. Both applications demand a precise control of the involved multiphase flows. The associated optimal control problems are characterized by specific mathematical programs with equilibrium constraints in function spaces, which lead to essentially degenerated sets of feasible state-control pairings. More precisely, Cahn–Hilliard–Navier–Stokes systems with nonsmooth homogeneous energy densities and Hele–Shaw systems with nonsmooth pinning conditions were used to model the underlying physical processes.

Based on previous results concerning ε-almost C-stationarity conditions for the optimal control problems, the group continued and expanded its research to establish the directional differentiability of the corresponding control-to-state operators and derive strong stationarity systems. Moreover, a numerical solver based on bundle-free implicit programming techniques was developed, analyzed and implemented. The solver was enhanced by an automated adaptive mesh refinement procedure utilizing a dual-weighted residual-based error estimator to guarantee a locally refined resolution of the processes at the interface, see [1]. The latter work was done in collaboration with the University of Hamburg within the DFG Priority Program SPP 1962.

The research in this field led to the comprehensive article [2], where different solution methods for the optimal control of geometric partial differential equations are compared and analyzed from an analytical and numerical point of view. These research efforts are a cornerstone for further developing analytical and numerical aspects of shape optimization problems with instationary fluid flow, which emerge, e.g., in the design of structural components in combustion engines and in the drag optimization of ship hulls.

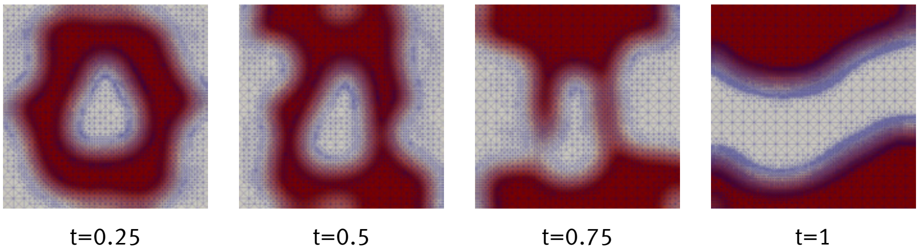

Fig. 3: *Numerical results for the control of a two-phase flow in order to form a curved channel out of an initially ring-shaped domain*

Further highlights in 2019

Regarding scientific events, the organization of the "Sixth International Conference on Continuous Optimization" ICCOPT 2019 in Berlin, August 3–8, 2019, with more than 900 participants and more than 840 scientific contributions, was the highlight of the year for RG 8. Michael Hintermüller was the Chair of both the Organizing and the Program Committees. The conference, which also included a 2-day summer school, was a great success and received hugely positive feedback from the optimization community. Apart from constituting the core of the Local Organization Committee, the group also participated actively in the scientific part, organizing several sessions as well as giving invited and contributed talks. Amal Alphonse was selected by the Best Paper Committee to be among the four finalists for the best paper competition [6].

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 its second phase. The annual meeting was held on October 10–12, 2019, at Hotel Sommerfeld in Kremmen and featured presentations that introduced the projects of the second period.

RG 8 has three currently running projects in the recently established Berlin Mathematics Research Center MATH+, an interdisciplinary Cluster of Excellence and cross-institutional venture of Freie Universität Berlin, Humboldt-Universität zu Berlin, Technische Universität Berlin, WIAS, and Zuse Institute Berlin (ZIB). These projects are: AA4-3 "Equilibria for energy markets with transport", EF3-3 "Optimal transport for imaging" and EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization". Additionally, Michael Hintermüller is a vice-speaker of the center, and a scientist-in-charge of MATH+ Emerging Field 3 (EF3) *Model-Based Imaging*.

The group participated in the "Synergistic Reconstruction Symposium" in Chester, UK, November 3–6, 2019, with an invited oral presentation and a poster. Kostas Papafitsoros received the 1st prize award in the corresponding poster competition ("Generating structure nonsmooth priors for image reconstruction").

Three members of the group participated in the special trimester "The Mathematics of Imaging" organized by the Institut Henri Poincaré in Paris, January–April, 2019. Within this trimester, Michael Hintermüller was invited to give a talk in the Workshop "Variational Methods and Optimization in Imaging", and Kostas Papafitsoros was invited to give a talk at the Young Researcher Colloquium. Guozhi Dong participated in the trimester's winter school in Marseille in January 2019 and gave a presentation there.

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[5] M. Hintermüller, K. Papafitsoros, *Chapter 11: Generating structured nonsmooth priors and associated primal-dual methods*, in: Vol. 20 of Handbook of Numerical Analysis, R. Kimmel, X.-C. Tai, eds., Elsevier, 2019, pp. 437–502, https://doi.org/10.1016/bs.hna.2019.08.001.

[6] A. Alphonse, M. Hintermüller, C.N. Rautenberg, *Directional differentiability for elliptic quasi-variational inequalities of obstacle type*, Calculus of Variations and Partial Differential Equations, 39 pages, **58**:1 (2019), published online on 24.01.2019, https://doi.org/10.1007/s00526-018-1473-0.

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

Head: Dr. Marita Thomas

Team: Priv.-Doz. Dr. Mohammad Hassan Farshbaf Shaker
Dr. Dirk Peschka
Sven Tornquist
Andrea Zafferi

Secretary: Andrea Eismann

Fig. 1: *Weierstrass Group in 2019, from left to right: M.H. Farshbaf-Shaker, A. Zafferi, S. Tornquist, M. Thomas, A. Eismann, D. Peschka*

WG 1 was established as one element of the Flexible Research Platform at WIAS in April 2017; it is partially funded by WIAS budget resources for three years and will be evaluated in Spring 2020.

WG 1's research goal consists in developing mathematical methods for systems with bulk-interface processes. This concerns 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 evolution laws.

The analytical results form the basis for the development of numerical algorithms supporting simulations for applications with bulk-interface interaction. The applications treated by WG 1 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 WG 1's agenda:

(1) dissipative processes in elastic solids with bulk-interface interaction, such as, e.g., damage, fracture, plastification;
(2) optoelectronic processes in semiconductor devices;
(3) multiphase flows with free boundaries.

WG 1 also contributes to organizing the WIAS seminars on Materials Modeling and Semiconductors.

In the following, a summary of the results and events within these three topics in 2019 is given:

Dissipative processes in elastic solids. The 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* studies the convergence of time- and space-discrete schemes for damage and fracture models with different types of coupled dynamics. In this context, to understand the fine properties of solutions to delamination models featuring a regularization of the delamination variable in terms of the perimeter of the "delaminated set", a simplified model for the rate-independent evolution of (delaminated) sets of finite perimeter was analyzed in [1]. Therein, the evolution of the admissible sets is driven by that of a given time-dependent set, which has to include the admissible sets and, hence, is to be understood as an external force. The process is driven by the competition between perimeter minimization and minimization of volume changes. Based on a time-discrete scheme, solutions of the problem are characterized by a stability condition, the validity of an energy-dissipation balance is

SPP 1748

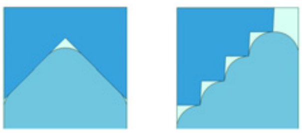

Fig. 2: *Partial C^1-regularity of (light-blue) solution sets for convex (left) and non-convex (right) force sets (dark-blue); cf. [1]*

obtained in specific cases, and fine properties of the solution sets with regard to convexity and regularity are deduced.

Beyond that, in collaboration with RG 4 *Nonlinear Optimization and Inverse Problems*, an optimal control problem with uncertain data and probabilistic terminal constraints for a vibrating string was investigated in [2]. On account of the uncertainty of the initial state, one seeks for controls that steer the system into a given neighborhood of the desired terminal state with sufficiently high probability. The method leads to optimal controls that are robust against uncertainties of the initial state. Such results are novel in the context of PDEs and can be extended to other control problems with uncertain data and probabilistic constraints.

Optoelectronic processes in semiconductor devices. In collaboration with RG 1 *Partial Differential Equations* and RG 3 *Numerical Mathematics and Scientific Computing*, WG 1 contributed to initiating the ECMI Special Interest Group *Modeling, Simulation, and Optimization in Electrical Engineering (MSOEE)* and to organizing the kick-off meeting held at WIAS on January 31 – February 1, see page 63.

Multiphase flows with free boundaries. WG 1 develops mathematical methods for multiphase flows with a focus on free boundary problems, transport of mixtures and suspensions, and also aims at their extension to applications in geosciences, e.g., within project C09 “Dynamics of rock dehydration on multiple scales” in the DFG-funded CRC 1114 *Scaling Cascades in Complex Systems*.

SFB 1114

Together with RG 1, WG 1 carried out the scientific workshop “PDE 2019: Partial Differential Equations in Fluids and Solids” held at WIAS on September 9–13 with more than 70 participants from 13 different countries and also hosted the annual assembly of the GAMM activity group *Analysis of Partial Differential Equations*, see page 61. Moreover, Dirk Peschka and Andreas Münch (Oxford University) jointly organized the Minisymposium “Recent Advances in Understanding Suspensions and Granular Media Flow” at the ICIAM 2019 (July 15–19, Valencia) with two sessions on recent experimental and mathematical aspects.

In February 2019, Mohammad Hassan Farshbaf Shaker started his position within the recently granted project AA2-4 “Modeling and analysis of suspension flows” funded by the DFG within the MATH+ cluster of excellence. This joint project of Dirk Peschka, Marita Thomas, Barbara Wagner (RG 7), Volker Mehrmann (TU Berlin), and Matthias Rosenau (Geoforschungszentrum Potsdam) aims at the development and justification of a unified continuum mechanical suspension flow model, which 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 and experimental data.

MATH+

Dirk Peschka successfully applied for the project “Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows” within the DFG-funded Priority Program 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates*, which started in September 2019. The project focuses on the consistent coupling of free boundary problems with moving contact lines to processes at the fluid-substrate interface (friction, reactions) and to processes inside the substrate (elasticity, porous medium flow). In [3], a joint work with RG 7 *Thermo-*

SPP 2171

dynamic Modeling and Analysis of Phase Transitions, it was shown that even a simple interface coupling can have a drastic impact on pattern formation in dewetting flows. In order to advance numerical methods for free boundary problems, Prof. Luca Heltai (SISSA, Trieste, Italy), a renowned expert in modeling and numerics for fluid-structure interaction problems, was invited as a visiting researcher by WG 1 from June 1 to July 31, 2019.

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, Posters, and Contributions to Exhibitions
- 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. K. Disser, W2 Professorship, August 28, Universität Kassel, Fachbereich Mathematik und Naturwissenschaften.
2. P. Pigato, Junior Professorship, October 22, (professorship corresponding to the German junior professorship) Tor Vergata University of Rome, Department of Economics and Finance.
3. C. Rautenberg, Assistant Professorship, August 1, George Mason University, Fairfax, USA, Department of Mathematical Sciences.
4. M. Redmann, Junior Professorship, August 5, Martin-Luther-Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II – Chemie, Physik und Mathematik.

A.1.2 Awards and Distinctions

1. J. Sprekels, *Member of the Scientific Advisory Committee of the Centrum Wiskunde & Informatika (CWI) in Amsterdam, the Netherlands*, 2019.
2. A. Alphonse, *Best paper finalist at ICCOPT 2019*, August 5, 2019.
3. M. Hintermüller, *Co-chair and Member of the Council of the Berlin Mathematics Research Center MATH+*.
4. ———, *Member of the Integrative Research Institute for the Sciences IRIS Adlershof of the Humboldt-Universität zu Berlin*.
5. ———, *Member of the Scientific Advisory Board of the INM – Leibniz-Institut für Neue Materialien, Saarbrücken*.
6. ———, *Spokesperson of Forschungsverbund Berlin e.V.*
7. D. Hömberg, *Chair of Cost Action TD1409 (Mi-NET)*.
8. ———, *Past President and Board Member of the European Consortium for Mathematics in Industry (ECMI)*.
9. ———, *Vice Chair of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization*.
10. V. John, *SeMA Journal Best Paper Prize 2018, Sociedad Española de Matemática Aplicada*, July 15, 2019.
11. H.-Chr. Kaiser, *Deputy Spokesperson of the Representative Bodies for Disabled Employees of the Leibniz Association*.
12. W. König, *Member of the Council of the Berlin Mathematics Research Center MATH+*.
13. A. Mielke, *Head of the Secretariat of the International Mathematical Union (IMU)*.
14. ———, *Member of the Council of the Berlin Mathematics Research Center MATH+*.
15. ———, *Treasurer of IMU*.
16. V. Spokoiny, *Member of the Council of the Berlin Mathematics Research Center MATH+*.
17. M. Thomas, *Member of the Council of the Berlin Mathematics Research Center MATH+*.

A.1.3 Habilitations

1. CH. BAYER, *Stochastic numerics and applications in rough paths and finance*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, June 19.

A.1.4 Defenses of Ph.D. Theses

1. L. ADAMYAN, *Adaptive weights community detection*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, February 18.
2. S. BERGMANN, *Derivation, asymptotic analysis and numerical solution of atomistically consistent phase-field models*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Prof. Dr. B. Wagner, Prof. E. Meca Álvarez, October 24.
3. T. GONZÁLEZ GRANDÓN, *Stochastic optimization under probust and dynamic probabilistic constraints: With applications to energy management*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. R. Henrion, May 31.
4. E. KLOCHKOV, *Influencer dynamics in opinion networks*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, August 1.
5. A. KOZIUK, *Re-sampling in instrumental variables regression*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, September 13.
6. B. STEMPER, *Rough volatility models: Monte Carlo, asymptotics and deep calibration*, Technische Universität zu Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Dr. Ch. Bayer, March 14.
7. A.J. TÓBIÁS, *Message routeing and percolation in interference limited multihop networks*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 27.
8. N. ALIA, *Optimal control of ladle stirring*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 31.
9. S. EYDAM, *Mode locking in systems of globally-coupled phase oscillators*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Dr. M. Wolfrum, June 12.
10. TH. FRENZEL, *On the derivation of effective gradient systems via EDP-convergence*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, June 26.
11. K. HOPF, *On the singularity formation and long-time asymptotics in a class of nonlinear Fokker–Planck equations*, University of Warwick, Mathematics and Statistics Doctoral Training Centre, supervisor: Prof. Dr. J.L. Rodrigo, October 21.
12. P. VÁGNER, *Thermodynamic modeling of solid oxide cells*, Charles University, Mathematical Institute, supervisor: Prof. F. Maršík, June 19.

A.1.5 Supervision of Bachelors and Masters Theses

1. F.F.A. BETHKE, *Second-order analysis for a bilinear optimal control problem governed by the linear damped wave equation* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Dr. A. Kröner, Prof. Dr. M. Hintermüller, October 30.
2. D. FRERICHS, *Zur Druckrobustheit und Adaptivität einer Virtuellen-Elemente-Methode für das Stokes-Problem* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Dr. Ch. Merdon, Prof. Dr. C. Carstensen, September 13.

3. F. Fumagalli, *Adaptive weights classification* (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. V. Spokoiny, February 1.
4. I. Hamoumi, *Accessibility assistance for the interactive navigation of texts* (master's thesis), Technische Universität Hamburg, Institut für Mathematik, supervisor: Dr. P. Farrell, February 5.
5. S. Kasaj, *One-level preconditioners for saddle point problems* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Caiazzo, December 11.
6. D. Kohn, *Die Kapazität in einem hochdichten D2D-Netzwerk* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, November 24.
7. F. Krause, *Ausdünnung eines Punktprozesses und Sendestrategien* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, October 8.
8. K. Krenz, *Existenzanalysis und numerische Simulation von Optimalsteuerungsproblemen zu linearen und nichtlinearen Schrödingergleichungen* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Prof. Dr. M. Hintermüller, Dr. A. Kröner, December 16.
9. H. Langhammer, *Clustergrößenverteilung eines zufälligen Graphen* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, November 18.
10. B. Lichtblau, *Image segmentation with parametric active contours in hip arthroplasty* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, February 21.
11. R. Löffler, *Percolation phase for the SINR model with random powers* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, June 14.
12. M. Lübbering, *Predicting stock prices based on press release sentiment: A comparison of naïve Bayes classifiers and support vector machines* (master's thesis), Technischen Universität Hamburg, Institut für Mathematik, supervisor: Dr. P. Farrell, January 8.
13. M. Messerschmid, *Sampling auf der Sphäre mit Anwendungen auf die stochastische Optimierung* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Priv.-Doz. Dr. R. Henrion, August 28.
14. J.-L. Mönning, *Asymptotic estimates for the chemical master equation* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Dr. M. Liero, Prof. Dr. A. Mielke, September 24.
15. J. Müller, *Ein diskretes Modell für Nachrichtentrajektorien* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, November 24.
16. D. Ni, *Sequentielle Beobachtung eines stochastischen Prozesses* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. M. Scheutzow, June 13.
17. J. Paikert, *Der Ginibre-Punktprozess* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, March 17.
18. M. Savova, *Lamplighter Irrfahrten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. N. Kurt, Prof. Dr. W. König, June 19.

19. S. Saydan, *Solvers for saddle point problems arising from finite element discretizations of the Darcy equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Caiazzo, December 13.
20. St. Schindler, *Spektren von Operatoren auf allgemeinen Hilberträumen und deren Verknüpfung mit Gradientenflüssen* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. M. Renger, October 31.
21. J. Schubert, *Zufällige Nachrichtenhopentscheidungen in einem Telekommunikationssystem* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. B. Jahnel, August 15.
22. N. Sharifian, *Zeitliche Behandlung des nichtlinearen Konvektionsterms in inkompressiblen Navier-Stokes-Gleichungen* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. A. Caiazzo, November 6.
23. A. Skënder Këndezi, *Extremwerte von stationären Folgen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. N. Kurt, Prof. Dr. W. König, February 1.
24. J. Trantow, *A pseudo time-stepping approach for the evolution of elastic curves* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 10.
25. F. Wunderlich, *The asymptotic strong Feller property. Enhancing conditions* (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Dr. O. Butkovsky, October 10.

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 and ended in September 2019. 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 were jointly carried out, providing a unique interdisciplinary and inter-sectorial training opportunity. The research focused on three major topics: induction heating, phase transformations in steel alloys, and gas stirring in steelmaking ladles. MIMESIS had a budget of 2.1 million euros and was 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 was a full partner within the Eurostars project E!10524 "High power composites of edge emitting semiconductor lasers" (HIP-Lasers, 2016–2019), which aimed 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)"** was a COST-funded action, which aimed to facilitate more effective widespread application of mathematics to all industrial sectors, by encouraging greater interaction between mathematicians and industrialists. It was chaired by RG 4 and ended in April 2019.

[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 is 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 supported enterprises in the research and development of innovative laser beam sources and components with a large application and market potential. RG 2 acted 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**

  "rDesign – Robust Topology-Optimization for SME in Industry 4.0" (September 1, 2018, to August 31, 2019) was a spin-off in preparation of WIAS Berlin (RG 3). It was 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

- **Excellence Strategy of the Federal and the State Governments (DFG)**

MATH+

The Berlin Mathematics Research Center MATH+

The highlight of the collaboration with the mathematical institutions in Berlin since January 2019 was the joint operation of the Berlin Mathematics Research Center MATH+.

MATH+ is a cross-institutional and transdisciplinary Cluster of Excellence with the aim to explore and further develop new approaches in application-oriented mathematics. Emphasis is placed on mathematical principles for using ever larger amounts of data in life and material sciences, in energy and network research, and in the humanities and social sciences. The Research Center is funded by the DFG for a first period of seven years since January 2019. It is a joint project of Freie Universität Berlin, Humboldt-Universität zu Berlin, Technische Universität Berlin, WIAS, and the Zuse Institute Berlin (ZIB). MATH+ continues the success stories of the renowned Research Center MATHEON and the Excellence-Graduate School Berlin Mathematical School (BMS).

In 2019, WIAS dedicated considerable financial and personal resources to the Center: Its director, Prof. M. Hintermüller (RG 8) was one of the three spokespersons and a member of the Executive Board of MATH+. He and his deputy directors, Prof. A. Mielke (RG 1) and Prof. W. König (RG 5), as well as Prof. P. Friz (RG 6), Prof. V. Spokoiny (RG 6), and Dr. M. Thomas (WG 1) were members of the MATH+ Council; Prof. A. Mielke (RG 1), Scientist in Charge of the Application Area AA2 “Materials, Lights, Devices”, Prof. M. Hintermüller (RG 8) and Prof. V. Spokoiny (RG 6) Scientists in Charge of the Emerging Field EF3 “Model-based Imaging”, and Prof. P. Friz (RG 6) and Prof. W. König Scientists in Charge of the Emerging Field EF4 “Particles and Agents” ; and WIAS members participated in the successful running of the following subprojects:

SE17: “Stochastic methods for the analysis of lithium-ion batteries” (ECMath-financed MATHEON project; in RG3, RG 6, and RG 7)

SE18: “Models for heat and charge-carrier flow in organic electronics” (MATH+ transition project; in RG 1)

AA2-1 “Hybrid models for the electrothermal behavior of organic semiconductor devices” (in RG 1)

AA2-3 “Quantum-classical simulation of quantum dot nanolasers” (in RG 2)

AA2-4 “Modeling and analysis of suspension flows” (in WG 1 and RG 7)

AA2-5 “Data-driven electronic structure calculations for nanostructures” (in RG 1)

AA2-6 “Multi-material electrocatalysis” (in RG 3 and RG 7)

AA4-1 “PDAEs with uncertainties for the analysis, simulation and optimization of energy networks” (in RG 4)

AA4-2 “Optimal control in energy markets using rough analysis and deep networks” (in RG 6)

AA4-3 “Equilibria for energy markets with transport” (in RG 8)

EF1-5 “On robustness of deep neural networks” (in RG 6)

EF2-4 “Conforming regular triangulations” (in RG 3)

EF3-1 “Model-based geometry reconstruction from TEM images” (in RG 1 and RG 6)

EF3-3 “Optimal transport for imaging” (in RG 6 and RG 8)

EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization" (in RG 8)

EF4-1 "Influence of mobility on connectivity" (in RG 5)

IP-TB-3 "Understanding doping variations in silicon crystals" (in LG 5)

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

  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).

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

  This collaborative research center began its work on January 1, 2008. In the third funding period (2016–2019), WIAS participated 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).

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

  In 2019, the SFB started with its third and last funding period. This interdisciplinary SFB combines groups from theoretical physics, applied mathematics, and computational neuroscience from four universities and research institutes in Berlin. WIAS participates with two subprojects. Subproject A3 "Self-organization and control in coupled networks and time-delayed systems" in RG 2 is focused on high-dimensional dynamics and localization phenomena in complex network systems and delay differential equations. Subproject A5 "Pattern formation in coupled parabolic systems" in RG 1 studies pattern formation in reaction-diffusion systems and in models of fluid dynamics.

- **Collaborative Research Center (SFB) 1114: "Skalenkaskaden in komplexen Systemen" (Scaling Cascades in Complex Systems)**, Freie Universität Berlin

  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 materials and 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 WG 1).

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

  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 nonparametric 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 2016–2019 (in RG 5), the interest was concentrated in 2019 on the analysis of branching processes in random environments on particular discrete 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 participated 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 aimed at assessing and improving numerical methods for population balance systems. In particular, a coupled stochastic-deterministic method for solving population balance systems was developed.

- **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. The second funding period until 2022 started in 2019.

  WIAS participated in the first funding period with the subprojects "Generalized Nash equilibrium problems with partial differential operators: Theory, algorithms and risk aversion" (until 31.12.2019), "Optimal control of elliptic and parabolic quasi-variational inequalities" (until 31.08.2019), and "Simulation and control of a nonsmooth Cahn–Hillard Navier–Stokes system with variable fluid densities" (until 31.12.2019), and participates in the second funding period with the subprojects "A non-smooth phase-field approach to shape optimization with instationary fluid flow" (from 01.07.2019), "Constrained mean field games: Analysis and algorithms" (from 01.07.2019), and "A unified approach to optimal uncertainty quantification and risk-averse optimization with quasi-variational inequality constraints" (from 01.07.2019) (all in RG 8).

- **Priority Program SPP 2171: "Dynamic Wetting of Flexible, Adaptive, and SwitchableSubstrates"**, Universität Münster

  The dynamic process of liquids that wet or dewet substrates is relevant in nature and for many technological applications. Processes that involve lubrication, adhesives, or surface coatings, depend on the dynamics of wetting processes. Recent developments in areas like microelectronics or 3D printing demonstrated the need to also understand cases in which the hydrodynamics and substrate dynamics are strongly coupled. This holds true especially on microscopic and mesoscopic length scales, where (non-)equilibrium surface phenomena dominate.

  WIAS participates in this first funding period with the two subprojects "Mathematische Modellierung und Simulation der Wechselwirkung von Substraten mit Strömungen durch verallgemeinerte Gradientenflüsse" (Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows; in WG 1; duration Sep. 2019 – Aug. 2022) and the tandem project "Dynamisches Benetzen und Entnetzen von viskosen flüssigen Tropfen/Filmen auf viskoelastischen Substraten" (Dynamic wetting and dewetting of viscous liquid droplets/films on viscoelastic substrates; in RG 7) in cooperation with Ralf Seemann (Universität des Saarlandes) (duration: Jan. 2020 – Dec. 2022).

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

  The first phase of this research unit has been funded since 2016, the second phase since 2019. 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.

- **GAČR-DFG Cooperation: Joint German-Czech Research Projects**

  "Electrochemical double layers in solid oxide cells (EDLSOC)" (in RG 3): This is a joint project of the Weierstrass Institute and the University of Chemistry and Technology, Prague, Czechia. The main goal of the EDLSOC project is to establish a detailed, experimentally validated thermodynamic description of the interface processes occurring in the electrodes of solid oxide cells. Model development and comparison to experimental data is supported by numerical models.

- **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)

"Mathematische Modellierung und Simulation der Wechselwirkung von Substraten mit Strömungen durch verallgemeinerte Gradientenflüsse" (Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows; Dr. D. Peschka)

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)

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.
- Two DAAD Fellowship holders (in RG 3 and RG 5); see page 171

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

- One Humboldt Research Fellowship holder (in RG 8); see page 171

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)
- Orange Labs Research, Paris, France:
  "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)
  "Connectivity improvements in mobile device-to-device networks" (01.12.2019–30.11.2020; 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. Ch. Bayer, Managing Editor, Quantitative Finance, Taylor & Francis Online, London, UK.
5. P. Friz, Editor-in-Chief, Annals of Applied Probability, The Institute of Mathematical Statistics, Beachwood, OH, USA.
6. ———, Editorial Board, Electronic Journal of Probability, Institute of Mathematical Statistics, Bethesda, USA.
7. R. Henrion, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
8. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
9. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
10. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
11. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
12. M. Hintermüller, Editorial Board, Interfaces and Free Boundaries, European Mathematical Society Publishing House, Zurich, Switzerland.
13. ———, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
14. ———, Editorial Board, ESAIM: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
15. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, 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. ———, Editorial Board, Foundations of Data Science, American Institute of Mathematical Sciences, Springfield, USA.
19. ———, Series Editor, International Series of Numerical Mathematics, Springer-Verlag, Basel, Switzerland.
20. ———, Series Editor, Handbook of Numerical Analysis, Elsevier, Amsterdam, Netherlands.
21. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
22. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.

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

23. W. KÖNIG, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
24. ———, Editorial Board, Bernoulli Journal, International Statistical Institute/Bernoulli Society for Mathematical Statistics and Probability, The Hague, Netherlands.
25. ———, Series Editor, Pathways in Mathematics, Birkhäuser, Basel, Switzerland.
26. P. MATHÉ, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
27. ———, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, Netherlands.
28. A. MIELKE, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
29. ———, Co-Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
30. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
31. M. RADZIUNAS, Editorial Board, Mathematical Modelling and Analysis, Vilnius, Lithuania.
32. J.G.M. SCHOENMAKERS, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
33. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
34. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
35. V. SPOKOINY, Co-Editor, Stochastic Processes and their Applications, Elsevier, Amsterdam, Netherlands.
36. ———, Editor, Theory of Probability and its Applications, SIAM, Philadelphia, Pennsylvania, USA.
37. M. THOMAS, Associate Editor, Discrete & Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences, Springfield, 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.

A.4 Conferences, Colloquia, and Workshops

18th GAMM Seminar on Microstructures
Berlin, January 18–19
Organized by: WIAS (RG 1), HU Berlin
Supported by: CRC 1114, HU Berlin

The series of "GAMM Seminars on Microstructures" was initiated to bring together engineers and mathematicians working on multiscale problems, mostly related to solid mechanics and material sciences. The workshops focus on

- mathematical and mechanical modeling materials with microstructure (plasticity, damage, phase transitions, electro-magneto-mechanics),
- experimental results on the formation and evolution of microstructure,
- mathematical analysis, variational formulations, non-convex problems, relaxation methods,
- and multiscale methods and computational tools for the determination of effective properties of micro-heterogeneous materials.

This workshop gave the opportunity to discuss and to compare different approaches to the above-mentioned fields and provided a platform for the interaction among young and established researchers in solid mechanics, mathematics, and material sciences.

There were 6 invited speakers from Germany, Europe, and the USA and all in all 43 participants. The workshop hosted the annual meeting of the GAMM Activity Group *Analysis of Microstructures*.

Kick-off Meeting of the ECMI Special Interest Group "Modelling, Simulation and Optimization in Electrical Engineering"
Berlin, January 31 – February 1
Organized by: WIAS (RG 1, RG 3, and WG 1)
Supported by: European Consortium for Mathematics in Industry (ECMI)

Recently, ECMI's research and innovation committee agreed to establish a special interest group on "Modeling, Simulation and Optimization in Electrical Engineering" (MSOEE). It is currently maintained by Stefan Kurz and Sebastian Schöps. The kickoff meeting at WIAS was the first joint meeting in which aims and methodologies of the MSOEE were discussed by all participants. There were four main talks concerned with previous collaborations in computational electronics, industry perspectives and possible European grants for which MSOEE aims to apply. There were also two round table discussions: The first one established the long-term goals of the MSOEE, e.g., joint projects between academia and industry, challenge workshops, book series about progress in the field. The second one established short-term goals of the MSOEE, e.g., a monthly newsletter, minisymposia, and conferences. There was an important discussion about antitrust ground rules and code of conduct, which nowadays have become an essential part of good practices for collaboration of academia and industry.

There were 27 participants from 4 European countries, 4 main talks given by Prof. Sebastian Schöps (TU Darmstadt), Prof. Michael Günther (Bergische Universität Wuppertal), Prof. Stefan Kurz (TU Darmstadt and Robert Bosch GmbH), and Prof. Wil Schilders (TU Eindhoven).

New Directions in Stochastic Analysis: Rough Paths, SPDEs and Related Topics
Berlin, March 18–22
Organized by: WIAS (RG 6), TU Berlin, HU Berlin, ZIB
Supported by: WIAS, ZIB, DFG FOR 2402, ERC

The conference was organized in order to highlight the topics of DFG FOR 2402, also marking the 65th birthday of Terry Lyons (Oxford). Hence, the main emphasis was on the powerful insights of pathwise analysis (Lyons's 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 topics included signatures with its applications to statistics and deep learning.

The conference featured talks by 35 invited speakers, including world leaders in the field such as Martin Hairer, and attracted more than 140 participants from all over the world. In particular, the conference highlighted the strong collaboration between stochastics groups in Berlin and Oxford and fit perfectly into the new strategic partnership between Berlin and Oxford.

The workshop was jointly organized by the WIAS research group *Stochastic Algorithms and Nonparametric Statistics* (P. Friz, Ch. Bayer), Humboldt-Universität zu Berlin (N. Perkowski), TU Berlin (P. Friz, W. Stannat), and Universität Bielefeld (M. Hofmanova), and funded by the DFG (FOR 2402) the and European Research Council.

Leibniz MMS Days 2019
Kühlungsborn, March 20–22
Organized by: IAP Kühlungsborn, WIAS
Supported by: Leibniz Association

The fourth 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. 47 scientists from 24 scientific institutions took part in the workshop. The goal was to further exploit the potential of modern methods of MMS and create synergistic effects. A special emphasis was given to the topics
– Systems biology and genetics as well as
– Computational and geophysical fluid dynamics.

The three keynote talks were given by:
– Carsten Marr (Helmholtz Zentrum München): "Computational models of stem cell decisions"
– Klaus Neymeyr (Universität Rostock): "How nonnegative matrix factorizations can help to decompose spectral mixture data"
– Juha Vierinen (The Arctic University of Norway, Tromsø): "Estimation of the mesospheric wind field correlation and structure functions using multistatic specular meteor radars"

11th Annual Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis
Berlin, May 23–25
Organized by: WIAS (RG 6), TU Berlin, Oxford University
Supported by: WIAS, DFG FOR 2042, European Research Council

Running now for many years, the 11th Berlin-Oxford meeting on Applied Stochastic Analysis took place at WIAS Berlin in Spring 2019. As in previous years, there was an emphasis on the powerful insights of pathwise analysis (Lyons's rough paths, Hairer's regularity structures, paracontrolled distributions à la Gubinelli–Imkeller–Perkowski), especially in the context of nonlinear (stochastic) partial differential equations. Further topics included expected signatures with its applications to statistics and deep learning.

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.

The workshop was jointly organized by the WIAS Research Group RG 6 *Stochastic Algorithms and Nonparametric Statistics*, P. Friz (ERC- and DFG-funded), T. Lyons (ERC-funded), Torstein Kastberg Nilssen (DFG-funded), and Michele Coghi (ECMath-funded).

Workshop on Mathematics and Materials Science for Steel Production and Manufacturing
Skien, June 4–5
Organized by: WIAS (RG 4), EFD Induction Skien
Supported by: European Industrial Doctorate ITN-EID project "Mimesis"

The final consortium meeting of the EID project Mimesis was embedded in an international "Workshop on Mathematics and Materials Science for Steel Production and Manufacturing" held at the production site of the industrial partner EFD Induction in Skien/Norway. Beside the MIMESIS members, several well-known experts in the research area of materials science as well as mathematical modeling, simulation, and optimization with applications in steel production were invited.

WORKSHOP ON PHASE TRANSITIONS AND PARTICLE SYSTEMS
Berlin, June 24–26
Organized by: WIAS (RG 5)
Supported by: MATH+, SFB 1114

The purpose of the workshop was to give an overview on recent developments in dynamic and static problems involving stochastic systems of several interacting components. In this field, the mathematical questions that can be posed and answered appear quite diverse, and the workshop aimed to highlight shared interests and tools, fostering the interaction among researchers. Most of the talks concerned either Gibbs measures or scaling limits of stochastic particle systems, and participants acknowledged the success in having two somehow separated research communities meeting.

This three-day workshop featured two minicourses taught by two world-class experts (one from France and one from the US) and eight invited research talks by distinguished speakers from well-known research institutions all over Europe. A poster session held on the first day gave the opportunity to many young researchers to present their work and it stimulated multiple scientific discussions among participants. The workshop attracted more than 50 scientists, gathering researchers working on the topic in the Berlin area, but also from Germany and abroad.

This workshop was organized by three members of the WIAS Research Group RG 5 Luisa Andreis, Wolfgang König, and Robert Patterson.

SIXTH INTERNATIONAL CONFERENCE ON CONTINUOUS OPTIMIZATION (ICCOPT 2019)
Berlin, August 3–8
Organized by: WIAS (RG 8 and RG 4), HU Berlin, TU Berlin
Supported by: DFG, Gurobi, HU Berlin, MATH+, MOS, SIAM, SPP 1962, Springer, TU Berlin, Two Sigma, WIAS

The ICCOPT is a flagship conference of the Mathematical Optimization Society (MOS), organized every three years.

ICCOPT 2019 was hosted by the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) Berlin. It included a Summer School (August 3–4) and a Conference (August 5–8) with a series of plenary and semi-plenary talks, organized and contributed sessions, as well as poster sessions. The overall organization was mainly done by members of WIAS, and by the Local Organizing Committee.

As a major event of MOS, ICCOPT aims to promote research in mathematical optimization. There were in total 776 scientific talks scheduled in 274 schedule sessions comprising four plenary talks, eight semi-plenary talks, and 178 organized sessions with three to eight talks each. At the poster session, 30 scientific posters were presented. Furthermore, 869 scientists registered for the conference, and 208 attended the Summer School.

The highlights included four plenaries, eight semi-plenaries, with speakers from Germany, Europe, Asia, and North America. This conference was a big success, with a number of attendee 50% higher than expected.

OPTICAL SOLITONS AND FREQUENCY COMB GENERATION
Berlin, September 18–20
Organized by: WIAS (RG 2)
Supported by: SFB 787, WIAS

The workshop "Optical Solitons and Frequency Comb Generation", organized with the support of SFB 787, brought together renowned national and international experts, both theoreticians and experimentalists, working on optical pulses, nonlinear localized structures in photonic devices, and frequency combs. They got an excellent opportunity to present the latest developments and to exchange knowledge with their colleagues and young scientists in the field of nonlinear optics and optoelectronics. A balance between theory, experiment, and numerics was kept.

The following topics were covered:

- Short optical pulses in photonics devices,
- Optical frequency comb generation in semiconductor mode-locked lasers and optical microcavities,
- Temporal and spatial cavity solitons in active and passive optical systems,
- Stability, interaction, and mobility properties of optical solitons,
- Microlasers and nanolasers,
- Solitons in optical systems with delayed feedback,
- Dispersion, nonlinearity, and solitons in ring and multi-section lasers,
- Generation and propagation of pulses in fiber lasers and optical waveguides,
- Localized structures in PT-symmetric optical systems,
- Model reduction, bifurcations and singular perturbations in nonlinear optics.

The program featured 23 invited and 9 contributed talks presented by speakers. The workshop was attended by 41 registered participants from 11 countries.

Foundations of Modern Statistics
Berlin, November 6–8
Organized by: WIAS (RG 6), HU Berlin, U Heidelberg, U Paris-Est Marne-la-Vallée
Supported by: DFG Research Unit 1735, IRTG 1792, WIAS

This workshop was organized on the occasion of the 60th birthday of Professor Vladimir Spokoiny. As the central theme, recent results on modern mathematical statistics and their applications were presented and discussed. The program featured 15 invited lectures by internationally renowned scientists active in Professor Spokoiny's scientific area.

The Conference was attended by about 64 participants mainly from Germany and Russia as well as from France, Switzerland, Singapore, and the United States.

Workshop on Mathematics of Deep Learning
Berlin, December 3–5
Organized by: WIAS (RG 4 and RG 6), TU Berlin
Supported by: WIAS, MATH+

Deep Learning has become a central topic in industry and science with a wide range of applications related to the processing and interpretation of large amounts of data. With presentations from experts of different fields of mathematics and computer science, the workshop with more than 60 participants focused on the current state of a mathematically rigorous understanding of deep learning architectures and their application.

PDE 2019: Partial Differential Equations in Fluids and Solids
Berlin, September 9–13
Organized by: WIAS (RG 1 and WG 1), U Regensburg, TU Darmstadt
Supported by: DFG, MATH+, WIAS

The international workshop PDE 2019 attracted 71 participants from 13 nations — among them 17 Ph.D. students — and hosted 20 invited lectures (45 min) as well as 18 contributed lectures (30 min). In addition, PDE 2019 hosted a meeting of the GAMM Activity Group "Analysis of Partial Differential Equations".

The workshop PDE 2019 fused expertise on the analysis of PDEs in solids, fluid dynamics, complex fluids, and interaction of fluids with solid structure. It thus created synergies among these fields and advanced analytical methods in current research related to systems with bulk-interface interaction, geometrically nonlinear materials, and fluid-structure interaction. This concerns, e. g., Lagrangian and Eulerian descriptions, free boundaries and moving domains, and variational approaches via energy/entropy methods.

Based on the positive feedback of the participants, conference proceedings will be collected and published as a special issue in the journal “Discrete and Continuous Dynamical Systems – Series S”.

Workshop on Probability, Analysis and Applications (PAA)
Accra, September 30 – October 4
Organized by: WIAS (RG 5), AIMS Ghana
Supported by: DAAD, AvH, BMBF

This workshop was part of the efforts of the members of RG 5 to develop and foster personal scientific contacts between African and German researchers. It was embedded in a three-week stay by Wolfgang König and Benedikt Jahnel as the lecturers in an intense lecture course at *The African Institute for Mathematical Sciences at Accra* (AIMS) Ghana. The main goal was to acquaint African researchers, in particular Ph.D. students and young postdocs, with some of the main research areas of the German guests, to inform the German participants about research topics that are under investigation in Africa, and to offer to the most developed African researchers a platform for giving international talks. There were eight speakers: three from Africa and five from Germany. The subjects of the talks ranged from optimization problems in stochastic analysis for finance to stochastic geometry for telecommunication models to phase transitions in statistical mechanics.

The workshop was organized within the framework of the German Research Chair Program at AIMS Ghana, supported by the Alexander von Humboldt Foundation (AvH) and the German Ministry of Education and Research (BMBF), and was supported by the DAAD. The organizers were Wolfgang König (RG 5), *Dirk Becherer* (Humboldt-Universität zu Berlin), and Olivier Menoukeu Pamen *(AIMS Ghana)*.

Kickoff Meeting of the DFG Priority Programme 1962
Sommerfeld, October 10–12
Organized by: WIAS (RG 8), HU Berlin
Supported by: DFG SPP 1962

The Kickoff Meeting of the Second Phase 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 10 to 12 in Sommerfeld near Berlin. A total of 41 participants attended the annual meeting of whom 39 were from outside WIAS. Each of the newly defended/approved 21 scientific projects in the SPP was represented by a talk of 25 minutes where a presentation of the aims and objectives of the project was given. 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. 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’ workshop or conference for the younger SPP members in late 2020 or early 2021, depending on the current world events. In summary, the meeting was very well attended by old and new members involved in the new (or continuing) projects.

MMS Summer School 2019 on Modern Programming Languages for Science and Statistics: R and Julia
Oberwolfach Research Institute for Mathematics, October 28 – November 1
Organized by: WIAS
Supported by: Leibniz Association

The development and the application of software that relies on certain mathematical and statistical algorithms is widespread in institutes of all sections of the Leibniz Association. Applications are the statistical analysis of experimental and observational data, the simulation of complex models, or the optimization of engineering devices.

The second Ph.D. Summer School of the Leibniz Network “Mathematical Modeling and Simulation” provided an introduction and an overview about two modern open source programming languages for science and statistics, namely R and Julia, which offer powerful tools for scientists.

The six speakers were Chris Rackauckas (JuliaLab/MIT), Patricio Farrell, Jürgen Fuhrmann, Alexander Linke, Jörg Polzehl, and Karsten Tabelow (all WIAS).

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

1. A. Alphonse, C.N. Rautenberg, co-organizers of the Session "Quasi-Variational Inequalities and Generalized Nash Equilibrium Problems", *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.
2. A. Caiazzo, organizer of the Minisymposium "Data-Driven Computational Fluid Dynamics", *European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019)*, Eindhoven University of Technology, Netherlands, September 30 – October 4.
3. P. Dvurechenskii, co-organizer of the Session "Recent Advances in Distributed Optimization", *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.
4. P. Farrell, N. Rotundo, co-organizers of the Minisymposium "Computational and Numerical Methods in Electronics", *SIAM Conference on Computational Science and Engineering (CSE19)*, Spokane, Washington, USA, February 25 – March 1.
5. ———, co-organizers of the Minisymposia MS ME-0-5 7 & 8 "Simulation, Modeling and Analysis of Semiconductors", *9th International Congress on Industrial and Applied Mathematics (ICIAM)*, Valencia, Spain, July 15–19.
6. P. Friz, co-organizer, *Berlin-Leipzig Workshop in Analysis and Stochastics*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 16–18.
7. ———, co-organizer, *Harmonic Analysis and Rough Paths*, Hausdorff Research Institute for Mathematics, Bonn, November 18–19.
8. J. Fuhrmann, co-organizer of the Minisymposium "Entwicklung von Policies und Richtlinien für Forschungssoftware", *deRSE19 – Konferenz für ForschungssoftwareentwicklerInnen in Deutschland*, Albert Einstein Wissenschaftspark Potsdam, June 4–6.
9. R. Henrion, M. Hintermüller, D. Hömberg, C. Löbhard, C.N. Rautenberg, members of the Organizing Committee, *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.
10. M. Hintermüller, co-organizer, *Thematic Programme "Modern Maximal Monotone Operator Theory: From Nonsmooth Optimization to Differential Inclusions", including workshops "Nonsmooth and Variational Analysis" (Jan. 28 to Feb. 1) and "Numerical Algorithms in Nonsmooth Optimization" (Feb. 25 to March 1), and 3 Lecture Series*, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, January 28 – March 8.
11. ———, organizer of the presentation of the DFG Priority Programme 1962 "Non Smooth and Complementarity-Based Distributed Parameter Systems: Simulation and Hierarchical Optimization", *90th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM)*, Technische Universität Wien, Austria, February 18–22.
12. ———, head of the Program Committee and of the Scientific Committee, *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.
13. M. Hintermüller, K. Papafitsoros, co-organizers of the Session "Bilevel Optimization in Image Processing", *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.
14. D. Hömberg, organizer of the Minisymposium "Success Stories from the COST Math in Industry Network", *British Applied Mathematics Colloquium 2019 (BAMC 2019)*, University of Bath, UK, April 24–26.
15. T. Keil, co-organizer of the Session "Optimal Control of Phase Field Models", *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.

16. Th. Koprucki, co-organizer of the Minisymposium "FAIRmath: Opening Mathematical Research Data for the Next Generation", *Annual DMV Meeting 2019*, KIT – Karlsruher Institut für Technologie, September 23–26.
17. ———, member of the Programme Committee, *International Symposium "Semiconductor Nanophotonics" 2019, CRC 787*, Technische Universität Berlin, November 4–5.
18. O. Marquardt, co-organizer, *Sondierungsworkshop MPIE/WIAS "Elektrochemie, Halbleiternanostrukturen und Metalle"*, Max-Planck-Institut für Eisenforschung GmbH Düsseldorf, October 14–15.
19. Ch. Merdon, co-organizer of the Minisymposia MS FE-1-2 5 & 6 & 7 "Divergence-Free and Pressure-Robust Discretizations for the Navier–Stokes Equations", *9th International Congress on Industrial and Applied Mathematics (ICIAM)*, Valencia, Spain, July 15–19.
20. D. Peschka, co-organizer of the Minisymposia MS ME-0-7 5 "Recent Advances in Understanding Suspensions and Granular Media Flow", *9th International Congress on Industrial and Applied Mathematics (ICIAM 2019)*, Valencia, Spain, July 15–19.
21. M. Radziunas, member of the International Program Committee, *24th International Conference on Mathematical Modelling and Analysis*, Tallinn University of Technology, European Consortium for Mathematics in Industry, Vilnius Gediminas Technical University and Tallinn University, Tallinn, Estonia, May 28–31.
22. C.N. Rautenberg, co-organizer of the Session "Fractional/Nonlocal PDEs: Applications, Control, and Beyond", *ICCOPT 2019 – Sixth International Conference on Continuous Optimization*, Berlin, August 5–8.
23. N. Rotundo, co-organizer of the Minisymposium IM FT-2-3 2 "Modeling, Simulation and Optimization in Electrical Engineering", *9th International Congress on Industrial and Applied Mathematics (ICIAM 2019)*, Valencia, Spain, July 15–19.
24. V. Spokoiny, organizer, *New Frontiers in High-dimensional Probability and Statistics 2*, Higher School of Economics, Moscow, Russian Federation, February 22–23.
25. ———, co-organizer, *Structural Inference in High-Dimensional Models 2*, National Research University Higher School of Economics, HDILab, St. Petersburg, Russian Federation, August 26–30.
26. N. Tapia, co-organizer, *Algebraic and Analytic Perspectives in the Theory of Rough Paths and Signatures*, University of Oslo, Department of Mathematics, Norway, November 14–15.

A.6 Publications

A.6.1 Monographs

[1] J. Polzehl, K. Tabelow, *Magnetic Resonance Brain Imaging: Modeling and Data Analysis using R*, Series: Use R!, Springer International Publishing, Cham, 2019, 231 pages. https://www.wias-berlin.de/publications/books/Rbook/.

[2] U. Wilbrandt, *Stokes–Darcy Equations – Analytic and Numerical Analysis*, Lecture Notes in Mathematical Fluid Mechanics, Birkhäuser, Basel, 2019, 212 pages.

Monographs (to appear)

[1] B. Jahnel, W. König, *Probabilistic Methods in Telecommunications*, Compact Textbooks in Mathematics, Springer/Birkhäuser.

A.6.2 Editorship of Proceedings and Collected Editions

[1] P. Friz, W. König, Ch. Mukherjee, St. Olla, eds., *Probability and Analysis in Interacting Physical Systems. In Honor of S.R.S. Varadhan, Berlin, August, 2016*, vol. 283 of Springer Proceedings in Mathematics & Statistics, Springer International Publishing, Cham, 2019, 294 pages.

[2] M. Hintermüller, M. Hinze, J. Sokołowski, St. Ulbrich, eds., *Special issue to honour Guenter Leugering on his 65th birthday*, vol. 1 of Control & Cybernetics, Systems Research Institute, Polish Academy of Sciences, Warsaw, 2019.

[3] M. Hintermüller, J.F. Rodrigues, eds., *Topics in Applied Analysis and Optimisation – Partial Differential Equations, Stochastic and Numerical Analysis*, CIM Series in Mathematical Sciences, Springer Nature Switzerland AG, Cham, 2019, 396 pages.

[4] V.A. Garanzha, L. Kamenski, H. Si, eds., *Numerical Geometry, Grid Generation and Scientific Computing. Proceedings of the 9th International Conference, NUMGRID 2018 / Voronoi 150, Celebrating the 150th Anniversary of G.F. Voronoi, Moscow, Russia, December 2018*, vol. 131 of Lecture Notes in Computational Science and Engineering, Springer Nature Switzerland AG, Cham, 2019, 319 pages.

Proceedings and Collected Editions (to appear)

[1] A. Stephan, *On EDP-convergence for gradient systems with different time scales*, Proceedings in Applied Mathematics and Mechanics (PAMM), Wiley.

A.6.3 Outstanding Contributions to Collected Editions

[1] M. Hintermüller, K. Papafitsoros, *Chapter 11: Generating Structured Nonsmooth Priors and Associated Primal-dual Methods, in: Processing, Analyzing and Learning of Images, Shapes, and Forms: Part 2*, R. Kimmel, X.-Ch. Tai, eds., vol. 20 of Handbook of Numerical Analysis, Elsevier, 2019, pp. 437–502.

[2] H. Neidhardt, A. Stephan, V.A. Zagrebnov, *Chapter 13: Trotter Product Formula and Linear Evolution Equations on Hilbert Spaces, in: Analysis and Operator Theory*, Th.M. Rassias, V.A. Zagrebnov, eds., vol. 146 of Springer Optimization and Its Applications, Springer, Cham, 2019, pp. 271–299.

A.6.4 Articles in Refereed Journals[3]

[1] P. Colli, G. Gilardi, J. Sprekels, *Deep quench approximation and optimal control of general Cahn–Hilliard systems with fractional operators and double obstacle potentials*, Discrete Contin. Dyn. Syst. Ser. S, published online on 21.12.2019, https://doi.org/10.3934/dcdss.2020213.

[2] ———, *A distributed control problem for a fractional tumor growth model*, Mathematics, 7 (2019), pp. 792/1–792/32. Open Access: https://www.mdpi.com/2227-7390/7/9/792.

[3] ———, *Optimal velocity control of a convective Cahn–Hilliard system with double obstacles and dynamic boundary conditions: A 'deep quench' approach*, J. Convex Anal., 26 (2019), pp. 485–514.

[4] ———, *Recent results on well-posedness and optimal control for a class of generalized fractional Cahn–Hilliard systems*, Control Cybernet., 48 (2019), pp. 153–197.

[5] ———, *Well-posedness and regularity for a fractional tumor growth model*, Adv. Math. Sci. Appl., 28 (2019), pp. 343–375.

[6] ———, *Well-posedness and regularity for a generalized fractional Cahn–Hilliard system*, Rend. Lincei Mat. Appl., 30 (2019), pp. 437–478.

[7] P. Colli, A. Signori, J. Sprekels, *Optimal control of a phase field system modelling tumor growth with chemotaxis and singular potentials*, Appl. Math. Optim., published online on 21.10.2019, https://doi.org/10.1007/s00245-019-09618-6.

[8] S.P. Frigeri, C.G. Gal, M. Grasselli, J. Sprekels, *Strong solutions to nonlocal 2D Cahn–Hilliard–Navier–Stokes systems with nonconstant viscosity, degenerate mobility and singular potential*, Nonlinearity, 32 (2019), pp. 678–727.

[9] G. Gilardi, J. Sprekels, *Asymptotic limits and optimal control for the Cahn–Hilliard system with convection and dynamic boundary conditions*, Nonlinear Analysis, 178 (2019), pp. 1–31.

[10] K.R. Schneider, *The point charge oscillator: Qualitative and analytical investigations*, Math. Model. Anal., 24 (2019), pp. 372–384. Open Access: https://journals.vgtu.lt/index.php/MMA/article/view/5387.

[11] J. Sprekels, H. Wu, *Optimal distributed control of a Cahn–Hilliard–Darcy system with mass sources*, Appl. Math. Optim., published online on 24.01.2019, https://doi.org/10.1007/s00245-019-09555-4.

[12] N. Alia, M. Pylvänäinen, V.-V. Visuri, V. John, S. Ollila, *Vibrations of a laboratory-scale gas-stirred ladle with two eccentric nozzles and multiple sensors*, J. Iron Steel Res. Int., 26 (2019), pp. 1031–1040. Open Access: https://doi.org/10.1007/s42243-019-00241-x.

[13] A. Alphonse, M. Hintermüller, C.N. Rautenberg, *Directional differentiability for elliptic quasi-variational inequalities of obstacle type*, Calc. Var. Partial Differ. Equ., 58 (2019), pp. 39/1–39/47.

[14] S. Amiranashvili, E. Tobisch, *Extended criterion for the modulation instability*, New J. Phys., 21 (2019), pp. 033029/1–033029/7. Open Access: https://iopscience.iop.org/article/10.1088/1367-2630/ab0130.

[15] S. Amiranashvili, M. Radziunas, U. Bandelow, R. Čiegis, *Numerical methods for accurate description of ultrashort pulses in optical fibers*, Commun. Nonlinear Sci. Numer. Simul., 67 (2019), pp. 391–402.

[16] L. Andreis, A. Asselah, P. Dai Pra, *Ergodicity of a system of interacting random walks with asymmetric interaction*, Ann. Inst. H. Poincare Probab. Statist., 55 (2019), pp. 590–606.

[17] C. Bartsch, V. John, R.I.A. Patterson, *Simulations of an ASA flow crystallizer with a coupled stochastic-deterministic approach*, Comput. Chem. Engng., 124 (2019), pp. 350–363.

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

[18] Ch. Bayer, J. Häppölä, R. Tempone, *Implied stopping rules for American basket options from Markovian projection*, Quant. Finance, 19 (2019), pp. 371–390.

[19] Ch. Bayer, P. Friz, P. Gassiat, J. Martin, B. Stemper, *A regularity structure for rough volatility*, Math. Finance, published online on 19.11.2019. Open Access: https://onlinelibrary.wiley.com/doi/full/10.1111/mafi.12233?af=R.

[20] Ch. Bayer, P. Friz, A. Gulisashvili, B. Horvath, B. Stemper, *Short-time near-the-money skew in rough fractional volatility models*, Quant. Finance, 19 (2019), pp. 779–798. Open Access: https://www.tandfonline.com/doi/full/10.1080/14697688.2018.1529420.

[21] C. Brée, V. Raab, J. Montiel-Ponsoda, G. Garre-Werner, K. Staliunas, U. Bandelow, M. Radziunas, *Beam-combining scheme of high-power broad-area semiconductor lasers with Lyot-filtered reinjection: Modeling, simulations, and experiments*, J. Opt. Soc. Amer. B Opt. Phys., 36 (2019), pp. 1721–1730.

[22] O. Butkovsky, L. Mytnik, *Regularization by noise and flows of solutions for a stochastic heat equation*, Ann. Probab., 47 (2019), pp. 165–212.

[23] L.O. Müller, A. Caiazzo, P.J. Blanco, *Reduced-order unscented Kalman filter with observations in the frequency domain: Application to computational hemodynamics*, IEEE Trans. Biomed. Eng., 66 (2019), pp. 1269–1276.

[24] L. Heltai, A. Caiazzo, *Multiscale modeling of vascularized tissues via non-matching immersed methods*, Internat. J. Numer. Methods Biomedical Engrg., 35 (2019), pp. 3264/1–3264/32.

[25] H. Bessaih, M. Coghi, F. Flandoli, *Mean field limit of interacting filaments for 3D Euler equations*, J. Statist. Phys., 174 (2019), pp. 562–578.

[26] M. Coghi, B. Gess, *Stochastic nonlinear Fokker–Planck equations*, Nonlinear Analysis, 187 (2019), pp. 259–278.

[27] K. Disser, J. Rehberg, *The 3D transient semiconductor equations with gradient-dependent and interfacial recombination*, Math. Models Methods Appl. Sci., 29 (2019), pp. 1819–1851.

[28] D.H. Doan, A. Glitzky, M. Liero, *Analysis of a drift-diffusion model for organic semiconductor devices*, Z. Angew. Math. Phys., 70 (2019), pp. 55/1–55/18.

[29] W. Dreyer, C. Guhlke, R. Müller, *The impact of solvation and dissociation on the transport parameters of liquid electrolytes: Continuum modeling and numerical study*, Eur. Phys. J. Special Topics, 227 (2019), pp. 2515–2538.

[30] D.R. Baimurzina, A. Gasnikov, E.V. Gasnikova, P. Dvurechensky, E.I. Ershov, M.B. Kubentaeva, A.A. Lagunovskaya, *Universal method of searching for equilibria and stochastic equilibria in transportation networks*, Comput. Math. Math. Phys., 59 (2019), pp. 19–33.

[31] A. Gasnikov, P. Dvurechensky, F. Stonyakin, A.A. Titov, *An adaptive proximal method for variational inequalities*, Comput. Math. Math. Phys., 59 (2019), pp. 836–841.

[32] S. Guminov, Y. Nesterov, P. Dvurechensky, A. Gasnikov, *Accelerated primal-dual gradient descent with linesearch for convex, nonconvex, and nonsmooth optimization problems*, Dokl. Math., 99 (2019), pp. 125–128.

[33] E.A. Vorontsova, A. Gasnikov, E.A. Gorbunov, P. Dvurechensky, *Accelerated gradient-free optimization methods with a non-Euclidean proximal operator*, Autom. Remote Control, 80 (2019), pp. 1487–1501.

[34] M. Eigel, R. Schneider, P. Trunschke, S. Wolf, *Variational Monte Carlo—Bridging concepts of machine learning and high dimensional partial differential equations*, Adv. Comput. Math., 45 (2019), pp. 2503–2532.

[35] I. Papaioannou, M. Daub, M. Drieschner, F. Duddeck, M. Ehre, L. Eichner, M. Eigel, M. Götz, W. Graf, L. Grasedyck, R. Gruhlke, D. Hömberg, M. Kaliske, D. Moser, Y. Petryna, D. Straub, *Assessment and*

design of an engineering structure with polymorphic uncertainty quantification, GAMM-Mitt., 42 (2019), pp. e201900009/1–e201900009/22.

[36] S. Eydam, M. Wolfrum, *The link between coherence echoes and mode locking*, Chaos, 29 (2019), pp. 103114/1–103114/10.

[37] S. Eydam, I. Franović, M. Wolfrum, *Leap-frog patterns in systems of two coupled FitzHugh–Nagumo units*, Phys. Rev. E, 99 (2019), pp. 042207/1–042207/9.

[38] P. Farrell, D. Peschka, *Nonlinear diffusion, boundary layers and nonsmoothness: Analysis of challenges in drift-diffusion semiconductor simulations*, Comput. Math. Appl., 78 (2019), pp. 3731–3747.

[39] P. Dondl, Th. Frenzel, A. Mielke, *A gradient system with a wiggly energy and relaxed EDP-convergence*, ESAIM Control Optim. Calc. Var., 25 (2019), pp. 68/1–68/45.

[40] C. Améndola, P. Friz, B. Sturmfels, *Varieties of signature tensors*, Forum Math. Sigma, 7 (2019), pp. e10/1–e10/54. Open Access: https://doi.org/10.1017/fms.2019.3.

[41] Y. Bruned, I. Chevyrev, P. Friz, R. Preiss, *A rough path perspective on renormalization*, J. Funct. Anal., 277 (2019), pp. 108283/1–108283/60. Open Access: https://doi.org/10.1016/j.jfa.2019.108283.

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[43] J. Fuhrmann, C. Guhlke, Ch. Merdon, A. Linke, R. Müller, *Induced charge electroosmotic flow with finite ion size and solvation effects*, Electrochim. Acta, 317 (2019), pp. 778–785.

[44] A. Glitzky, M. Liero, *Instationary drift-diffusion problems with Gauss–Fermi statistics and field-dependent mobility for organic semiconductor devices*, Comm. Math. Sci., 17 (2019), pp. 33–59.

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[48] F. Flegel, M. Heida, *The fractional p-Laplacian emerging from homogenization of the random conductance model with degenerate ergodic weights and unbounded-range jumps*, Calc. Var. Partial Differ. Equ., 59 (2020), pp. 8/1–8/39 (published online on 28.11.2019).

[49] H. Heitsch, *On probabilistic capacity maximization in a stationary gas network*, Optimization, 69 (2020), pp. 575–604 (published online on 10.06.2019).

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[51] S. Hajian, M. Hintermüller, C. Schillings, N. Strogies, *A Bayesian approach to parameter identification in gas networks*, Control Cybernet., 48 (2019), pp. 377–402.

[52] M. Hintermüller, N. Strogies, *Identification of the friction function in a semilinear system for gas transport through a network*, Optim. Methods Softw., 35 (2020), pp. 576–617 (published online on 10.12.2019).

[53] G. Dong, M. Hintermüller, K. Papafitsoros, *Quantitative magnetic resonance imaging: From fingerprinting to integrated physics-based models*, SIAM J. Imaging Sci., 2 (2019), pp. 927–971.

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A.7 Preprints, Reports

A.7.1 WIAS Preprints Series[4]

[1] P. Colli, G. Gilardi, J. Sprekels, *Asymptotic analysis of a tumor growth model with fractional operators*, Preprint no. 2625, WIAS, Berlin, 2019.

[2] ———, *A distributed control problem for a fractional tumor growth model*, Preprint no. 2616, WIAS, Berlin, 2019.

[3] ———, *Longtime behavior for a generalized Cahn–Hilliard system with fractional operators*, Preprint no. 2588, WIAS, Berlin, 2019.

[4] ———, *Well-posedness and regularity for a fractional tumor growth model*, Preprint no. 2613, WIAS, Berlin, 2019.

[5] P. Colli, A. Signori, J. Sprekels, *Optimal control of a phase field system modelling tumor growth with chemotaxis and singular potentials*, Preprint no. 2614, WIAS, Berlin, 2019.

[6] J. Elschner, G. Hu, *Inverse elastic scattering from rigid scatterers with a single incoming wave*, Preprint no. 2571, WIAS, Berlin, 2019.

[7] K.R. Schneider, A. Grin, *Global bifurcation analysis of limit cycles for a generalized van der Pol system*, Preprint no. 2639, WIAS, Berlin, 2019.

[8] ———, *Lower and upper bounds for the number of limit cycles on a cylinder*, Preprint no. 2638, WIAS, Berlin, 2019.

[9] A. Alphonse, M. Hintermüller, C.N. Rautenberg, *Existence, iteration procedures and directional differentiability for parabolic QVIs*, Preprint no. 2592, WIAS, Berlin, 2019.

[10] A. Alphonse, M. Hintermüller, C.N. Rautenberg, *Stability of the solution set of quasi-variational inequalities and optimal control*, Preprint no. 2582, WIAS, Berlin, 2019.

[11] L. Andreis, W. König, R.I.A. Patterson, *A large-deviations approach to gelation*, Preprint no. 2568, WIAS, Berlin, 2019.

[12] M.J. Arenas Jaén, D. Hömberg, R. Lasarzik, P. Mikkonen, Th. Petzold, *Modelling and simulation of flame cutting for steel plates with solid phases and melting*, Preprint no. 2670, WIAS, Berlin, 2019.

[13] U. Bandelow, S. Amiranashvili, S. Pickartz, *Stabilization of optical pulse transmission by exploiting fiber nonlinearities*, Preprint no. 2661, WIAS, Berlin, 2019.

[14] Ch. Bayer, Ch.B. Hammouda, R.F. Tempone, *Hierarchical adaptive sparse grids and quasi Monte Carlo for option pricing under the rough Bergomi model*, Preprint no. 2652, WIAS, Berlin, 2019.

[15] Ch. Bayer, R.F. Tempone, S. Wolfers, *Pricing American options by exercise rate optimization*, Preprint no. 2651, WIAS, Berlin, 2019.

[16] L. Blank, E. Meneses Rioseco, U. Wilbrandt, A. Caiazzo, *Modeling, simulation, and optimization of geothermal energy production from hot sedimentary aquifers*, Preprint no. 2656, WIAS, Berlin, 2019.

[17] C. Brée, V. Raab, J. Montiel-Ponsoda, G. Garre-Werner, K. Staliunas, U. Bandelow, M. Radziunas, *Beam combining scheme for high-power broad-area semiconductor lasers with Lyot-filtered reinjection: Modeling, simulations, and experiments*, Preprint no. 2586, WIAS, Berlin, 2019.

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

[18] C.K. Macnamara, A. Caiazzo, I. Ramis-Conde, M.A.J. Chaplain, *Computational modelling and simulation of cancer growth and migration within a 3D heterogeneous tissue: The effects of fibre and vascular structure*, Preprint no. 2597, WIAS, Berlin, 2019.

[19] A. Caiazzo, R. Maier, D. Peterseim, *Reconstruction of quasi-local numerical effective models from low-resolution measurements*, Preprint no. 2577, WIAS, Berlin, 2019.

[20] D. Janke, A. Caiazzo, N. Ahmed, N. Alia, O. Knoth, B. Moreau, U. Wilbrandt, D. Willink, Th. Amon, V. John, *On the feasibility of using open source solvers for the simulation of a turbulent air flow in a dairy barn*, Preprint no. 2644, WIAS, Berlin, 2019.

[21] M. Coghi, T. Nilssen, *Rough nonlocal diffusions*, Preprint no. 2619, WIAS, Berlin, 2019.

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[23] D.H. Doan, A. Fischer, J. Fuhrmann, A. Glitzky, M. Liero, *Drift-diffusion simulation of S-shaped current-voltage relations for organic semiconductor devices*, Preprint no. 2630, WIAS, Berlin, 2019.

[24] P.-É. Druet, *Global-in-time existence for liquid mixtures subject to a generalised incompressibility constraint*, Preprint no. 2622, WIAS, Berlin, 2019.

[25] P.-É. Druet, A. Jüngel, *Analysis of cross-diffusion systems for fluid mixtures driven by a pressure gradient*, Preprint no. 2646, WIAS, Berlin, 2019.

[26] D. Bothe, P.-É. Druet, *Mass transport in multicomponent compressible fluids: Local and global well-posedness in classes of strong solutions for general class-one models*, Preprint no. 2658, WIAS, Berlin, 2019.

[27] A. Kroshnin, D. Dvinskikh, P. Dvurechensky, A. Gasnikov, N. Tupitsa, C.A. Uribe, *On the complexity of approximating Wasserstein barycenter*, Preprint no. 2665, WIAS, Berlin, 2019.

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[29] M. Ebeling-Rump, D. Hömberg, R. Lasarzik, Th. Petzold, *Topology optimization subject to additive manufacturing constraints*, Preprint no. 2629, WIAS, Berlin, 2019.

[30] M. Eigel, L. Grasedyck, R. Gruhlke, D. Moser, *Low rank surrogates for polymorphic fields with application to fuzzy-stochastic partial differential equations*, Preprint no. 2580, WIAS, Berlin, 2019.

[31] M. Drieschner, M. Eigel, R. Gruhlke, D. Hömberg, Y. Petryna, *Comparison of monomorphic and polymorphic approaches for uncertainty quantification with experimental investigations*, Preprint no. 2579, WIAS, Berlin, 2019.

[32] M. Eigel, R. Gruhlke, M. Marschall, *Low-rank tensor reconstruction of concentrated densities with application to Bayesian inversion*, Preprint no. 2672, WIAS, Berlin, 2019.

[33] S. Eydam, M. Wolfrum, *The link between coherence echoes and mode locking*, Preprint no. 2596, WIAS, Berlin, 2019.

[34] M. Lübbering, J. Kunkel, P. Farrell, *What company does my news article refer to? Tackling multiclass problems with topic modeling*, Preprint no. 2621, WIAS, Berlin, 2019.

[35] M.H. Farshbaf Shaker, M. Gugat, H. Heitsch, R. Henrion, *Optimal Neumann boundary control of a vibrating string with uncertain initial data and probabilistic terminal constraints*, Preprint no. 2626, WIAS, Berlin, 2019.

[36] Th. Frenzel, M. Liero, *Effective diffusion in thin structures via generalized gradient systems and EDP-convergence*, Preprint no. 2601, WIAS, Berlin, 2019.

[37] C. Cancès, C. Chainais-Hillairet, J. Fuhrmann, B. Gaudeul, *A numerical analysis focused comparison of several finite volume schemes for an unipolar degenerated drift-diffusion model*, Preprint no. 2620, WIAS, Berlin, 2019.

[38] J. Fuhrmann, D.H. Doan, A. Glitzky, M. Liero, G. Nika, *Unipolar drift-diffusion simulation of S-shaped current-voltage relations for organic semiconductor devices*, Preprint no. 2660, WIAS, Berlin, 2019.

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[41] ———, *An existence result for a class of electrothermal drift-diffusion models with Gauss–Fermi statistics for organic semiconductors*, Preprint no. 2593, WIAS, Berlin, 2019.

[42] B. Franchi, M. Heida, S. Lorenzani, *A mathematical model for Alzheimer's disease: An approach via stochastic homogenization of the Smoluchowski equation*, Preprint no. 2595, WIAS, Berlin, 2019.

[43] M. Heida, St. Neukamm, M. Varga, *Stochastic homogenization of Lambda-convex gradient flows*, Preprint no. 2594, WIAS, Berlin, 2019.

[44] O. Souček, M. Heida, J. Málek, *On a thermodynamic framework for developing boundary conditions for Korteweg fluids*, Preprint no. 2599, WIAS, Berlin, 2019.

[45] M.J. Cánovas, M.J. Gisbert, R. Henrion, J. Parra, *Lipschitz lower semicontinuity moduli for linear inequality systems*, Preprint no. 2631, WIAS, Berlin, 2019.

[46] W. van Ackooij, R. Henrion, P. Pérez-Aros, *Generalized gradients for probabilistic/robust (probust) constraints*, Preprint no. 2569, WIAS, Berlin, 2019.

[47] A. Hinsen, B. Jahnel, E. Cali, J.-P. Wary, *Phase transitions for chase-escape models on Gilbert graphs*, Preprint no. 2642, WIAS, Berlin, 2019.

[48] G. Dong, M. Hintermüller, Y. Zhang, *A class of second-order geometric quasilinear hyperbolic PDEs and their application in imaging science*, Preprint no. 2591, WIAS, Berlin, 2019.

[49] M. Hintermüller, T. Keil, *Optimal control of geometric partial differential equations*, Preprint no. 2612, WIAS, Berlin, 2019.

[50] C. Grässle, M. Hintermüller, M. Hinze, T. Keil, *Simulation and control of a nonsmooth Cahn–Hilliard Navier–Stokes system with variable fluid densities*, Preprint no. 2617, WIAS, Berlin, 2019.

[51] M. Hintermüller, K. Papafitsoros, *Generating structured non-smooth priors and associated primal-dual methods*, Preprint no. 2611, WIAS, Berlin, 2019.

[52] M. Hintermüller, K. Papafitsoros, C.N. Rautenberg, *Variable step mollifiers and applications*, Preprint no. 2628, WIAS, Berlin, 2019.

[53] D. Gahururu, M. Hintermüller, St.-M. Stengl, Th.M. Surowiec, *Generalized Nash equilibrium problems with partial differential operators: Theory, algorithms, and risk aversion*, Preprint no. 2654, WIAS, Berlin, 2019.

[54] J.I. Asperheim, P. Das, B. Grande, D. Hömberg, Th. Petzold, *Numerical simulation of high-frequency induction welding in longitudinal welded tubes*, Preprint no. 2600, WIAS, Berlin, 2019.

[55] F. Auricchio, E. Bonetti, M. Carraturo, D. Hömberg, A. Reali, E. Rocca, *Structural multiscale topology optimization with stress constraint for additive manufacturing*, Preprint no. 2615, WIAS, Berlin, 2019.

[56] D. Hömberg, R. Lasarzik, *Weak entropy solutions to a model in induction hardening, existence and weak-strong uniqueness*, Preprint no. 2671, WIAS, Berlin, 2019.

[57] Ch. Hirsch, B. Jahnel, A. Tóbiás, *Lower large deviations for geometric functionals*, Preprint no. 2632, WIAS, Berlin, 2019.

[58] B. Jahnel, A. Tóbiás, *SINR percolation for Cox point processes with random powers*, Preprint no. 2659, WIAS, Berlin, 2019.

[59] A. Tóbiás, B. Jahnel, *Exponential moments for planar tessellations*, Preprint no. 2572, WIAS, Berlin, 2019.

[60] V. John, P. Knobloch, U. Wilbrandt, *Finite element pressure stabilizations for incompressible flow problems*, Preprint no. 2587, WIAS, Berlin, 2019.

[61] M. Kantner, *Generalized Scharfetter–Gummel schemes for electro-thermal transport in degenerate semiconductors using the Kelvin formula for the Seebeck coefficient*, Preprint no. 2605, WIAS, Berlin, 2019.

[62] M. Kantner, Th. Koprucki, *Non-isothermal Scharfetter–Gummel scheme for electro-thermal transport simulation in degenerate semiconductors*, Preprint no. 2664, WIAS, Berlin, 2019.

[63] M. Kantner, Th. Höhne, Th. Koprucki, S. Burger, H.-J. Wünsche, F. Schmidt, A. Mielke, U. Bandelow, *Multi-dimensional modeling and simulation of semiconductor nanophotonic devices*, Preprint no. 2653, WIAS, Berlin, 2019.

[64] M. Kantner, A. Mielke, M. Mittnenzweig, N. Rotundo, *Mathematical modeling of semiconductors: From quantum mechanics to devices*, Preprint no. 2575, WIAS, Berlin, 2019.

[65] S. Jansen, W. König, B. Schmidt, F. Theil, *Surface energy and boundary layers for a chain of atoms at low temperature*, Preprint no. 2589, WIAS, Berlin, 2019.

[66] H. Abels, J. Daube, Ch. Kraus, D. Kröner, *The sharp-interface limit for the Navier–Stokes–Korteweg equations*, Preprint no. 2663, WIAS, Berlin, 2019.

[67] H. Abels, J. Daube, Ch. Kraus, *Pressure reconstruction for weak solutions of the two-phase incompressible Navier–Stokes equations with surface tension*, Preprint no. 2662, WIAS, Berlin, 2019.

[68] R. Lasarzik, *Maximal dissipative solutions for incompressible fluid dynamics*, Preprint no. 2666, WIAS, Berlin, 2019.

[69] R. Lasarzik, E. Rocca, G. Schimperna, *Weak solutions and weak-strong uniqueness for a thermodynamically consistent phase-field model*, Preprint no. 2608, WIAS, Berlin, 2019.

[70] E. Emmrich, R. Lasarzik, *Existence of weak solutions to a dynamic model for smectic-A liquid crystals under undulations*, Preprint no. 2567, WIAS, Berlin, 2019.

[71] M. Akbas, Th. Gallouët, A. Gassmann, A. Linke, Ch. Merdon, *A gradient-robust well-balanced scheme for the compressible isothermal Stokes problem*, Preprint no. 2641, WIAS, Berlin, 2019.

[72] A.M. ter Elst, A. Linke, J. Rehberg, *On the numerical range of sectorial forms*, Preprint no. 2667, WIAS, Berlin, 2019.

[73] K.M. Gambaryan, T. Boeck, A. Trampert, O. Marquardt, *Nucleation chronology and electronic properties of In(As,Sb,P) graded composition quantum dots grown on InAs(100) substrate*, Preprint no. 2623, WIAS, Berlin, 2019.

[74] A. Mielke, A. Montefusco, M.A. Peletier, *Exploring families of energy-dissipation landscapes via tilting – Three types of EDP convergence*, Preprint no. 2668, WIAS, Berlin, 2019.

[75] A. Mielke, T. Roubíček, *Thermoviscoelasticity in Kelvin–Voigt rheology at large strains*, Preprint no. 2584, WIAS, Berlin, 2019.

[76] A. Mielke, A. Stephan, *Coarse-graining via EDP-convergence for linear fast-slow reaction systems*, Preprint no. 2643, WIAS, Berlin, 2019.

[77] G. Nika, B. Vernescu, *Multiscale modeling of magnetorheological suspensions*, Preprint no. 2598, WIAS, Berlin, 2019.

[78] F. Agnelli, A. Constantinescu, G. Nika, *Design and testing of 3D-printed micro-architectured polymer materials exhibiting a negative Poisson's ratio*, Preprint no. 2624, WIAS, Berlin, 2019.

[79] D. Heydecker, R.I.A. Patterson, *Bilinear coagulation equations*, Preprint no. 2637, WIAS, Berlin, 2019.

[80] S. Pickartz, *The role of the self-steepening effect in soliton compression due to cross-phase modulation by dispersive waves*, Preprint no. 2585, WIAS, Berlin, 2019.

[81] A. Pimenov, S. Amiranashvili, A.G. Vladimirov, *Temporal cavity solitons in a delayed model of a dispersive cavity ring laser*, Preprint no. 2581, WIAS, Berlin, 2019.

[82] Ch. Schelte, A. Pimenov, A.G. Vladimirov, J. Javaloyes, S.V. Gurevich, *Tunable Kerr frequency combs and temporal localized states in time-delayed Gires–Tournois interferometers*, Preprint no. 2650, WIAS, Berlin, 2019.

[83] J.-P. Koester, M. Radziunas, A. Zeghuzi, H. Wenzel, A. Knigge, *Simulation and design of a compact GaAs based tunable dual-wavelength diode laser system*, Preprint no. 2635, WIAS, Berlin, 2019.

[84] M. Radziunas, D.J. Little, D.M. Kane, *Numerical study of coherence of optical feedback in semiconductor laser dynamics*, Preprint no. 2604, WIAS, Berlin, 2019.

[85] A. Zeghuzi, M. Radziunas, H.-J. Wünsche, J.-P. Koester, H. Wenzel, U. Bandelow, A. Knigge, *Traveling wave analysis of non-thermal far-field blooming in high-power broad-area lasers*, Preprint no. 2633, WIAS, Berlin, 2019.

[86] A. Rathsfeld, *On a half-space radiation condition*, Preprint no. 2669, WIAS, Berlin, 2019.

[87] A.F.M. ter Elst, R. Haller-Dintelmann, J. Rehberg, P. Tolksdorf, *On the L^p -theory for second-order elliptic operators in divergence form with complex coefficients*, Preprint no. 2590, WIAS, Berlin, 2019.

[88] H. Meinlschmidt, Ch. Meyer, J. Rehberg, *Regularization for optimal control problems associated to nonlinear evolution equations*, Preprint no. 2576, WIAS, Berlin, 2019.

[89] A.F.M. ter Elst, H. Meinlschmidt, J. Rehberg, *Essential boundedness for solutions of the Neumann problem on general domains*, Preprint no. 2574, WIAS, Berlin, 2019.

[90] D.R.M. Renger, J. Zimmer, *Orthogonality of fluxes in general nonlinear reaction networks*, Preprint no. 2609, WIAS, Berlin, 2019.

[91] G. Alì, N. Rotundo, *Existence and uniqueness of solution for multidimensional parabolic PDAEs arising in semiconductor modeling*, Preprint no. 2607, WIAS, Berlin, 2019.

[92] D. Belomestny, M. Kaledin, J.G.M. Schoenmakers, *Semi-tractability of optimal stopping problems via a weighted stochastic mesh algorithm*, Preprint no. 2610, WIAS, Berlin, 2019.

[93] H. Si, *On decomposition of embedded prismatoids in R^3 without additional points*, Preprint no. 2602, WIAS, Berlin, 2019.

[94] A. Stephan, *Combinatorial considerations on the invariant measure of a stochastic matrix*, Preprint no. 2627, WIAS, Berlin, 2019.

[95] H. Stephan, *Millions of Perrin pseudoprimes including a few giants*, Preprint no. 2657, WIAS, Berlin, 2019.

[96] L. Taggi, *Uniformly positive correlations in the dimer model and phase transition in lattice permutations in $\mathbb{Z}^d, d > 2$, via reflection positivity*, Preprint no. 2647, WIAS, Berlin, 2019.

[97] N. Tapia, L. Zambotti, *The geometry of the space of branched rough paths*, Preprint no. 2645, WIAS, Berlin, 2019.

[98] J. Diehl, E.-F. Kurusch, N. Tapia, *Time-warping invariants of multidimensional time series*, Preprint no. 2603, WIAS, Berlin, 2019.

[99] R. Rossi, U. Stefanelli, M. Thomas, *Rate-independent evolution of sets*, Preprint no. 2578, WIAS, Berlin, 2019.

[100] P. Vágner, C. Guhlke, V. Miloš, R. Müller, J. Fuhrmann, *A continuum model for yttria-stabilised zirconia incorporating triple phase boundary, lattice structure and immobile oxide ions*, Preprint no. 2583, WIAS, Berlin, 2019.

[101] K. Chouk, W. van Zuijlen, *Asymptotics of the eigenvalues of the Anderson Hamiltonian with white noise potential in two dimensions*, Preprint no. 2606, WIAS, Berlin, 2019.

[102] A.G. Vladimirov, A.V. Kovalev, E.A. Viktorov, N. Rebrova, G. Huyet, *Dynamical regimes in a class A model of a nonlinear mirror mode-locked laser*, Preprint no. 2573, WIAS, Berlin, 2019.

[103] A. Münch, B. Wagner, *Self-consistent field theory for a polymer brush. Part I: Asymptotic analysis in the strong-stretching limit*, Preprint no. 2648, WIAS, Berlin, 2019.

[104] ———, *Self-consistent field theory for a polymer brush. Part II: The effective chemical potential*, Preprint no. 2649, WIAS, Berlin, 2019.

[105] S. Yanchuk, St. Ruschel, J. Sieber, M. Wolfrum, *Temporal dissipative solitons in time-delay feedback systems*, Preprint no. 2570, WIAS, Berlin, 2019.

[106] A. Zeghuzi, H.-J. Wünsche, H. Wenzel, M. Radziunas, J. Fuhrmann, A. Klehr, U. Bandelow, A. Knigge, *Time-dependent simulation of thermal lensing in high-power broad-area semiconductor lasers*, Preprint no. 2634, WIAS, Berlin, 2019.

A.7.2 Preprints/Reports in other Institutions

[1] V. Avanesov, *How to gamble with non-stationary x-armed bandits and have no regrets*, arXiv:1908.07636, Cornell University Library, arXiv.org, Ithaka, USA, 2019.

[2] ———, *Nonparametric change point detection in regression*, arXiv:1903.02603, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

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[21] D. Heydecker, R.I.A. Patterson, *Kac interaction clusters: A bilinear coagulation equation and phase transition*, arXiv:1902.07686, Cornell University Library, Ithaca, USA, 2019.

[22] M. Redmann, *An L^2_T-error bound for time-limited balanced truncation*, arXiv:1907.05478, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

[23] A. Kroshnin, V. Spokoiny, A. Suvorikova, *Statistical inference for Bures–Wasserstein barycenters*, arXiv:1901.00226, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

[24] V. Spokoiny, M. Panov, *Accuracy of Gaussian approximation in nonparametric Bernstein–von Mises theorem*, arXiv:1910.06028, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

[25] N. Puchkin, V. Spokoiny, *Structure-adaptive manifold estimation*, arXiv:1906.05014, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

[26] Y.-W. Sun, K. Papagiannouli, V. Spokoiny, *Online graph-based change-point detection for high dimensional data*, arXiv:1906.03001, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

[27] V. Betz, H. Schäfer, L. Taggi, *Interacting self-avoiding polygons*, arXiv:1902.08517, Cornell University Library, Ithaca, USA, 2019.

[28] E. Candellero, A. Stauffer, L. Taggi, *Abelian oil and water dynamics does not have an absorbing-state phase transition*, arXiv:1901.08425v1, Cornell University Library, Ithaca, USA, 2019.

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[30] J. Diehl, K. Ebrahimi-Fard, N. Tapia, *Time warping invariants of multidimensional time series*, arXiv:1906.05823, Cornell University Library, arXiv.org, Ithaca, USA, 2019.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Main and Plenary Talks

1. M. Eigel, *A statistical learning approach for parametric PDEs*, Workshop "Scientific Computation using Machine-Learning Algorithms", April 25–26, University of Nottingham, UK, April 26.
2. M. Hintermüller, *Generalized Nash games with PDEs and applications in energy markets*, French-German-Swiss Conference on Optimization (FGS'2019), September 17–20, Nice, France, September 20.
3. D. Hömberg, *From distortion compensation to 3D printing – A phase field approach to topology optimization*, The Hawassa Math & Stat Conference 2019, February 11–15, Hawassa University, Ethiopia, February 12.
4. V. John, *Finite elements for scalar convection-dominated equations and incompressible flow problems – A never ending story?*, Conference on Applied Mathematics, August 19–21, Lahore University of Management Sciences, Pakistan, August 19.
5. A. Mielke, *Gradient systems and evolutionary Gamma-convergence*, DMV-Jahrestagung 2019, September 23–26, KIT – Karlsruher Institut für Technologie, September 24.
6. M. Radziunas, *Efficient modeling and simulation of dynamics in high-power semiconductor lasers*, 24th International Conference on Mathematical Modelling and Analysis (MMA2019), May 28–31, Tallinn University of Technology, Estonia, May 31.
7. M. Wolfrum, *Temporal dissipative solitons in systems with time delay*, 11th Colloquium on the Qualitative Theory of Differential Equations, University of Szeged, Bolyai Institute, Hungary, June 20.

A.8.2 Scientific Talks (Invited)

1. J. Sprekels, *Optimal control of a Cahn–Hilliard–Darcy system with mass source modeling tumor growth*, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 14.
2. A. Alphonse, *Directional differentiability for elliptic quasi-variational inequalities*, Workshop "Surface, Bulk, and Geometric Partial Differential Equations: Interfacial, Stochastic, Non-local and Discrete Structures", January 20–26, Mathematisches Forschungsinstitut Oberwolfach, January 25.
3. ———, *Directional differentiability for elliptic quasi-variational inequalities*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Best Paper Session, August 5–8, Berlin, August 5.
4. S. Amiranashvili, *Controlling light by light*, Seminar for Theoretical Physics, Technische Universität Wien, Austria, January 23.
5. ———, *Controlling light by light*, Waves Côte d'Azur, June 4–7, Université Côte d'Azur, Nice, France, June 4.
6. L. Andreis, *A large-deviations approach to the multiplicative coagulation process*, Workshop "Woman in Probability", May 31 – June 1, Technische Universität München, Fakultät für Mathematik, May 31.
7. ———, *Coagulating particles and gelation phase transition: A large-deviation approach*, Second Italian Meeting on Probability and Mathematical Statistics, June 17–20, Vietri sul Mare, Italy, June 19.
8. ———, *Coagulation processes and gelation from a large deviation point of view*, BMS – BGSMath Junior Meeting 2019, June 26–28, Berlin Mathematical School (BMS), Barcelona Graduate School of Mathematics (BGSMath), Technische Universität Berlin, June 26.
9. ———, *Large-deviation approach to coagulation processes and gelation*, Workshop on Chemical Reaction Networks, July 1–3, Politecnico di Torino, Dipartimento di Scienze Matematiche "G. L. Lagrange", Italy, July 2.

10. ———, *Phase transitions in coagulation processes and random graphs*, Workshop “Welcome Home 2019”, December 19–20, Università di Torino, Dipartimento di Matematica “G. Peano”, Italy, December 19.

11. U. Bandelow, *Modeling and simulation of electrically driven quantum dot based single-photon sources*, Seminar NATEC II, Technical University of Denmark, Kgs. Lyngby, Denmark, June 7.

12. ———, *Ultrashort solitons and their interaction with dispersive waves in the regime of event horizons in nonlinear optical media*, 2nd International Conference on Photonics Research, November 4–9, Kocaeli University, Antalya, Turkey, November 8.

13. Ch. Bayer, *A regularity structure for rough volatility*, Vienna Seminar in Mathematical Finance and Probability, Technische Universität Wien, Research Unit of Financial and Actuarial Mathematics, Austria, January 10.

14. ———, *Pricing American options by exercise rate optimization*, Workshop on Financial Risks and Their Management, February 19–20, Ryukoku University, Wagenkan, Kyoto, Japan, February 19.

15. ———, *Numerics for rough volatility*, Stochastic Processes and Related Topics, February 21–22, Kansai University, Senriyama Campus, Osaka, Japan, February 22.

16. ———, *Deep calibration of rough volatility models*, SIAM Conference on Financial Mathematics & Engineering, June 4–7, Society for Industrial and Applied Mathematics, Toronto, Ontario, Canada, June 7.

17. ———, *Pricing American options by exercise rate optimization*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Session “Stochastic Optimization and Its Applications (Part III)”, August 5–8, Berlin, August 7.

18. ———, *Calibration of rough volatility models by deep learning*, 2 talks, Rough Workshop 2019, September 4–6, Technische Universität Wien, Financial and Actuarial Mathematics, Austria, September 5–6.

19. ———, *Learning rough volatility*, Algebraic and Analytic Perspectives in the Theory of Rough Paths and Signatures, November 14–15, University of Oslo, Department of Mathematics, Norway, November 14.

20. ———, *Pricing American options by exercise rate optimization*, Seminar, Imperial College London, Mathematical Finance Department, UK, December 16.

21. F. Besold, *Minimax clustering with adaptive weights*, New Frontiers in High-dimensional Probability and Statistics 2, February 20–23, Higher School of Economics, Moscow, Russian Federation, February 23.

22. ———, *Manifold clustering*, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, October 28.

23. ———, *Adaptive manifold clustering*, Rencontres de Statistiques Mathématiques, December 16–20, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, December 19.

24. O. Butkovsky, *Regularization by noise for SDEs and SPDEs with applications to numerical methods*, Seminar Wahrscheinlichkeitstheorie, Universität Mannheim, Probability & Statistics Group, October 16.

25. ———, *Regularization by noise for SDEs and related systems: A tale of two approaches*, Hausdorff Junior Trimester, Universität Bonn, Hausdorff Research Institute for Mathematics (HIM), November 26.

26. ———, *New coupling techniques for exponential ergodicity of SPDEs in hypoelliptic and effectively elliptic settings*, Oberseminar Stochastik, Universität Bonn, Hausdorff Research Center, Institut für Angewandte Mathematik (IAM), November 28.

27. ———, *Approximation of SDE*, LSA Winter Meeting 2019, December 2–6, Higher School of Economics, National Research University, Laboratory of Stochastic Analysis and its Applications, Moscow, Russian Federation, December 3.

28. ———, *Numerical methods for SDEs: A stochastic sewing approach*, 12th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 5–6, University of Oxford, Mathematical Institute, UK, December 6.

29. ———, *New coupling techniques for exponential ergodicity of stochastic delay equations and SPDEs*, Probability Seminar, Swansea University, Department of Mathematics, UK, December 9.

30. A. Caiazzo, *Multiscale hybrid modeling and simulation of cancer growth within a 3D heterogeneous tissue*, Canada-Germany Workshop Mathematical Biology and Numerics, June 24–26, Universität Heidelberg, June 26.

31. M. Coghi, *Pathwise McKean–Vlasov theory*, Oberseminar Partielle Differentialgleichungen, Universität Konstanz, Fachbereich Mathmatik und Statistik, February 6.

32. ———, *Stochastic nonlinear Fokker–Planck equations*, 11th Annual ERC Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis, May 23–25, WIAS Berlin, May 23.

33. ———, *Mean field limit of interacting filaments for 3D Euler equations*, Second Italian Meeting on Probability and Mathematical Statistics, June 17–20, Università degli Studi di Salerno, Dipartimento di Matematica, Vietri sul Mare, Italy, June 20.

34. ———, *Rough nonlocal diffusions*, Recent Trends in Stochastic Analysis and SPDEs, July 17–20, University of Pisa, Department of Mathematics, Italy, July 18.

35. P.-É. Druet, *Multicomponent diffusion in fluids: Some mathematical aspects*, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, April 3.

36. ———, *The low Mach number limit for complex fluids: Recent results on strong and weak solvability*, PDE 2019: Partial Differential Equations in Fluids and Solids, September 9–13, WIAS, Berlin, September 9.

37. D. Dvinskikh, *Introduction to decentralized optimization*, Summer School “Big Data”, July 15–18, Sirius Educational Centre, Sochi, Russian Federation, July 16.

38. ———, *Complexity rates for accelerated primal-dual gradient method for stochastic optimisation problem*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Session “Primal-Dual Methods for Structured Optimization”, August 5–8, Berlin, August 7.

39. P. Dvurechensky, *Distributed calculation of Wasserstein barycenters*, Huawei, Shanghai, China, June 6.

40. ———, *A unifying framework for accelerated randomized optimization methods*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Session “Large-Scale Stochastic First-Order Optimization (Part I)”, August 5–8, Berlin, August 6.

41. ———, *On the complexity of optimal transport problems*, Optimal Transportation Meeting, September 23–27, Higher School of Economics, Moscow, Russian Federation, September 26.

42. ———, *HDI Lab: Optimization methods for optimal transport*, 4 talks, HSE-Yandex Autumn School on Generative Models, November 26–29, Higher School of Economics, National Research University, Moscow, Russian Federation, November 26–27.

43. M. Ebeling-Rump, *Topology optimization subject to additive manufacturing constraints*, INdAM Workshop MACH2019 “Mathematical Modeling and Analysis of Degradation and Restoration in Cultural Heritage”, March 25–29, Istituto Nazionale di Alta Matematica “Francesco Severi”, Rome, Italy, March 26.

44. ———, *Topology optimization subject to additive manufacturing constraints*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Session “Infinite-Dimensional Optimization of Nonlinear Systems (Part III)”, August 5–8, Berlin, August 6.

45. M. Eigel, *A statistical learning approach for parametric PDEs*, École Polytechnique Fédérale de Lausanne (EPFL), Scientific Computing and Uncertainty Quantification, Lausanne, Switzerland, May 14.

46. ———, *Some thoughts on adaptive stochastic Galerkin FEM*, Sixteenth Conference on the Mathematics of Finite Elements and Applications (MAFELAP 2019), Minisymposium 17 “Finite Element Methods for Efficient Uncertainty Quantification”, June 18–21, Brunel University London, Uxbridge, UK, June 18.

47. ———, *A statistical learning approach for high-dimensional PDEs*, 3rd International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2019), Minisymposium 6–IV “Uncertainty Computations with Reduced Order Models and Low-Rank Representations”, June 24–26, Crete, Greece, June 25.

48. ———, *A machine learning approach for explicit Bayesian inversion*, Workshop 3 within the Special Semester on Optimization “Optimization and Inversion under Uncertainty”, November 11–15, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 12.

49. P. Farrell, *Solving PDEs numerically*, University of Exeter, Department of Mathematics, UK, April 11.

50. ———, *Modeling and simulation of charge carrier transport in semiconductors and electrolytes, Part II*, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, June 27.

51. ———, *Novel schemes for drift-diffusion semiconductor problems*, European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Minisymposium 15 “Novel Flux Approximation Schemes for Advection-Diffusion Problems (Part 2)”, September 30 – October 4, Eindhoven University of Technology, Netherlands, October 2.

52. ———, *Creating anisotropic meshes by combining RBFs and HDE*, International Conference of Kernel-based Methods and it’s Application, October 10–14, Xi’an Jiaotong-Liverpool University, Suzhou, China, October 13.

53. ———, *Konjugierte Gradienten*, Technische Universität Bergakademie Freiberg, Fakultät Mathematik und Informatik, November 27.

54. ———, *Simulating semiconductor devices in a physically correct and stable way*, Technische Universität Bergakademie Freiberg, Fakultät Mathematik und Informatik, November 27.

55. P. Friz, *Multiscale systems, homogenization and rough paths*, CRC 1114 Colloquium & Lectures, Collaborative Research Center CRC 1114 “Scaling Cascades in Complex Systems”, Freie Universität Berlin, June 13.

56. ———, *Rough semimartingales*, Paths between Probability, PDEs, and Physics: Conference 2019, July 1–5, Imperial College London, July 2.

57. ———, *Rough paths, rough volatility and regularity structures*, 2 talks, Mini-course consisting of two sessions, Mathematics and CS Seminar, Institute of Science and Technology Austria, Klosterneuburg, Austria, July 4–5.

58. ———, *Rough paths, rough volatility, regularity structures*, 2 talks, Rough Workshop 2019, September 4–6, Technische Universität Wien, Financial and Actuarial Mathematics, Austria, September 4–5.

59. ———, *Rough transport, revisited*, Algebraic and Analytic Perspectives in the Theory of Rough Paths and Signatures, November 14–15, University of Oslo, Department of Mathematics, Norway, November 14.

60. ———, *Some perspectives on harmonic analysis and rough paths*, Harmonic Analysis and Rough Paths, November 18–19, Hausdorff Research Institute for Mathematics, Bonn, November 18.

61. J. Fuhrmann, *Modeling and simulation of charge carrier transport in semiconductors and electrolytes, Part I*, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, June 27.

62. ———, *Modified exponential fitting schemes for degenerate semiconductors and electrolytes*, European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Minisymposium 15 “Novel Flux Approximation Schemes for Advection-Diffusion Problems (Part 2)”, September 30 – October 4, Eindhoven University of Technology, Netherlands, October 2.

63. R. Gruhlke, *Bayesian upscaling with application to failure analysis of adhesive bonds in rotor blades*, 3rd International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2019), Minisymposium 6–II "Uncertainty Computations with Reduced Order Models and Low-Rank Representations", June 24–26, Crete, Greece, June 24.

64. M. Heida, *The SQRA operator: Convergence behaviour and applications*, Politechnico di Milano, Dipartimento di Matematica, Italy, March 13.

65. M. Heida, *The SQRA operator: Convergence behaviour and applications*, Universität Wien, Fakultät für Mathematik, Lehrstuhl Analysis, Austria, March 19.

66. H. Heitsch, *On probabilistic capacity maximization in a stationary gas network*, 9th International Congress on Industrial and Applied Mathematics (ICIAM), Minisymposium MS A6-1-1 4 "Mathematical Optimization and Gas Transport Networks: Academic Developments II", July 15–19, Valencia, Spain, July 16.

67. ———, *Optimal Neumann boundary control of the vibrating string with uncertain initial data and probabilistic terminal constraints*, The XV International Conference on Stochastic Programming (ICSP XV), Minisymposium "Nonlinear Programming with Probability Functions", July 29 – August 2, Norwegian University of Science and Technology, Trondheim, Norway, July 30.

68. R. Henrion, *Robust control of a sweeping process with probabilistic end-point constraints*, Workshop "Nonsmooth and Variational Analysis", January 28 – February 1, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, January 31.

69. ———, *Problèmes d'optimisation sous contraintes en probabilité*, 4 talks, Spring School in Nonsmooth Analysis and Optimization, April 16–18, Université Mohammed V, Rabat, Morocco, April 16–18.

70. ———, *Chance constraints then and now*, International Conference on Stochastic Optimization and Related Topics, April 25–26, Mühlheim an der Ruhr, April 26.

71. ———, *On some extended models of chance constraints*, Workshop "Mathematical Optimization of Systems Impacted by Rare, High-Impact Random Events", June 24–28, Institute for Computational and Experimental Research in Mathematics (ICERM), Providence, USA, June 24.

72. ———, *Robust control of a sweeping process with probabilistic end-point constraints*, The XV International Conference on Stochastic Programming (ICSP XV), Minisymposium "Nonlinear Programming with Probability Functions", July 29 – August 2, Norwegian University of Science and Technology, Trondheim, Norway, July 30.

73. ———, *Optimal Neumann boundary control of the vibrating string with uncertain initial data*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Session "PDE-constrained Optimization under Uncertainty (Part I)", August 5–8, Berlin, August 8.

74. ———, *Optimal Neumann boundary control of the vibrating string under random initial conditions*, OVA9: 9th International Seminar on Optimization and Variational Analysis, Universidad Miguel Hernández, Elche, Spain, September 2.

75. ———, *Optimization problems with probust constraints: Theory, applications and algorithmic solution*, XXXVIII Spanish Conference on Statistics and Operations Research, September 3–6, Universitat Politècnica de València, Alcoi, Spain, September 5.

76. ———, *On derivatives of probability functions*, Workshop "Statistics, Risk & Optimization", Universität Wien, Austria, September 27.

77. ———, *Probabilistic constraints in optimization with PDEs*, Workshop 3 within the Special Semester on Optimization "Optimization and Inversion under Uncertainty", November 11–15, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 13.

78. ———, *Nonsmoothness in the context of probability functions*, Workshop 4 within the Special Semester on Optimization "Nonsmooth Optimization", November 25–27, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 25.

79. ———, *Optimal probabilistic control of the vibrating string under random initial conditions*, PGMO DAYS 2018, Session 1E "Stochastic Optimal Control", December 3–4, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF'Lab Paris-Saclay, Palaiseau, France, December 4.

80. A. Hinsen, *Introduction to interacting particles systems (IPS)*, Workshop on Probability, Analysis and Applications (PAA), September 23 – October 4, African Institute for Mathematical Sciences — Ghana (AIMS Ghana), Accra, October 2.

81. ———, *IPS in telecommunication I*, Workshop on Probability, Analysis and Applications (PAA), September 23 – October 4, African Institute for Mathematical Sciences — Ghana (AIMS Ghana), Accra, October 4.

82. ———, *IPS in telecommunication II*, Workshop on Probability, Analysis and Applications (PAA), September 23 – October 4, African Institute for Mathematical Sciences — Ghana (AIMS Ghana), Accra, October 4.

83. M. Hintermüller, *Applications in image processing*, Workshop on Efficient Operator Splitting Techniques for Complex System and Large Scale Data Analysis, January 15–18, Sanya, China, January 14.

84. ———, *A function space framework for structural total variation regularization with applications in inverse problems*, Thematic Programme "Modern Maximal Monotone Operator Theory: From Nonsmooth Optimization to Differential Inclusions", Workshop "Nonsmooth and Variational Analysis", January 28 – February 1, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, February 1.

85. ———, *Lecture Series: Optimal control of nonsmooth structures*, 4 talks, Thematic Programme "Modern Maximal Monotone Operator Theory: From Nonsmooth Optimization to Differential Inclusions", February 4–7, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, February 6–7.

86. ———, *(Pre)Dualization, dense embeddings of convex sets, and applications in image processing*, Thematic Programme "Modern Maximal Monotone Operator Theory: From Nonsmooth Optimization to Differential Inclusions", Workshop "Numerical Algorithms in Nonsmooth Optimization", February 25 – March 1, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, February 28.

87. ———, *Generalized Nash equilibrium problems with application to spot markets with gas transport*, Workshop "Electricity Systems of the Future: Incentives, Regulation and Analysis for Efficient Investment", March 18–22, Isaac Newton Institute, Cambridge, UK, March 21.

88. ———, *Optimal control of multiphase fluids and droplets*, Colloquium of the Mathematical Institute, University of Oxford, UK, June 7.

89. ———, *A function space framework for structural total variation regularization with applications in inverse problems*, 71st Workshop: Advances in Nonsmooth Analysis and Optimization (NAO2019), June 25–30, International School of Mathematics "Guido Stampacchia", Erice, Italy, June 26.

90. ———, *Generalized Nash equilibrium problems with PDEs connected to spot markets with (gas) transport*, 9th International Congress on Industrial and Applied Mathematics (ICIAM 2019), Session MS ME-1-4 1 "Recent Advances in PDE-constrained Optimization", July 15–19, Valencia, Spain, July 15.

91. ———, *A physically oriented method for quantitative magnetic resonance imaging*, 9th International Congress on Industrial and Applied Mathematics (ICIAM 2019), Session MS A1-1-3 5 "Computationally Efficient Methods for Large-scale Inverse Problems in Imaging Applications", July 15–19, Valencia, Spain, July 17.

92. ———, *Optimal control problems involving nonsmooth structures*, 3 talks, Autumn School 2019 "Optimal Control and Optimization with PDEs" (ALOP), October 7–10, Universität Trier, October 7.

93. ———, *Optimal control of multiphase fluids and droplets*, Polish Academy of Sciences, Systems Research Institute, Warsaw, Poland, December 3.

94. D. Hömberg, *MSO for steel production and manufacturing*, 9th International Congress on Industrial and Applied Mathematics (ICIAM), Minisymposium IM FT-4-2 1 "Academia-Industry Case Studies from MI-NET and ECMI", July 15–19, Valencia, Spain, July 15.

95. ———, *Optimal pre-heating strategies for the flame cutting of steel plates*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Session "Infinite-Dimensional Optimization of Nonlinear Systems (Part III)", August 5–8, Berlin, August 6.

96. ———, *Mathematics for steel production and manufacturing*, Conference "Dynamics, Equations and Applications (DEA 2019)", Session "D442 Complex Systems in Material Science", September 16–20, AGH University of Science and Technology, Kraków, Poland, September 17.

97. ———, *Maths for digital factory*, Polytechnic of Leiria, Center for Rapid and Sustainable Product Development, Marinha Grande, Portugal, October 10.

98. ———, *Mathematics for steel production and manufacturing*, Sondierungsworkshop MPIE/WIAS "Elektrochemie, Halbleiternanostrukturen und Metalle", October 14–15, Max-Planck-Institut für Eisenforschung GmbH Düsseldorf, October 14.

99. B. Jahnel, *Is the Mathern process Gibbs?*, Workshop on Stochastic Modeling of Complex Systems, GWOT '19, April 8–12, Universität Mannheim, Institut für Mathematik, April 9.

100. ———, *Dynamical Gibbs-non-Gibbs transitions for the continuum Widom–Rowlinson model*, The 41st Conference on Stochastic Processes and their Applications 2019 (SPA 2019), July 8–12, Northwestern University Evanston, USA, July 9.

101. ———, *Continuum percolation in random environment*, 4 talks, Workshop on Probability, Analysis and Applications (PAA), September 23 – October 4, African Institute for Mathematical Sciences — Ghana (AIMS Ghana), Accra, September 23 – October 4.

102. ———, *Attractor properties for irreversible and reversible interacting particle systems*, Quaid-i-Azam University Islamabad, Department of Mathematics, Pakistan, November 19.

103. V. John, *Finite element methods for incompressible flows*, 5 talks, Workshop on Computational Modeling and Numerical Analysis (WCMNA 2019), February 25–28, Laboratório Nacional de Computação Científica, Petrópolis, Brazil, February 25–28.

104. ———, *Algebraic finite element stabilizations for convection-diffusion equations*, Workshop on Computational Modeling and Numerical Analysis (WCMNA 2019), February 25–28, Laboratório Nacional de Computação Científica, Petrópolis, Brazil, February 26.

105. ———, *Algebraic finite element stabilizations for convection-diffusion equations*, Workshop "Towards Computable Flows", April 26–27, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, April 26.

106. ———, *On $L^2(\Omega)$ estimates for finite element methods for evolutionary convection-dominated problems*, PIMS-Germany Workshop on Discretization of Variational Eigenvalue and Flow Problems, June 24–26, Universität Heidelberg, June 25.

107. ———, *Variational Multiscale (VMS) methods for the simulation of turbulent incompressible flows*, University of Groningen, Bernoulli Institute, Computational Mechanics & Numerical Mathematics, Netherlands, September 23.

108. ———, *Variational Multiscale (VMS) methods for the simulation of turbulent incompressible flows*, Indian Institute of Science, Department of Computational and Data Science, Bangalore, India, November 28.

109. ———, *Finite elements for scalar convection-dominated equations and incompressible flow problems – A never ending story?*, Indo-German Conference on Computational Mathematics (IGCM), December 2–4, Indian Institute of Science, Department of Computer and Data Sciences, Bangalore, India, December 3.

110. M. Kantner, *Hybrid modeling of quantum light emitting diodes: Self-consistent coupling of drift-diffusion, Schrödinger–Poisson, and quantum master equations*, SPIE Photonics West, February 5–7, San Francisco, USA, February 6.

111. W. König, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Workshop on Spectral Properties of Disordered Systems, January 7–11, Paris, France, January 11.

112. ———, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Berlin–Leipzig Workshop in Analysis and Stochastics, January 16–18, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 17.

113. ———, *A large-deviations approach to the multiplicative coalescent*, Math Probability Seminar Series, New York University Shanghai, Institute of Mathematical Sciences, China, February 19.

114. ———, *A large-deviations approach to coagulation*, Workshop on Stochastic Modeling of Complex Systems, GWOT '19, April 8–12, Universität Mannheim, Institut für Mathematik, April 10.

115. ———, *A large-deviations approach to the multiplicative coalescent*, 18. Erlanger-Münchner Tag der Stochastik / Probability Day 2019, Friedrich-Alexander-Universität Erlangen–Nürnberg, Department Mathematik, May 10.

116. ———, *Cluster size distribution in a classical many-body system*, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln, June 18.

117. ———, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Workshop on Dynamics, Random Media and Universality of Complex Physical Systems, August 26–30, Westfälische Wilhelms-Universität Münster, Department of Mathematics and Computer Science, August 27.

118. ———, *Micro-macro phase transitions in coagulating particle systems*, 4 talks, Workshop on Probability, Analysis and Applications (PAA), September 23 – October 4, African Institute for Mathematical Sciences — Ghana (AIMS Ghana), Accra, September 23 – October 4.

119. ———, *A large-deviations approach to the multiplicative coalescent*, Oberseminar Wahrscheinlichkeitstheorie, Universität München, Mathematisches Institut, November 25.

120. ———, *A large-deviations approach to coagulation*, Maxwell Analysis Seminar, Harriot Watt University, The Maxwell Institute for Mathematical Sciences, Edinburgh, UK, December 27.

121. Th. Koprucki, *Multi-dimensional modeling and simulation of semiconductor devices*, Physikalisches Kolloquium, Technische Universität Chemnitz, Institut für Physik, November 27.

122. M. Landstorfer, *Theory and validation of the electrochemical double layer*, PC Seminar, AG Prof. Baltruschat, Universität Bonn, Abt. Elektrochemie, March 8.

123. ———, *Modelling porous intercalation electrodes with continuum thermodynamics and multi-scale asymptotics*, Oxford Battery Modelling Symposium, March 18–19, University of Oxford, Pembroke College, UK, March 18.

124. R. Lasarzik, *Weak entropic solutions to a model in induction hardening: Existence and weak-strong uniqueness*, Decima Giornata di Studio Università di Pavia – Politecnico di Milano Equazioni Differenziali e Calcolo delle Variazioni, Politecnico di Milano, Italy, February 21.

125. ———, *Optimal control via relative energies*, Workshop "Recent Trends in Optimal Control of Partial Differential Equations", February 25–27, Technische Universität Berlin, February 27.

126. ———, *Weak entropy solutions in the context of induction hardening*, 9th International Congress on Industrial and Applied Mathematics (ICIAM), Minisymposium CP FT-1-7 9 "Partial Differential Equations VII", July 15–19, Valencia, Spain, July 19.

127. A. LINKE, *Towards a pressure robust computation of computable flows*, Workshop ”Towards Computable Flows”, April 26–27, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, April 27.

128. ———, *On high-order pressure-robust space discretisations, their advantages for incompressible high Reynolds number generalised Beltrami flows and beyond*, Conference “POEMs — POlytopal Element Methods in Mathematics and Engineering”, April 29 – May 3, CIRM – Luminy, Centre International de Rencontres Mathématiques, Marseille, France, April 29.

129. ———, *On high-order pressure-robust space discretisations, their advantages for incompressible high Renolds number generalised Beltrami flows and beyond*, PIMS-Germany Workshop on Discretization of Variational Eigenvalue and Flow Problems, June 24–26, Universität Heidelberg, June 26.

130. ———, *On high Reynolds number flows, pressure-robustness and high-order methods*, Technische Universität Darmstadt, Fachbereich Mathematik, August 28.

131. ———, *On high-order pressure-robust space discretisations, their advantages for incompressible high Reynolds number generalised Beltrami flows and beyond*, European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Minisymposium 23 “Recent Advances in Numerical Simulation of Incompressible Flows (Part 3)”, September 30 – October 4, Eindhoven University of Technology, Netherlands, October 2.

132. ———, *Robust discretization of advective linear transport, based on a complete flux scheme and entropy principles*, European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Minisymposium 15 “Novel Flux Approximation Schemes for Advection-Diffusion Problems (Part 1)”, September 30 – October 4, Eindhoven University of Technology, Netherlands, October 2.

133. O. MARQUARDT, *Modelling the electronic properties of semiconductor nanowires*, Engineering Physics Seminar, McMaster University, Hamilton, Canada, July 12.

134. M. MARSCHALL, *Random domains in PDE problems with low-rank surrogates. Forward and backward*, Physikalisch-Technische Bundesanstalt, Arbeitsgruppe 8.41 “Mathematische Modellierung und Datenanalyse”, Berlin, April 10.

135. ———, *Complexity reduction in Bayesian inverse problems by low-rank tensor representation*, Robert Bosch GmbH, Corporate Research – Advanced Engineering Computer Vision Systems (CR/AEC4), Hildesheim, April 16.

136. ———, *Adaptive low-rank approximation in Bayesian inverse problems*, 3rd International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2019), Minisymposium 6–IV “Uncertainty Computations with Reduced Order Models and Low-Rank Representations”, June 24–26, Crete, Greece, June 25.

137. ———, *Low-rank surrogates in Bayesian inverse problems*, 19th French-German-Swiss Conference on Optimization (FGS’2019), Minisymposium 1 “Recent Trends in Nonlinear Optimization 1”, September 17–20, Nice, France, September 17.

138. P. MATHÉ, *Relating direct and inverse Bayesian problems via the modulus of continuity*, Stochastic Computation and Complexity (ibcparis2019), April 15–16, Institut Henri Poincaré, Paris, France, April 16.

139. ———, *The role of the modulus of continuity in inverse problems*, Forschungsseminar Inverse Probleme, Technische Universität Chemnitz, Fachbereich Mathematik, August 13.

140. ———, *Relating direct and inverse problems via the modulus of continuity*, The Chemnitz Symposium on Inverse Problems 2019, September 30 – October 2, Technische Universität Chemnitz, Fakultät für Mathematik, Frankfurt a. M., October 1.

141. CH. MERDON, *Pressure-robust mixed finite element methods and refined a posteriori error control for the Stokes problem*, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, January 29.

142. ———, *Pressure-robust finite element discretisations for the Navier–Stokes problem*, Technische Universität Dresden, Fachbereich Mathematik, April 11.

143. ———, *Pressure-robustness in the discretisation of the Navier–Stokes equations*, University of Twente, Institute of Nanotechnology, Enschede, Netherlands, September 30.

144. ———, *A gradient-robust, well-balanced discretisation for the compressible barotropic Stokes problem*, European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Minisymposium 23 "Recent Advances in Numerical Simulation of Incompressible Flows (Part 1)", September 30 – October 4, Eindhoven University of Technology, Netherlands, October 1.

145. A. Mielke, *Evolutionary Gamma-convergence for gradient systems*, Mathematisches Kolloquium, Albert-Ludwigs-Universität Freiburg, January 24.

146. ———, *Effective kinetic relations and EDP convergence for gradient systems*, Necas Seminar on Continuum Mechanics, Charles University, Prague, Czech Republic, March 18.

147. ———, *Thermodynamical modeling via GENERIC: From quantum mechanics to semiconductor devices*, Institute of Thermomechanics's Seminar, Czech Academy of Sciences, Prague, March 21.

148. ———, *Effective kinetic relations and EDP convergence*, COPDESC-Workshop "Calculus of Variation and Nonlinear Partial Differential Equations", March 25–28, Universität Regensburg, March 28.

149. ———, *Transport versus growth and decay: The (spherical) Hellinger–Kantorovich distance between arbitrary measures*, Optimal Transport: From Geometry to Numerics, May 13–17, Erwin Schrödinger International Institute for Mathematics and Physics, Universität Wien, Austria, May 17.

150. ———, *Gradient systems and the derivation of effective kinetic relations via EDP convergence*, Material Theories, Statistical Mechanics, and Geometric Analysis: A Conference in Honor of Stephan Luckhaus' 66th Birthday, June 3–6, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, June 5.

151. ———, *EDP convergence for the membrane limit in the porous medium equation*, 9th International Congress on Industrial and Applied Mathematics (ICIAM 2019), Thematic Minisymposium MS ME-1-3 9 "Entropy Methods for Multi-dimensional Systems in Mechanics", July 15–19, Valencia, Spain, July 19.

152. ———, *Gamma convergence of dissipation functionals and EDP convergence for gradient systems*, 6th Applied Mathematics Symposium Münster: Recent Advances in the Calculus of Variations, September 16–19, Westfälische Wilhelms-Universität Münster, September 17.

153. ———, *Variational methods in time-dependent material models with finite-strain deformations*, 4 talks, Hausdorff School on Modeling and Analysis of Evolutionary Problems in Materials Science, September 23–27, Hausdorff Center for Mathematics, Universität Bonn, September 26–27.

154. ———, *An existence result for thermoviscoelasticity at finite strains*, Mathematics for Mechanics, October 29 – November 1, Czech Academy of Sciences, Institute for Information Theory and Automation, Prague, Czech Republic, November 1.

155. ———, *On initial-boundary value problems for materials with internal variables or temperature dependence*, Workshop on Mathematical Methods in Continuum Physics and Engineering: Theory, Models, Simulation, November 6–7, Technische Universität Darmstadt, November 6.

156. ———, *Pattern formation in coupled parabolic systems on extended domains*, Fundamentals and Methods of Design and Control of Complex Systems – Introductory Lectures 2019/20 of CRC 910, Technische Universität Berlin, November 25.

157. R. Müller, *Transport phenomena in electrolyte within a battery cell*, Battery Colloquium, Technische Universität Berlin, April 18.

158. G. Nika, *Homogenization for a multi-scale model of magnetorheological suspension*, 9th International Congress on Industrial and Applied Mathematics (ICIAM 2019), Minisymposium MS ME-1-3 1 "Emerging Problems in the Homogenization of Partial Differential Equations", July 15–19, Valencia, Spain, July 15.

159. T. Orenshtein, *Random walks in random environment as rough paths*, Probability Seminar, New York University Shanghai, Institute of Mathematical Sciences, Shanghai, China, November 26.

160. K. Papafitsoros, *Generating structure non-smooth priors for image reconstruction*, Young Researchers in Imaging Seminars, March 20–27, Henri Poincaré Institute, Paris, France, March 27.

161. ———, *A function space framework for structural total variation regularization with applications in inverse problems*, Applied Inverse Problems Conference, Minisymposium "Multi-Modality/Multi-Spectral Imaging and Structural Priors", July 8–12, Grenoble, France, August 8.

162. ———, *Quantitative MRI: From fingerprinting to integrated physics-based models*, Synergistic Reconstruction Symposium, November 3–6, Chester, UK, November 4.

163. R.I.A. Patterson, *Interaction clusters for the Kac process*, Berlin–Leipzig Workshop in Analysis and Stochastics, January 16–18, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 18.

164. ———, *Kinetic interaction clusters*, Oberseminar, Martin-Luther-Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II – Chemie, Physik und Mathematik, April 17.

165. ———, *Flux large deviations*, Seminar, Statistical Laboratory, University of Cambridge, Faculty of Mathematics, UK, May 7.

166. ———, *A novel simulation method for stochastic particle systems*, Seminar, Department of Chemical Engineering and Biotechnology, University of Cambridge, Faculty of Mathematics, UK, May 9.

167. ———, *Interaction clusters for the Kac process*, Workshop on Effective Equations: Frontiers in Classical and Quantum Systems, June 24–28, Hausdorff Research Institute for Mathematics, Bonn, June 28.

168. ———, *Flux large deviations*, Workshop on Chemical Reaction Networks, July 1–3, Politecnico di Torino, Dipartimento di Scienze Matematiche "G. L. Lagrange", Italy, July 2.

169. ———, *Fluctuations and confidence intervals for stochastic particle simulations*, First Berlin–Leipzig Workshop on Fluctuating Hydrodynamics, August 26–30, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, August 29.

170. D. Peschka, *Dynamic contact angles via generalized gradient flows*, Modelling of Thin Liquid Films – Asymptotic Approach vs. Gradient Dynamics, April 28 – May 3, Banff International Research Station for Mathematical Information and Discovery, Canada, April 30.

171. ———, *Gradient formulations with flow maps – Mathematical and numerical approaches to free boundary problems*, Kolloquium des Graduiertenkollegs 2339 "Interfaces, Complex Structures, and Singular Limits", Universität Regensburg, May 24.

172. ———, *Mathematical modeling of fluid flows using gradient systems*, Seminar in PDE and Applications, Delft University of Technology, Netherlands, May 28.

173. ———, *Steering pattern formation of viscous flows*, DMV-Jahrestagung 2019, Sektion "Differentialgleichungen und Anwendungen", September 23–26, KIT - Karlsruher Institut für Technologie, September 23.

174. P. Pigato, *Density and tube estimates for diffusion processes under Hormander-type conditions*, Statistics Seminars, Università di Bologna, Italy, February 28.

175. ———, *Precise asymptotics of rough stochastic volatility models*, 11th Annual ERC Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis, May 23–25, WIAS Berlin, May 23.

176. ———, *Rough stochastic volatility models*, Università degli Studi di Roma "Tor Vergata", Dipartimento di Economia e Finanza, Italy, June 26.

177. ———, *Precise asymptotics: Robust stochastic volatility models*, Forschungsseminar Wahrscheinlichkeitstheorie, Universität Potsdam, July 1.

178. ———, *Parameters estimation in a threshold diffusion*, 62nd ISI World Statistics Congress 2019, IPS-26 “Perspectives on Statistical Methods for Time Dependent Processes”, August 18–23, Kuala Lumpur, Malaysia, August 21.

179. ———, *Applications of stochastic analysis to volatility modelling*, Università degli Studi di Roma “Tor Vergata”, Dipartimento di Economia e Finanza, Italy, September 27.

180. J. Polzehl, *R Introduction, visualization and package management / Exploring functional data*, 3 talks, Leibniz MMS Summer School 2019, October 28 – November 1, Mathematisches Forschungsinstitut Oberwolfach, October 28 – November 1.

181. C.N. Rautenberg, *Parabolic quasi-variational inequalities with gradient and obstacle type constraints*, Thematic Programme “Modern Maximal Monotone Operator Theory: From Nonsmooth Optimization to Differential Inclusions”, January 28 – February 1, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, January 31.

182. M. Redmann, *Numerical approximations for rough and stochastic differential equations*, Technische Universität Bergakademie Freiberg, Fakultät für Mathematik und Informatik, April 1.

183. ———, *Numerical approximations for rough and stochastic differential equations*, Technische Universität Dresden, Fakultät Mathematik, April 12.

184. J. Rehberg, *An extrapolation for the Lax–Milgram isomorphism for second order divergence operators*, Oberseminar “Angewandte Analysis”, Technische Universität Darmstadt, February 7.

185. ———, *Well-posedness for the Keller–Segel model – based on a pioneering result of Herbert Amann*, International Conference “Nonlinear Analysis” in Honor of Herbert Amann’s 80th Birthday, June 11–14, Scuola Normale Superiore di Pisa, Cortona, Italy, June 11.

186. ———, *Maximal parabolic regularity for the treatment of real world problems*, 12th Workshop on Analysis and Advanced Numerical Methods for Partial Differential Equations (not only) for Junior Scientists (AANMPDE 12), July 1–5, Österreichische Akademie der Wissenschaften, St. Wolfgang / Strobl, Austria, July 2.

187. ———, *Explicit and uniform estimates for second order divergence operators on L^p spaces*, Evolution Equations: Applied and Abstract Perspectives, October 28 – November 1, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, October 31.

188. D.R.M. Renger, *Reaction fluxes*, Applied Mathematics Seminar, University of Birmingham, School of Mathematics, UK, April 4.

189. ———, *A generic formulation of a chemical reaction network from Onsager–Machlup theory*, Conference to Celebrate 80th Jubilee of Miroslav Grmela, May 18–19, Czech Technical University, Faculty of Nuclear Sciences and Physical Engineering, Prague, May 19.

190. ———, *Macroscopic fluctuation theory of chemical reaction networks*, Workshop on Chemical Reaction Networks, July 1–3, Politecnico di Torino, Dipartimento di Scienze Matematiche “G. L. Lagrange“, Italy, July 2.

191. J.G.M. Schoenmakers, *Tractability of continuous time optimal stopping problems*, Séminaire du Groupe de Travail “Finance Mathématique, Probabilités Numériques et Statistique des Processus”, Université Paris Diderot, LPSM-Equipe Mathématiques Financières et Actuarielles, Probabilités Numériques, France, June 27.

192. H. Si, *An introduction to unstructured mesh generation and adaptation*, Universidad de Chile, Department of Computer Science, Santiago, Chile, April 28.

193. ———, *Instructor for the course “An Introduction to Mesh Generation Methods and Software for Scientific Computing”*, 8 talks, BAIHANG University International Summer School 2019, July 1–26, Beijing, China, July 1–26.

194. ———, *Unstructured mesh generation and its applications*, Beihang University, School of Mathematics and Systems Science, Beijing, China, November 22.

195. ———, *An introduction to mesh generation methods and softwares for scientific computing*, 8 talks, Zhejiang University, Center for Engineering & Scientific Computation, Hangzhou, China, December 15–26.

196. V. Spokoiny, *Inference for spectral projectors*, RTG Kolloquium, Universität Heidelberg, Institut für Angewandte Mathematik, January 10.

197. ———, *Optimal stopping via reinforced regression*, HUB-NUS FinTech Workshop, March 18–21, National University of Singapore, Institute for Mathematical Science, Singapore, March 21.

198. ———, *Optimal stopping and control via reinforced regression*, Optimization and Statistical Learning, March 25–28, Les Houches School of Physics, France, March 26.

199. ———, *Advanced statistical methods*, 2 talks, Higher School of Economics, National Research University, Moscow, Russian Federation, April 9–11.

200. ———, *Statistical inference for barycenters*, Optimal Transportation Meeting, September 23–27, Higher School of Economics, National Research University, Moscow, Russian Federation, September 26.

201. ———, *Bayesian inference vs stochastic optimization*, HSE-Yandex Autumn School on Generative Models, November 26–29, Higher School of Economics, National Research University, Moscow, Russian Federation, November 29.

202. ———, *Bayesian inference for nonlinear inverse problems*, Rencontres de Statistiques Mathématiques, December 16–20, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, December 19.

203. K. Tabelow, *Speaker of Neuroimaging Workshop*, 6 talks, Workshop in Advanced Statistics: Good Scientific Practice for Neuroscientists, February 13–14, University of Zurich, Center for Reproducible Science, Switzerland, February 13–14.

204. ———, *Quantitative MRI for in-vivo histology*, Doktorandenseminar, Berlin School of Mind and Brain, April 1.

205. ———, *Adaptive smoothing data from multi-parameter mapping*, 7th Nordic-Baltic Biometric Conference, June 3–5, Vilnius University, Faculty of Medicine, Lithuania, June 5.

206. ———, *Quantitative MRI for in-vivo histology*, Neuroimmunological Colloquium, Charité-Universitätsmedizin Berlin, November 11.

207. ———, *Model-based imaging for quantitative MRI*, KoMSO Challenge-Workshop Mathematical Modeling of Biomedical Problems, December 12–13, Friedrich-Alexander-Universität Erlangen-Nürnberg, December 12.

208. L. Taggi, *Critical density in activated random walks*, Horowitz Seminar on Probability, Ergodic Theory and Dynamical Systems, Tel Aviv University, School of Mathematical Sciences, Israel, May 20.

209. ———, *Essential enhancements for activated random walks*, Second Italian Meeting on Probability and Mathematical Statistics, June 17–20, Vietri sul Mare, Italy, June 19.

210. ———, *Non-decay of correlations in the dimer model and phase transition in lattice permutations in $Z^d, d > 2$ via reflection positivity*, Meeting of the Swiss Mathematical Society: Recent Advances in Loop Models and Height Functions, September 2–4, Université Fribourg, Switzerland, September 3.

211. ———, *Absorbing-state phase transition in activated random walk and oil and water*, Probability Seminars, Università degli Studi "La Sapienza" di Roma, Italy, October 1.

212. ———, *Uniformly positive correlations in the dimer model and phase transition in lattice permutations in $Z^d, d > 2$, via reflection positivity*, Seminaire Probabilités et Statistiques, Université Claude Bernard Lyon 1, Institut Camille Jordan (ICJ), France, November 14.

213. ———, *Phase transition in lattice permutations and uniformly positive correlations in the dimer model in $\mathbb{Z}^d, d > 2$, via reflection positivity*, Kolloquium des Fachbereichs Mathematik, Technische Universität Darmstadt, December 5.

214. N. Tapia, *Algebraic aspects of signatures*, SciCADE 2019, International Conference on Scientific Computation and Differential Equations, July 22–26, Innsbruck, Austria, July 24.

215. ———, *Signatures in shape analysis*, 4th Conference on Geometric Science of Information (GSI 2019), August 27–29, École Nationale de l'Aviation Civile, Toulouse, France, August 27.

216. ———, *Non-commutative Wick polynomials*, Rencontre GDR Renormalisation, September 30 – October 4, L'Université du Littoral Côte d'Opale, Laboratoire de Mathématiques Pures et Appliquées Joseph Liouville, Calais, France, October 3.

217. ———, *Iterated-sums signature, quasi-symmetric functions and time series analysis*, 12th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 4–6, University of Oxford, Mathematical Institute, UK, December 5.

218. M. Thomas, *Analysis for the discrete approximation of gradient-regularized damage models*, Mathematics Seminar Brescia, Università degli Studi di Brescia, Italy, March 13.

219. ———, *Analysis for the discrete approximation of gradient-regularized damage models*, PDE Afternoon, Universität Wien, Austria, April 10.

220. ———, *Coupling of rate-independent and rate-dependent systems*, 5 talks, MURPHYS-HSFS 2019 Summer School on Multi-Rate Processes, Slow-Fast Systems and Hysteresis, June 17–19, Politecnico di Torino, Turin, Italy, June 17–19.

221. ———, *Analytical and numerical aspects for the approximation of gradient-regularized damage models*, 9th International Congress on Industrial and Applied Mathematics (ICIAM 2019), Thematic Minisymposium MS A3-2-26 "Phase-Field Models in Simulation and Optimization", July 15–19, Valencia, Spain, July 17.

222. ———, *Gradient structures for flows of concentrated suspensions*, 9th International Congress on Industrial and Applied Mathematics (ICIAM 2019), Thematic Minisymposium MS ME-7-75 "Recent Advances in Understanding Suspensions and Granular Media Flow", July 15–19, Valencia, Spain, July 17.

223. ———, *Analytical and numerical aspects of rate-independent gradient-regularized damage models*, Conference "Dynamics, Equations and Applications (DEA 2019)", Session D444 "Topics in the Mathematical Modelling of Solids", September 16–20, AGH University of Science and Technology, Kraków, Poland, September 19.

224. ———, *Coupling of rate-independent and rate-dependent systems with application to delamination processes in solids*, Seminar "Applied and Computational Analysis", University of Cambridge, UK, October 10.

225. ———, *GENERIC structures with bulk-interface interaction*, SFB 910 Symposium "Energy Based Modeling, Simulation and Control", October 25, Technische Universität Berlin, October 25.

226. ———, *Coupling of rate-independent and rate-dependent systems with application to delamination processes in solids*, Mathematics for Mechanics, October 29 – November 1, Czech Academy of Sciences, Prague, Czech Republic, October 31.

227. P. Vágner, *Thermodynamic modeling of the YSZ metal gas electrode interface dynamics*, University of Chemistry and Technology, Institute of Anorganic Technology, Prague, Czech Republic, July 15.

228. W. van Zuijlen, *Mass-asymptotics for the parabolic Anderson model in 2D*, Berlin–Leipzig Workshop in Analysis and Stochastics, January 16–18, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 18.

229. ———, *The parabolic Anderson model in 2D, mass- and eigenvalue asymptotics*, Stochastic Analysis Seminar, University of Oxford, Mathematical Institute, UK, February 4.

230. ———, *The parabolic Anderson model in 2D, mass- and eigenvalue asymptotics*, Analysis and Probability Seminar, Imperial College London, Department of Mathematics, UK, February 5.

231. ———, *Bochner integrals in ordered vector spaces*, Analysis Seminar, University of Canterbury, Department of Mathematics and Statistics, UK, March 1.

232. ———, *Mini-course on Besov spaces I–III*, 3 talks, Junior Trimester Program: Randomness, PDEs and Nonlinear Fluctuations (Sept. 2 to Dec. 19, 2019), Hausdorff Research Institute for Mathematics (HIM), Bonn, October 16 – November 6.

233. ———, *From periodic to Dirichlet and Neumann on boxes*, 12th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 4–6, University of Oxford, Mathematical Institute, UK, December 6.

234. A.G. Vladimirov, *Nonlinear wave phenomena in delay differential models of multimode lasers*, Waves Côte d'Azur 2019, June 4–7, Faculté des Sciences de l'Université de Nice, France, June 6.

235. B. Wagner, *Mathematical modeling of real world processes*, 2 talks, CERN Academic Training Programme 2018–2019, CERN, Geneva, Switzerland, March 14–15.

236. ———, *Free boundary problems of active and driven hydrogels*, PIMS-Germany Workshop on Modelling, Analysis and Numerical Analysis of PDEs for Applications, June 24–26, Universität Heidelberg, Interdisciplinary Center for Scientific Computing and BIOQUANT Center, June 24.

237. ———, *Ill-posedness of two-phase flow models of concentrated suspensions*, 9th International Congress on Industrial and Applied Mathematics ICIAM2019, Minisymposium MS ME-0-7 6 "Recent Advances in Understanding Suspensions and Granular Media Flow – Part 2", July 15–19, Valencia, Spain, July 17.

238. ———, *Free boundary problems of active and driven hydrogels*, EUROMECH 604, Fluid and Solid Mechanics for Issue Engineering, September 23–25, University of Oxford, Mathematical Institute, UK, September 24.

239. M. Wolfrum, *The relation of Chimeras, bump states, and Turing patterns in arrays of coupled oscillators*, School and Workshop on Patterns of Synchrony: Chimera States and Beyond, May 6–17, International Centre for Theoretical Physics, Trieste, Italy, May 16.

240. ———, *Patterns in discrete media*, Fundamentals and Methods of Design and Control of Complex Systems – Introductory Lectures 2019/20 of CRC 910, Technische Universität Berlin, December 2.

A.8.3 Talks for a More General Public

1. S. Bergmann, *LabSlam*, SCIENCE DAY 2019, Forschungsverbund Berlin e.V., June 13.

2. J.A. Brüggemann, *Mathematische Lösungen für komplexe Probleme: Forschung in Angewandter Mathematik am Weierstraß-Institut für Angewandte Analysis und Stochastik*, Girls'Day at WIAS, March 28.

3. M. Eigel, *Mathematik des Lichts: Licht, Form, Zufall in der Echtzeitgrafik*, MathInside – Mathematik ist überall, Urania, Berlin, May 21.

4. W. König, *Das Internet der Dinge — Neue Herausforderungen an die Mathematik*, MathInside – Mathematik ist überall, Urania, Berlin, January 29.

5. ———, *Das Internet der Dinge — Neue Herausforderungen an die Mathematik*, 24. Berliner Tag der Mathematik, Beuth Hochschule für Technik Berlin, May 11.

6. ———, *Paradoxien der Wahrscheinlichkeitstheorie*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2019, WIAS at Leibniz Association Headquarters, Berlin, June 15.

7. ———, *Paradoxa in der Wahrscheinlichkeitsrechnung*, 2 talks, Tag der Wissenschaften 2019, Weinberg-Gymnasium Kleinmachnow, November 8.
8. D.R.M. Renger, *Schallwellen in elektronischer Musik*, 24. Berliner Tag der Mathematik, Beuth Hochschule für Technik Berlin, May 11.
9. H. Stephan, *Mathematische Kleinigkeiten von großer Bedeutung*, Girls' Day at WIAS, March 28.
10. K. Tabelow, *Die Vermessung des Gehirns*, 24. Berliner Tag der Mathematik, Beuth Hochschule für Technik Berlin, May 11.

A.8.4 Posters

1. N. Alia, M.J. Arenas Jaén, *Revealing secrets of industrial processes with Math*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2019, WIAS at Leibniz Headquarters, Berlin, June 15.
2. V. Avanesov, *Nonparametric change point detection in regression*, SFB 1294 Spring School 2019, Dierhagen, March 18–22.
3. F. Besold, *Manifold clustering with adaptive weights*, Structural Inference in High-Dimensional Models 2, National Research University Higher School of Economics, HDILab, St. Petersburg, Russian Federation, August 26–30.
4. ———, *Manifold clustering with adaptive weights*, Joint Workshop of BBDC, BZML and RIKEN AIP, Fraunhofer Institute HHI, September 9–10.
5. C. Brée, V. Raab, J. Montiel, G.G. Werner, K. Staliunas, U. Bandelow, M. Radziunas, *Lyot spectral filter for polarization beam combining of high-power, broad-area diode lasers: Modeling, simulations, and experiments*, CLEO/Europe-EQEC 2019, Munich, June 23–27.
6. C. Brée, V. Raab, D. Gailevičius, V. Purlys, J. Montiel, G.G. Werner, K. Staliunas, A. Rathsfeld, U. Bandelow, M. Radziunas, *Genetically optimized photonic crystal for spatial filtering of reinjection into broad-area diode lasers*, CLEO/Europe-EQEC 2019, Munich, June 23–27.
7. J.A. Brüggemann, *Elliptic obstacle-type quasi-variational inequalities (QVIs) with volume constraints motivated by a contact problem in biomedicine*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Berlin, August 5–8.
8. G. Dong, *Direct reconstruction of biophysical parameters using dictionary learning and robust regularization*, 1st MATH+ Day, Berlin, December 13.
9. D. Dvinskikh, *Distributed decentralized (stochastic) optimization for dual friendly functions*, Optimization and Statistical Learning, Les Houches, France, March 24–29.
10. ———, *Decentralized and parallelized primal and dual accelerated methods*, Structural Inference in High-Dimensional Models 2, National Research University Higher School of Economics, HDILab, St. Petersburg, Russian Federation, August 26–30.
11. A. Kroshnin, N. Tupitsa, D. Dvinskikh, P. Dvurechensky, A. Gasnikov, C.A. Uribe, *On the complexity of approximating Wasserstein barycenters*, Thirty-sixth International Conference on Machine Learning, ICML 2019, Long Beach, CA, USA, June 9–15.
12. P. Dvurechensky, *Distributed optimization for Wasserstein barycenter*, Optimization and Statistical Learning, Les Houches, France, March 24–29.
13. ———, *On the complexity of optimal transport problems*, Computational and Mathematical Methods in Data Science, Berlin, October 24–25.

14. A. Gasnikov, P. Dvurechensky, E. Gorbunov, E. Vorontsova, D. Selikhanovych, C.A. Uribe, *Optimal tensor methods in smooth convex and uniformly convex optimization*, Conference on Learning Theory, COLT 2019, Phoenix, Arizona, USA, June 24–28.

15. S. Eydam, A. Gerdes, *Extensive chaos, cluster and chimera states in globally-coupled Stuart–Landau systems*, SFB 910: Workshop on "Control of Self-Organizing Nonlinear Systems", Lutherstadt Wittenberg, August 20–22.

16. M.H. Farshbaf Shaker, D. Peschka, M. Thomas, *Modeling and analysis of suspension flows*, Visit of the Scientific Advisory Board of MATH+, November 11.

17. ———, *Modeling and analysis of suspension flows*, 1st MATH+ Day, Berlin, December 13.

18. J. Fuhrmann, A. Linke, Ch. Merdon, R. Müller, *Induced charge electroosmotic flow including finite ion size effects*, 13th International Symposium on Electrokinetics (ELKIN), Cambridge, USA, June 12–14.

19. M. Heida, A. Mielke, A. Stephan, *Effective models for materials and interfaces with multiple scales*, SCCS Days 2019 of the Collaborative Research Center - CRC 1114, Zeuthen, May 20–22.

20. A. Hinsen, *The White Knight model — An epidemic on a spatial random network*, Bocconi Summer School in Advanced Statistics and Probability, Lake Como School of Advanced Studies, Lake Como, Italy, July 8–19.

21. D. Hömberg, *European collaboration in industrial and applied mathematics*, EMMC International Workshop 2019 "European Materials Modelling Council", Vienna, Austria, February 25–27.

22. W. König, *EF4: Particles and Agents*, 1st MATH+ Day, Berlin, December 13.

23. M. Landstorfer, *Mathematical modeling of intercalation batteries with non-equilibrium thermodynamics and homogenization theory*, ModVal 2019 – 16th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies, Braunschweig, March 12–13.

24. S. Cap, M. Landstorfer, D. Klein, R. Schlägl, N. Nickel, *Silicon thin films deposited by low pressure chemical vapor deposition on planer current collectors as model system for lithium ion batteries*, Advanced Lithium Batteries for Automobile Applications (ABAA 12), Ulm, October 6–9.

25. A. Maltsi, Th. Koprucki, T. Streckenbach, K. Tabelow, J. Polzehl, *Model-based geometry reconstruction of quantum dots from TEM*, BMS Summer School 2019: Mathematics of Deep Learning, Berlin, August 19–30.

26. ———, *Model-based geometry reconstruction of quantum dots from TEM*, Microscopy Conference 2019, Poster session IM 4, Berlin, September 1–5.

27. P.P. Bawol, Ch. Merdon, H. Baltruschat, J. Fuhrmann, *Rotating ring-disc electrode simulations: A comparison of classical finite differences to fully implicit finite volume scheme*, ModVal 2019 – 16th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies, Braunschweig, March 12–13.

28. D. Peschka, *Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flow*, Begutachtungskolloquium für die Anträge des SPP 2171 "Dynamische Benetzung flexibler, adaptiver und schaltbarer Oberflächen", Mainz, February 7–8.

29. ———, *Dynamic contact angles via gradient flows*, 694. WE-Heraeus-Seminar "Wetting on Soft or Microstructured Surfaces", Bad Honnef, April 10–13.

30. A. Pimenov, *Temporal solitons in a delayed model of a semiconductor laser*, Waves Côte d'Azur, Nice, France, June 4–7.

31. J. Polzehl, K. Tabelow, *Analyzing neuroimaging experiments within R*, 2019 OHBM Annual Meeting, Organization for Human Brain Mapping, Rome, Italy, June 9–13.

32. M. Opper, S. Reich, V. Spokoiny, V. Avanesov, D. Maoutsa, P. Rozdeba, *Approximative Bayesian inference and model selection for stochastic differential equations*, CRC 1294 Annual Meeting 2019, Universität Potsdam, Campus Griebnitzsee, September 23.
33. St.-M. Stengl, M. Hintermüller, *On the convexity of optimal control problems involving nonlinear PDEs or VIs*, ICCOPT 2019 – Sixth International Conference on Continuous Optimization, Berlin, August 5–8.
34. S. Tornquist, *Towards the analysis of dynamic phase-field fracture*, Spring School on Variational Analysis 2019, Paseky, Czech Republic, May 19–25.
35. ———, *Towards the analysis of dynamic phase-field fracture*, MURPHYS-HSFS 2019 Summer School on Multi-Rate Processes, Slow-Fast Systems and Hysteresis, Turin, Italy, June 17–21.
36. P. Vágner, *A detailed double layer model of solid oxide cell electrolyte-electrode interface*, ModVal 2019 – 16th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies, Braunschweig, March 12–13.
37. P. Vágner, M. Pavelka, *Dielectric polarization in GENERIC*, Joint European Thermodynamics Conference (JETC 2019), Barcelona, Spain, May 21–24.
38. B. Wagner, S. Reber, J. Iglesias, A. Fritsch, E. Meca, *Hierarchical spindle assembly: Sequence-dependent energy landscapes for a cytoplasmic condensate*, Kick-Off Meeting DFG SPP 2191 “Molecular Mechanisms of Functional Phase Separation”, Heidelberg, June 6–7.
39. A. Münch, B. Wagner, *Nonlinear visco-elastic effects of polymer and hydrogel layers sliding on liquid substrates*, 694. WE-Heraeus-Seminar, Bad Honnef, April 11–13.
40. A. Zafferi, *Dynamics of rock dehydration on multiple scales*, SCCS Days 2019 of the Collaborative Research Center - CRC 1114, Zeuthen, May 20–22.
41. ———, *An approach to multi-phase flows in geosciences*, MURPHYS-HSFS 2019 Summer School on Multi-Rate Processes, Slow-Fast Systems and Hysteresis, Turin, Italy, June 17–21.

A.9 Visits to other Institutions[5]

1. J. Sprekels, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 12–19.
2. L. Andreis, Junior Trimester Program: Randomness, PDEs and Nonlinear Fluctuations, Hausdorff Research Institute for Mathematics (HIM), Bonn, September 2 – December 19.
3. Ch. Bayer, Technische Universität Wien, Research Unit of Financial and Actuarial Mathematics, Austria, January 7–10.
4. ———, Osaka University, Graduate School of Engineering Science, Japan, February 12–22.
5. ———, Université Grenoble, Laboratoire Jean Kuntzmann, France, June 24–27.
6. ———, Rheinisch-Westfälische Technische Hochschule Aachen, Aachen Institute for Advanced Study in Computational Engineering Science (AICES), August 5–10.
7. ———, September 22–26.
8. F. Besold, Higher School of Economics (HSE), Faculty of Computer Science, Moscow, Russian Federation, February 20–23.
9. ———, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, October 24–30.
10. O. Butkovsky, Universität Bonn, Hausdorff Research Institute for Mathematics, October 1–5.
11. ———, Universität Bonn, Hausdorff Research Institute for Mathematics (HIM), November 25–29.
12. M. Coghi, Universität Konstanz, Fachbereich Mathematik und Statistik, February 4–8.
13. P.-É. Druet, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, April 1–4.
14. D. Dvinskikh, Moscow Institute of Physics and Technology, Department of Control/Management and Applied Mathematics, Moscow, Russian Federation, February 9 – March 2.
15. ———, July 8–13.
16. P. Dvurechensky, Moscow Institute of Physics and Technology, Department of Control/Management and Applied Mathematics, Russian Federation, April 18–24.
17. M. Eigel, Università della Svizzera italiana, Institute of Computational Science, Lugano, Switzerland, July 8–15.
18. P. Farrell, Xi'an Jiaotong-Liverpool University, Department of Mathematical Sciences, Suzhou, China, October 6–16.
19. M. Heida, Politechnico Milano, Dipartimento di Matematica, Italy, March 11–15.
20. ———, Guest Professorship, Technische Universität München, Fachbereich Analysis und Modellbildung, October 1, 2019 – March 31, 2020.
21. M. Hintermüller, University of Oxford, Mathematical Institute, UK, June 5–8.
22. ———, Polish Academy of Sciences, Systems Research Institute, Warsaw, Poland, December 2–5.
23. D. Hömberg, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, March 6–26.
24. ———, November 9–14.
25. ———, November 16–24.

[5] Only stays of more than three days are listed.

26. V. JOHN, Lahore University of Management Sciences, Department of Mathematics, Pakistan, August 22–30.
27. ———, Mathematisches Forschungsinstitut Oberwolfach, September 8–21.
28. ———, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, India, November 25 – December 5.
29. W. KÖNIG, New York University Shanghai, Institute of Mathematical Sciences, Shanghai, China, February 18 – March 1.
30. ———, Université de Nantes, Laboratoire Jean Leray, France, May 13–17.
31. R. LASARZIK, Università degli Studi di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, February 18–22.
32. P. MATHÉ, Technische Universität Chemnitz, Fachbereich Mathematik, August 12–16.
33. ———, Fudan University, School of Mathematical Sciences, Shanghai, China, October 7–25.
34. A. MIELKE, Charles University, Prague, Czech Republic, March 18–22.
35. G. NIKA, École Polytechnique, Laboratoire de Mécanique des Solides, Paris, France, March 18–22.
36. T. ORENSHTEIN, New York University Shanghai, Institute of Mathematical Sciences, Shanghai, China, November 12 – December 30.
37. R.I.A. PATTERSON, University of Cambridge, Faculty of Mathematics, UK, May 3–11.
38. C.N. RAUTENBERG, Philipps Universität Marburg, Fachbereich Mathematik und Informatik, May 14–17.
39. J. REHBERG, Technische Universität Darmstadt, Fachbereich Mathematik, February 4–8.
40. N. ROTUNDO, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, February 18–22.
41. ———, Università della Calabria, Cosenza, Italy, September 27 – October 4.
42. H. SI, Universidad de Chile, Department of Computer Science, Santiago, Chile, March 25 – April 5.
43. ———, Zhejiang University, Center for Engineering & Scientific Computation, Hangzhou, China, November 11–16.
44. ———, BeiHang University, School of Mathematics and Systems Science, Beijing, China, November 17–29.
45. V. SPOKOINY, Higher School of Economics (HSE), Faculty of Computer Science, Moscow, Russian Federation, February 18 – March 2.
46. ———, April 9–13.
47. ———, Huawei, Shanghai, China, June 4–8.
48. ———, Higher School of Economics (HSE), Faculty of Computer Science, Moscow, Russian Federation, July 17–31.
49. ———, September 14 – October 4.
50. L. TAGGI, Institute for Advanced Study, School of Mathematics, Princeton, USA, April 26 – May 11.
51. ———, Tel Aviv University, School of Mathematical Sciences, Israel, May 19–26.
52. ———, Université Paris-Est Créteil Val de Marne, Laboratoire d’Analyse et de Mathématiques Appliquées (LAMA) - UMR, France, July 7–12.
53. ———, Università degli Studi Roma Tre, Dipartimento di Matematica e Fisica, Italy, September 26 – October 4.
54. ———, Université Claude Bernard Lyon 1, Institut Camille Jordan (ICJ), France, November 12–15.

55. ———, Technische Universität Darmstadt, Fachbereich Mathematik, December 4–7.
56. M. Thomas, Università degli Studi di Brescia, Dipartimento di Ingegneria Civile Ambiente, Territorio Architettura e Matematica, Italy, March 11–14.
57. ———, Universität Wien, Fakultät für Mathematik, Austria, April 8–12.
58. ———, Guest Professorship, Universität Kassel, FB 10 Mathematik und Naturwissenschaften, October 1, 2019 – March 31, 2020.
59. ———, University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK, October 8–11.
60. P. Vágner, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, April 3–9.
61. ———, June 17–21.
62. ———, University of Chemistry and Technology, Institute of Anorgani-Technology, Prague, Czech Republic, July 9–23.
63. ———, December 16–20.
64. W. van Zuijlen, Université de Nantes, Laboratoire Jean Leray, France, May 13–17.
65. ———, Radboud University Nijmegen, Department of Mathematics, Netherlands, August 22–26.
66. ———, Junior Trimester Program: Randomness, PDEs and Nonlinear Fluctuations, Hausdorff Research Institute for Mathematics (HIM), Bonn, September 2 – November 30.
67. ———, Radboud University Nijmegen, Department of Mathematics, Netherlands, December 19–30.
68. B. Wagner, University of Oxford, Mathematical Institute, UK, June 27 – July 5.

A.10 Academic Teaching[6]

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. 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. W. König, *Analysis III für Mathematikerinnen und Mathematiker* (lecture), Technische Universität Berlin, 4 SWS.
16. O. Marquardt, *Grundlagen der medizinischen Messtechnik* (lecture), Beuth Hochschule für Technik Berlin, 2 SWS.
17. B. Moreau, *Computational Fluid Dynamics* (practice), Beuth Hochschule für Technik Berlin, 2 SWS.
18. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
19. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
21. M. Wolfrum, B. Fiedler, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

[6] SWS = semester periods per week

Summer Semester 2019

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. A. Caiazzo, *Analysis 1* (lecture), Freie Universität Berlin, 4 SWS.
4. ———, *Analysis 1* (practice), Freie Universität Berlin, 2 SWS.
5. P. Friz, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
6. ———, *Maß- und Integrationstheorie* (practice), Technische Universität Berlin, 2 SWS.
7. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
8. P. Friz, M. Coghi, *Maß- und Integrationstheorie* (lecture), Technische Universität Berlin, 4 SWS.
9. A. Glitzky, A. Mielke, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
10. M. Heida, *Analysis I und Lineare Algebra für Ingenieurwissenschaften* (lecture), Technische Universität Berlin, 4 SWS.
11. ———, *Analysis I und Lineare Algebra für Ingenieurwissenschaften* (practice), Technische Universität Berlin, 2 SWS.
12. M. Hintermüller, *Ausgewählte Themen der Optimierung* (lecture), Humboldt-Universität zu 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. D. Hömberg, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
15. B. Jahnel, W. König, *Introduction to Probability (15 two-hour lectures from Sep. 16 to Oct. 4)* (lecture), African Institute for Mathematical Sciences — Ghana (AIMS Ghana), – SWS.
16. V. John, *Numerik III* (lecture), Freie Universität Berlin, 4 SWS.
17. R. Lasarzik, *Differentialgleichungen III* (lecture), Technische Universität Berlin, 4 SWS.
18. O. Marquardt, *Brückenkurs Physik (10 ninety-minute lectures from March 23 to 27, 2019)* (lecture), Beuth Hochschule für Technik Berlin, - SWS.
19. ———, *Brückenkurs Physik (10 ninety-minute lectures from September 23 to 27, 2019)* (lecture), Beuth Hochschule für Technik Berlin, - SWS.
20. A. Mielke, *Partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
21. K. Papafitsoros, *Ausgewählte Themen der Optimierung* (practice), Humboldt-Universität zu Berlin, 1 SWS.
22. V. Spokoiny, *Mathematische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
23. ———, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
24. ———, *Mathematische Statistik* (practice), Humboldt-Universität zu Berlin, 2 SWS.
25. V. Spokoiny, W. Härdle, M. Reiss, G. Blanchard, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
26. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.

27. M. Wolfrum, B. Fiedler, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin, 2 SWS.

Winter Semester 2019/2020

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. P. Dvurechensky, *Recent Developments in Optimization Methods and Machine Learning Applications* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
3. ———, *Recent Developments in Optimization Methods and Machine Learning Applications* (practice), Humboldt-Universität zu Berlin, 1 SWS.
4. M.H. Farshbaf Shaker, *Optimalsteuerung bei partiellen Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS.
5. P. Friz, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
6. ———, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
7. P. Friz, Ch. Bayer, *Rough Volatility, Rough Paths and Related Topics* (lecture), Technische Universität Berlin, 2 SWS.
8. J. Fuhrmann, *Wissenschaftliches Rechnen (Scientific Computing)* (lecture), Technische Universität Berlin, 4 SWS.
9. A. Glitzky, *Ausgewählte Themen der Optimierung (M23): Einführung in die Kontrolltheorie und optimale Steuerung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. ———, *Ausgewählte Themen der Optimierung (M23): Einführung in die Kontrolltheorie und optimale Steuerung* (practice), Humboldt-Universität zu Berlin, 1 SWS.
11. A. Glitzky, A. Mielke, B. Zwicknagl, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
12. M. Heida, *Homogenization* (lecture), Technische Universität München, 2 SWS.
13. ———, *Nonlinear Analysis* (lecture), Technische Universität München, 4 SWS.
14. ———, *Nonlinear Analysis* (practice), Technische Universität München, 2 SWS.
15. M. Hintermüller, *Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
16. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
17. O. Klein, *Ausgewählte Themen der angewandten Analysis (M38): Mathematische Modellierung von Hystereseeffekten* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
18. ———, *Ausgewählte Themen der angewandten Analysis (M38): Mathematische Modellierung von Hystereseeffekten* (practice), Humboldt-Universität zu Berlin, 1 SWS.
19. A. Mielke, *Mehrdimensionale Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
20. ———, *Mehrdimensionale Variationsrechnung* (practice), Humboldt-Universität zu Berlin, 2 SWS.
21. D. Peschka, *Numerische Mathematik II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
22. H. Si, *Block Lecture: Introduction to Unstructured Mesh Generation Methods (32 forty-minute lectures from December 16 to 26, 2019)* (lecture), Zhejiang University, – SWS.

23. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.

24. V. Spokoiny, W. Härdle, M. Reiss, S. Greven, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/Universität Potsdam/WIAS Berlin, 2 SWS.

25. H. Stephan, *Funktionalanalytische Methoden in der klassischen Physik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.

26. ———, *Funktionalanalytische Methoden in der klassischen Physik* (practice), Humboldt-Universität zu Berlin, 1 SWS.

27. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.

28. M. Thomas, *Funktionalanalysis* (lecture), Universität Kassel, 4 SWS.

29. ———, *Nichtlineare Funktionalanalysis* (lecture), Universität Kassel, 4 SWS.

30. 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. A. Acharya, Carnegie Mellon University, Civil and Environmental Engineering, Pittsburgh, USA, June 15–20.
2. N. Ahmed, Lahore University of Management Sciences, Department of Mathematics, Syed Babar Ali School of Sciences & Engineering, Pakistan, January 7–18.
3. G. Alì, University of Calabria, Department of Physics, Cosenza, Italy, January 28 – February 7.
4. G. Antunes Monteiro, Tschechische Akademie der Wissenschaften, Prag, Czech Republic, June 3–7.
5. R. Arndt, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – September 30.
6. D. Belomestny, Universität Duisburg-Essen, Fachbereich Mathematik, Essen, May 28 – June 3.
7. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, August 16–26.
8. H. Berthold, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Optimierung, Kaiserslautern, February 18–22.
9. M. Brokate, Technische Universität München, Zentrum Mathematik, Garching, July 8 – December 31.
10. C. Butucea, Université Paris-Est Marne-la-Vallée, Laboratoire d'Analyse et de Mathématiques Appliquées, Marne-la-Vallée, France, November 5–9.
11. D. Camargo, The Weizmann Institute of Science, Faculty of Mathematics and Computer Science, Rehovot, Israel, January 6–12.
12. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modelling, Vilnius, Lithuania, February 4–8.
13. ———, June 10–21.
14. P. Colli, Università di Pavia, Dipartimento di Matematica "F. Casorati", Pavia, Italy, May 19–25.
15. P. Das, EFD Induction AS, Skien, Norway, November 19, 2018 – January 23, 2019.
16. ———, April 8–20.
17. ———, December 9–12.
18. G. Dong, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – October 31.
19. R. Eisenberg, Rush University Chicago, Department of Physiology & Biophysics, USA, May 8–18.
20. I. Franovic, University of Belgrade, Institute of Physics Belgrade, Serbia, June 2–15.
21. K. Gambaryan, Yerevan State University, Faculty of Radiophysics, Chair of Semiconductor and Microelectronics, Armenia, July 5 – September 1.
22. A. Gasnikov, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, January 2 – February 7.
23. ———, August 2–25.
24. ———, September 30 – October 10.
25. ———, November 4–21.
26. B. Gaudeul, Université de Lille, Laboratoire Paul Painlevé, France, November 4–15.

[7] Only stays of more than three days are listed.

27. A.K. Giri, Indian Institute of Technology Roorkee, Department of Mathematics, India, June 22 – July 14.
28. B. Grund, University of Minnesota, School of Statistics, Minneapolis, USA, July 8–19.
29. S. Guminov, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, August 1–16.
30. P. Hager, Technische Universität Berlin, Institut für Mathematik, May 6, 2019 – April 30, 2020.
31. A. Hajizadeh, Leibniz-Institut für Neurobiologie Magdeburg, Speziallabor Nicht-Invasive Bildgebung, March 25 – April 11.
32. ———, June 24–28.
33. E.J. Hall, Rheinisch-Westfälische Technische Hochschule Aachen, Fachgruppe Mathematik, Aachen, January 21–25.
34. M. Heinkenschloss, Rice University, Department of Computational and Applied Mathematics, Houston, Texas, USA, March 13–16.
35. L. Heltai, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, January 28 – February 1.
36. ———, April 23 – May 3.
37. ———, June 1 – July 31.
38. ———, October 21 – November 8.
39. M. Hennessy, University of Oxford, Mathematical Institute, Oxford, UK, July 23–26.
40. Ch. Hirsch, Universität Mannheim, Institut für Mathematik, June 18–21.
41. ———, December 20–23.
42. N. Hitschfeld Kahler, Universdad de Chile, Department of Computer Science, Santiago, Chile, December 1–13.
43. H. Hoel, King Abdullah University of Science and Technology, Department of Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, January 21–25.
44. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, Chemnitz, March 11–15.
45. J. Holley, Robert Bosch GmbH, April 1, 2017 – March 31, 2020.
46. G. Hu, Beijing Computational Science Research Center, China, September 20 – October 20.
47. O. Huber, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – December 31.
48. A. Ivanova, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, August 1–16.
49. T. Jahn, Goethe-Universität Frankfurt am Main, Informatik und Mathematik, Frankfurt, October 28 – November 1.
50. L. Jie, University of Cambridge, Department of Engineering, UK, April 14–20.
51. A. Jüngel, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, October 22–25.
52. D. Kamzolov, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, August 19–31.
53. A. Kebaier, Université Paris 13, Laboratoire Analyse, Géométrie et Applications, Villetaneuse, France, January 20–23.

54. V. Kempf, Universität der Bundeswehr München, Institut für Mathematik und Computergestützte Simulation, Neubiberg, February 25 – March 1.
55. Y. Klochkov, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, International Research Training Group (IRTG) 1792 “High Dimensional Non Stationary Time Series”, January 1 – March 31.
56. M. Kniely, Institute of Science and Technology Austria (IST Austria), Klosterneuburg, Austria, November 4–29.
57. R. Kravchenko, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, July 1, 2019 – December 31, 2021.
58. J. Lelong, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, St Martin d’Hères, France, April 15–18.
59. M. Malamud, Peoples’ Friendship University of Russia (RUDN University), Moscow, Russian Federation, April 30 – May 5.
60. E. Meca Álvarez, University of Cordoba, Agronomy Department, Spain, October 23–26.
61. M. Milicevic, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, April 22–26.
62. Ch. Mönch, Johannes-Gutenberg-Universität, Institut für Mathematik, Mainz, October 14–17.
63. A. Montefusco, Eidgenössische Technische Hochschule Zürich, Institut für Polymere, Zürich, Switzerland, November 4–8.
64. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, April 1–17.
65. ———, July 23 – August 2.
66. ———, December 9–13.
67. Ch. Onyi, Nnamdi Azikiwe University Awka, Department of Mathematics, Awka, Nigeria, September 26, 2017 – November 29, 2019.
68. P. Pigato, University of Rome Tor Vergata, Department of Economics and Finance, Rome, Italy, November 28, 2019 – February 29, 2020.
69. Ch. Rackauckas, Massachusetts Institute of Technology, Department of Mathematics, University of Maryland, Center for Translational Medicine, Baltimore, USA, November 2–6.
70. S. Ramesh Babu, SSAB Europe Oy, Raahe, Finland, January 2–12.
71. V. Romano, University of Catania, Department of Mathematics and Informatics, Catania, Italy, January 27 – February 2.
72. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, November 18 – December 18.
73. Ch. Schelte, University of the Balearic Islands, Department of Physics, Palma, Spain, February 1 – April 2.
74. St. Schulz, Tyndall National Institute, Integrated ICT Hardware & Systems, Cork, Ireland, January 21–25.
75. O. Sekulovic, Crnogorski Telecom, Podgorica, Montenegro, May 5–12.
76. U. Sharma, CERMICS, École des Ponts ParisTech, Marne-la-Vallée, France, June 18–21.
77. E. Shulgin, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, August 2–23.
78. R. Soares dos Santos, New York University Shanghai, Institute of Mathematical Sciences, Institute of Mathematical Sciences, Pudong Xinqu, Shanghai Shi, China, July 22 – August 3.
79. G. Stadler, New York University, Courant Institute of Mathematical Sciences, New York, USA, June 3 – July 31.

80. Y. Sun, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, October 1, 2018 – September 30, 2020.
81. Th. Surowiec, Philipps-Universität Marburg, Mathematik und Informatik, Marburg, July 5–8.
82. A. Suvorikova, Universität Potsdam, Institut für Mathematik, September 1, 2018 – August 31, 2019.
83. F.J.E. Telschow, University of California San Diego, Department of Family and Preventive Medicine, La Jolla CA, USA, March 1 – December 31.
84. R.F. Tempone, King Abdullah University of Science and Technology, Department of Applied Mathematics and Computational Science, Thuwal, Saudi Arabia, January 16–22.
85. A. ter Elst, The University of Auckland, Department of Mathematics, New Zealand, November 2–30.
86. P. Tolksdorf, Université Paris-Est — Créteil Val-de-Marne, Laboratoire d'Analyse et de Mathématiques Appliquées, France, May 28 – June 6.
87. N. Torri, Université Paris Nanterre, Laboratoire d'Analyse et de Mathématiques, Nanterre, France, October 28 – November 1.
88. B. Vignaud, University Claude Bernard Lyon 1, Department of Mathematics, Villeurbanne, France, April 8 – August 9.
89. A. Visintin, Università di Trento, Dipartimento di Matematica, Trento, Italy, July 8–14.
90. M. Walloth, Technische Universität Darmstadt, Fachbereich Mathematik, Arbeitsgruppe Numerik und Wissenschaftliches Rechnen, May 12–17.
91. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, October 2–8.
92. Y.-X. Yuan, Chinese Academy of Sciences, AMSS, Beijing, China, August 2–9.
93. M. Zajnulina, Aston University, School of Engineering and Applied Science, UK, October 7–25.
94. J. Zimmer, University of Bath, Mathematical Sciences, UK, November 4 – December 18.

A.11.2 Scholarship Holders

1. A.K. Giri, Indian Institute of Technology Roorkee, Department of Mathematics, Roorkee, India, DAAD Fellowship, June 22 – July 14.
2. A. Jha, New Delhi, India, Berlin Mathematical School, October 1, 2017 – December 31, 2019.
3. Ch. Kwofie, University of Energy and Natural Resources, Sunyani, Ghana, DAAD Fellowship, February 1, 2018 – June 30, 2021.
4. J. Neumann, Berlin, EXIST Business Start-up Grant, September 1, 2018 – August 31, 2019.
5. Ch. Onyi, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, Berlin Mathematical School, October 1, 2017 – November 29, 2019.
6. A. Visram, Berlin, EXIST Business Start-up Grant, September 1, 2018 – August 31, 2019.
7. 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 – February 18.

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 1–30.
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 – March 31.
7. R. KRAVCHENKO, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. V. Spokoiny, MATH+, doctoral candidate, July 1 – December 31.
8. 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. Acharya, Carnegie Mellon University, Civil and Environmental Engineering, Pittsburgh, USA, *Line defect dynamics and solid mechanics*, June 18.
2. N. Ahmed, Lahore University of Management Sciences, Department of Mathematics, Syed Babar Ali School of Sciences & Engineering, Pakistan, *Numerical comparisons of finite element stabilized methods for a 2D vortex dynamics simulation at high Reynolds number*, January 10.
3. G. Antunes Monteiro, Tschechische Akademie der Wissenschaften, Prag, Czech Republic, *On the convergence of viscous approximation for rate-independent processes with regulated inputs*, June 4.
4. M.S. Aronna, Technische Universität Berlin, Institut für Mathematik, *On second order optimality conditions for control-affine problems: The finite and infinite dimensional case*, January 23.
5. D. Belomestny, Universität Duisburg-Essen, Fachbereich Mathematik, Essen, *Density deconvolution under general assuptions on measurement error distribution*, May 29.
6. P. Berg, University of Alberta, Department of Science, Canada, *Energy conversion in electrokinetic flow through charged and viscoelastic nanochannels*, May 17.
7. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, *Homogenization problems with non-separated scales*, January 18.
8. M. Brokate, Technische Universität München, Zentrum Mathematik, Garching, *Sensitivity in rate independent evolutions*, September 26.
9. D. Camargo, The Weizmann Institute of Science, Faculty of Mathematics and Computer Science, Rehovot, Israel, *The meteor process stationary distribution*, January 11.
10. M. Chernysheva, Leibniz Institute of Photonic Technology, Ultrafast Fiber Lasers, Jena, *Highlights of pulse generation and dynamics in mode-locked all-fibre and SOA-based fibre lasers*, May 23.
11. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modelling, Vilnius, Lithuania, *Numerical simulation of models with the memory effects: Diffusion, heat conduction, nonlinear optics*, February 7.
12. P. Colli, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Pavia, Italy, *Well-posedness, regularity and asymptotic analyses for a fractional phase field system*, May 22.
13. F. Della Porta, Max-Planck-Institut für Mathematik in den Naturwissenschaften Leipzig, Research Group “Rigidity and Flexibility in PDEs”, *The nonlocal Cahn–Hilliard–Hele–Shaw system with regular and singular potential*, June 12.
14. E.V. Denning, Technical University of Denmark, Department of Photonics Engineering, Kgs. Lyngby, Denmark, *Accurate few-mode models of highly structured photonic reservoirs*, August 19.
15. G. Dong, Humboldt-Universität zu Berlin, Institut für Mathematik, *Quantitative magnetic resonance imaging: From fingerprinting to integrated physics-based models*, June 3.
16. R. Eisenberg, Rush University Chicago, Department of Physiology & Biophysics, USA, *Voltage sensors of biological channels are nanomachines that perfectly conserve current, as Maxwell defined it*, May 16.
17. Y. Fournier, Leibniz-Institut für Astrophysik Potsdam, Kosmische Magnetfelder, Magnetohydrodynamik und Turbulenz, *Non-local effects in the solar dynamo*, September 3.
18. Ch. Freysoldt, Max-Planck-Institut für Eisenforschung GmbH, Computergestütztes Materialdesign, Düsseldorf, *Concepts and algorithms in SPHInX*, May 9.
19. S. Gailus, Hausdorff Institute for Mathematics/Boston University, Bonn, *Homogenization of multiscale diffusion processes with small noise*, December 18.

20. N. Gantert, Technische Universität München, Fakultät für Mathematik, *Consensus and disagreement in opinion dynamics*, June 26.

21. V.A. Garanzha, Federal Research Center “Computer Science and Control” of the Russian Academy of Sciences, Dorodnicyn Computing Center, Moscow, Russian Federation, *Moving adaptive meshes based on the hyperelastic stress deformation*, January 23.

22. A. Gasnikov, Moscow Institute of Physics and Technology (MIPT), Department of Control/Management and Applied Mathematics, Dolgoprudny, Moscow Region, Russian Federation, *Adaptive accelerated stochastic gradient descent*, January 15.

23. B. Gaudeul, Université de Lille, Laboratoire Paul Painlevé, France, *Some numerical schemes for a reduced case of a Nernst–Planck–Poisson model*, November 7.

24. A.K. Giri, Indian Institute of Technology Roorkee, Department of Mathematics, India, *Recent developments in the theory of coagulation-fragmentation models*, July 2.

25. C. Gräser, Freie Universität Berlin, Institut für Mathematik, *Truncated nonsmooth Newton multigrid for nonsmooth minimization problems*, July 9.

26. J. Gravesen, Technical University of Denmark, Department of Applied Mathematics and Computer Science, Kgs. Lyngby, Denmark, *Differential geometry and dimension reduction for nano structures*, June 24.

27. M. Gunzburger, Florida State University, Dept. of Scientific Computing, Tallahassee, USA, *Four “better” ways to solve the Navier–Stokes equations: Simulation of Richardson pair dispersion, ensemble discretization methods, an auxiliary equation approach for UQ, and filtered regularizations*, October 31.

28. A. Hajizadeh, Leibniz-Institut für Neurobiologie Magdeburg, Speziallabor Nicht-Invasive Bildgebung, *Computational modelling of signal processing in the human auditory cortex: Analytical solutions based on cortical network structure and oscillatory dynamics*, March 28.

29. A. Hazra, Tata Institute of Fundamental Research, Centre for Applicable Mathematics, Bangalore, India, *Globally constraint-preserving FR/DG scheme for Maxwell’s equations up to fifth order of accuracy*, July 11.

30. L. Heltai, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, *Unconventional frameworks for the simulation of coupled bulk-interface problems*, June 25.

31. N. Hitschfeld Kahler, Universdad de Chile, Department of Computer Science, Santiago, Chile, *GPU computing and meshing*, December 12.

32. M. Holler, Universität Graz, Institute of Mathematics and Scientific Computing, Austria, *A variational model for learning convolutional image atoms from incomplete data*, October 23.

33. G. Hu, Beijing Computational Science Research Center, China, *Corner scattering theory and data-driven inversion schemes*, October 7.

34. L. Jie, University of Cambridge, Department of Engineering, UK, *Macroscopic model for head-on binary droplet collisions in a gaseous medium*, April 16.

35. A. Jüngel, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, *Cross-diffusion systems: From spin semiconductors to biological populations with stochastic forcing*, October 23.

36. A. Kebaier, Université Paris 13, Laboratoire Analyse, Géométrie et Applications, Villetaneuse, France, *Asymptotic properties of maximum likelihood estimator for the drift parameters of jump-type square root processes*, January 22.

37. M. Kniely, Institute of Science and Technology Austria (IST Austria), Klosterneuburg, Austria, *On the large-time behavior of a class of semiconductor equations*, November 13.

38. O. KRIVOROTKO, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, Russian Federation, *Regularization of multi-parametric inverse problems for differential equations arising in immunology, epidemiology and economy*, November 12.
39. B. LEES, University of Bristol, School of Mathematics, UK, *The phase transition for random loop models on trees*, December 11.
40. J. LELONG, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, St Martin d'Hères, France, *Pricing path-dependent Bermudan options using Wiener chaos expansion: An embarrassingly parallel approach*, April 16.
41. S. METZNER, Physikalisch-Technische Bundesanstalt / TU Berlin, Mathematics Department, *Approximate large-scale Bayesian inference with application to magnetic resonance fingerprinting*, June 3.
42. M. MILICEVIC, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, *The alternating direction method of multipliers with variable step sizes for the iterative solution of nonsmooth minimization problems and application to BV-damage evolution*, April 23.
43. CH. MÖNCH, Johannes-Gutenberg-Universität, Institut für Mathematik, Mainz, *Universality of persistence exponents for self-similar processes with stationary increments*, October 16.
44. P. NEIJJAR, Institute of Science and Technology Austria (IST Austria), Klosterneuburg bei Wien, Austria, *Product limit laws at shocks in (T)ASEP*, February 13.
45. M. PAVELKA, Charles University Prague, Mathematical Institute, Czech Republic, *Symmetric Hyperbolic Thermodynamically Compatible (SHTC) equations within GENERIC*, December 3.
46. V. ROMANO, University of Catania, Department of Mathematics and Informatics, Catania, Italy, *Charge and phonon transport in graphene*, January 29.
47. T. ROUBÍČEK, Charles University Prague, Mathematical Institute, Czech Republic, *Fully convective models of some processes in the Earth*, November 27.
48. CH. SCHELTE, University of the Balearic Islands, Department of Physics, Palma, Spain, *Bistability and solitons in an injected time-delayed Kerr microcavity*, March 28.
49. K. SCHRATZ, Heriot-Watt University Edinburgh, UK, Department of Mathematics, Edinburgh, UK, *Nonlinear Fourier integrators for dispersive equations and beyond*, December 9.
50. P. SCHROEDER, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *Building bridges: Pressure-robust FEM, Beltrami flows and structure preservation in incompressible CFD*, February 14.
51. ST. SCHULZ, Tyndall National Institute, Integrated ICT Hardware & Systems, Cork, Ireland, *Electronic, optical and transport properties of III-N alloys and heterostructures: Insights from and challenges for theoretical modelling*, January 24.
52. J. SCHWIENTEK, H. BERTHOLD, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Optimierung, Kaiserslautern, *Numerical methods for (general) semi-infinite optimization*, February 19.
53. J. SPREKELS, Humboldt-Universität zu Berlin, Institut für Mathematik, *Optimal control of a Cahn–Hilliard–Darcy system with mass source modeling tumor growth*, December 18.
54. B. SPRUNGK, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, *Noise-level robust sampling methods for Bayesian inverse problems*, May 28.
55. G. STADLER, New York University, Courant Institute of Mathematical Sciences, New York, USA, *Estimation of extreme event probabilities by combining large deviation theory and PDE-constrained optimization, with application to tsunami waves*, July 10.
56. ———, *Sparse optimal control of PDEs with uncertain coefficients*, July 11.

57. L. STRENGE, Technische Universität Berlin, Fachgebiet Regelungssysteme, *A multilayer, multi-timescale model approach for economic and frequency control in power grids using Julia*, December 19.

58. R. STYLE, ETH Zürich, Department of Materials, Zürich, Switzerland, *Arresting phase separation with polymer networks*, July 25.

59. F.J.E. TELSCHOW, University of California San Diego, Department of Family and Preventive Medicine, La Jolla, CA, USA, *Estimation of expected Euler characteristics of non-stationary Gaussian random fields*, May 21.

60. A.F.M. TER ELST, The University of Auckland, Department of Mathematics, New Zealand, *The Dirichlet-to-Neumann operator on* $C^{1+\kappa}$ *-domains*, November 20.

61. U. THIELE, Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, *Gradient dynamics models for films of complex fluids and beyond – Dewetting, line deposition and biofilms*, February 28.

62. P. TOLKSDORF, Université Paris-Est – Créteil Val-de-Marne, Laboratoire d'Analyse et de Mathématiques Appliquées, France, *On the Lp-theory for second-order elliptic operators in divergence-form with complex coefficients (Part 1)*, May 29.

63. ———, *On the Lp-theory for second-order elliptic operators in divergence-form with complex coefficients (Part 2)*, June 5.

64. N. TORRI, Université Paris Nanterre, Laboratoire d'Analyse et de Mathématiques, Nanterre, France, *Directed polymer in a heavy-tail random environment*, October 30.

65. G.L. TORRISI, Istituto per le Applicazioni del Calcolo "Mauro Picone" (C.N.R), Rome, Italy, *The Clark–Ocone formula for point processes*, March 27.

66. J. TRANTOW, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, *A pseudo time-stepping approach for the evolution of elastic curves*, July 30.

67. A. USCHMAJEW, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Tensors and Optimization, Leipzig, *Optimization on low-rank manifolds*, December 16.

68. M. WALLOTH, Technische Universität Darmstadt, Fachbereich Mathematik, Arbeitsgruppe Numerik und Wissenschaftliches Rechnen, *Reliable, efficient and robust a posteriori estimators for the variational inequality in fracture phase-field models*, May 14.

69. M. YAMAMOTO, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Inverse problems for first-order transport equations by Carleman estimates*, October 7.

70. Y.-X. YUAN, Chinese Academy of Sciences, Academy of Mathematics and Systems Science, Beijing, China, *Efficient optimization algorithms for large scale data analysis*, August 2.

71. J. ZIMMER, University of Bath, Mathematical Sciences, Bath, UK, *Regularisation and analysis of Dean–Kawasaki-type equations*, November 27.

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.

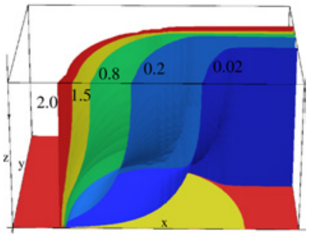
`ParMooN` is a joint development with the group of Prof. S. Ganesan (IISc Bangalore) and the group of Prof. G. Matthies (TU Dresden).

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

`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/.

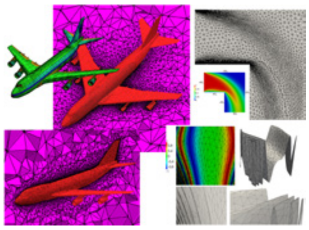


Concentration isosurfaces in a thin-layer flow cell (`pdelib`)

TetGen (contact: H. Si, phone: +49 30/20372-446, e-mail: hang.si@wias-berlin.de)

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

More information is available at https://www.wias-berlin.de/software/tetgen/.



Adapted tetrahedral meshes and anisotropic meshes for numerical methods and scientific computation

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).

`qmri` is the third R-package in this collection that contains functions for the analysis of magnetic resonance imaging data acquired in the multi-parameter mapping framework. This includes the estimation of quantitative model parameters, structural adaptive smoothing methods for noise reduction, and methods for performing a bias correction caused by the low signal-to-noise ratio.

The three R-packages of this collection are included in the Neuroconductor platform for reproducible computational imaging software (https://neuroconductor.org).