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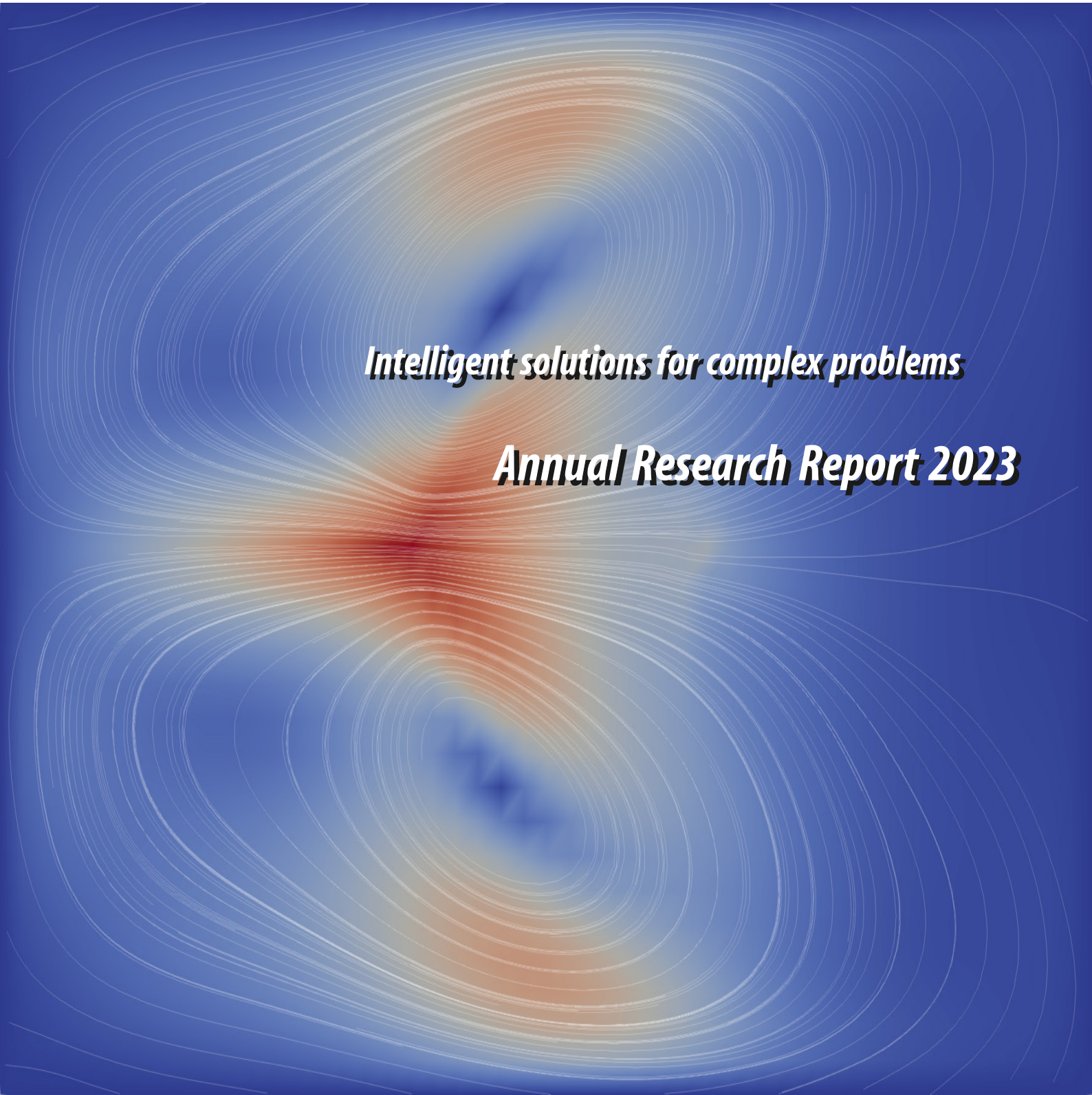

Intelligent solutions for complex problems

Annual Research Report 2023

Cover figure: The plot shows the simulated velocity field in an anisotropic electrolyte, where the flow is induced by an external, alternating electric field. The simulation is based on a finite element discretization of an anisotropic Navier–Stokes–Nernst–Planck–Poisson system and aims at visualizing the capability of this coupled nonlinear PDE system to capture experimentally observed flow properties of such an electrolyte.

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Prof. Michael Hintermüller, Director

The Weierstrass Institute for Applied Analysis and Stochastics, Leibniz Institute in Forschungsverbund Berlin e. V. (WIAS, member of the Leibniz Association), presents its Annual Research Report 2023. Besides a selection of our scientific highlights of the year, one finds figures and facts on the Institute's performance.

In 2023, several career-related strategic concepts and documents were passed. These include the new WIAS Human Resources Development Concept along with an agile list of measures, a buddy and mentoring program for the onboarding of new members and for supporting early-career researchers at WIAS, and, last but not least, the WIAS Alumni Program.

While WIAS currently has a percentage of 40% females among its Ph.D. students, there are still concerns about gender equality at later career stages. Consequently, the updated Equal Opportunities Plan for the years 2024–2027 develops corresponding goals and strategic measures—with the new Iris Runge Program being the most prominent and comprehensive one—to improve the situation.

Scientific research at WIAS was thriving also in 2023. Here, I only highlight (i) WIAS hosting the 175th European Study Group with Industry, Europe's leading workshop bringing together mathematicians and industrial companies, from September 18 to 22, 2023, (ii) the start of a new Weierstrass Group on *Multi-species Balance Laws*, led by Dr. Katharina Hopf, and (iii) the implementation of a new focus platform on *Simulation of Semiconductor Devices for Quantum Technologies* on WIAS's Flexible Research Platform.

The Mathematical Research Data Initiative (MaRDI) (a consortium of the National Research Data Infrastructure NFDI) coordinated by WIAS, published a white paper in accordance with the rules of the German Research Foundation (DFG) in order to support the DFG project application process concerning research data management plans. Also, WIAS finalized a document on its new software development concept.

Several exciting visits were highlights of the year 2023. These included in particular a one-day exchange with Prof. Martina Brockmeier, the President of the Leibniz Association, in June, and a very warm welcome for Prof. Christoph Sorger, the new Secretary General of the International Mathematical Union (IMU) for the period 2023–2026.

WIAS continues to be among the five cooperation partners of the Cluster of Excellence Berlin Mathematics Research Center MATH+, with its Director as its new Chair since November 2022. The reporting year brought WIAS seven new MATH+ projects starting 2024.

65 and 75: These two numbers stand for events in 2023 connecting the past, present, and future of our Institute and the WIAS community. 65: In autumn, Prof. Alexander Mielke, one of our scientific and leadership pillars, has retired and handed over the leadership of Research Group 1 *Partial Differential Equations* to Dr. Matthias Liero, who will act on this position until a successor has been found. Alexander Mielke has now accepted to be an Honorary Member of the Institute. 75: In a wonderful event in late autumn, we had the opportunity to celebrate the 75th birthday of the former WIAS Director, Prof. Jürgen Sprekels. The much enjoyed event gathered several generations of researchers.

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.

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 February 2024

M. Hintermüller

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1 Scientific Highlights

- Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes
- Phase Transitions in Random Graphs
- Spin-Qubit Shuttles for Scalable Semiconductor Quantum Computers: Modeling, Simulation and Optimal Control
- Symmetrization in Cross-diffusions
- Solving Parametric PDEs with Neural Networks
- Data-driven Regularization and Quantitative Imaging

1.1 Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes

Dirk Peschka and Marita Thomas

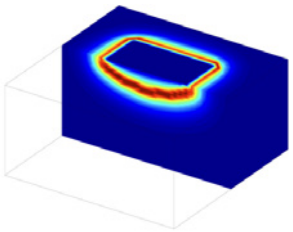


Fig. 1: *Numerical simulation of a conchoidal fracture, see 10.1002/zamm.201900288*

Modern devices and materials are heterogeneous and posses a bulk-interface structure. They are composed of different materials joined by thin interfacial layers—lower-dimensional substructures that substantially influence a system's overall functionality. For example, biological tissue is made of cells including fluidic phases and protein clusters, separated by semipermeable membranes. Metals and rocks consist of crystal grains with different orientation, forming grain boundaries between them. Electronic devices are made of layers of different semiconductor materials, forming interfaces where different materials meet. In all these examples, the interfaces strongly impact the functionality of the whole system: They influence and regulate heat and mass transport, chemical reactions, the response to mechanical forces, optical properties, and electric currents between neighboring bulk phases. Thus, interface processes and bulk processes are always coupled.

The shape of a sliding liquid droplet is determined by surface energies and by its interaction with an underlying substrate by interfacial friction; cf. Figure 5. The growth of cracks in solid materials can be seen as the creation of new material surfaces with complicated geometry that leads to a release of strain energy; cf. Figure 1. The optical emission of a laser can be substantially enhanced by suitably including thin insulating layers to guide electronic charges into the optically active region; cf. Figure 2. These are only three of the examples of systems with bulk-interface interaction that have been studied mathematically by the Weierstrass Group "Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes" (WG BIP) within several third-party-funded projects, in particular within the DFG Priority Programs SPP 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates*, SPP 1748 *Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretisation Methods, Mechanical and Mathematical Analysis*, SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*, the DFG Research Center MATHEON, ECMath – Einstein Center for Mathematics Berlin, and the Berlin Mathematics Research Center MATH+.

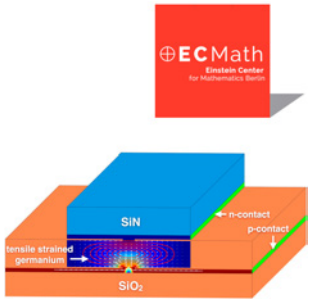
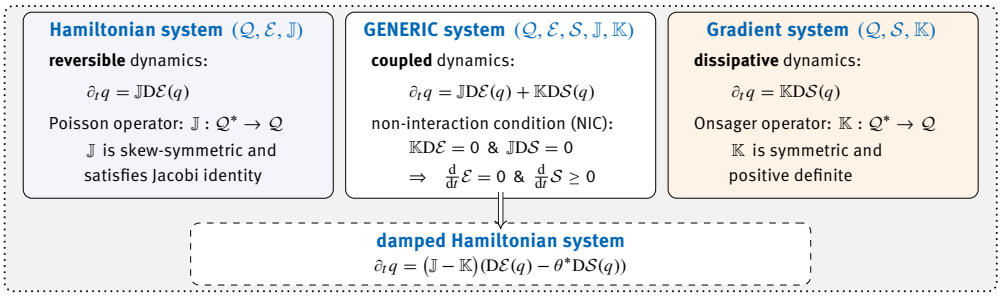


Fig. 2: *Ge laser: Thin insulating layers guide charges into the optically active region of the laser and enhance its light emission; see 10.1109/JPHOT.2015.2427093*

The Weierstrass Group WG BIP was funded for the period 04/2017–06/2023, and it was devoted to the development of mathematical methods for systems with bulk-interface interaction in different applications. For this, an overarching goal of WG BIP was the formulation of a general mathematical structure that supports the mathematical modeling and analysis of processes with bulk-interface coupling in a variational framework. This article highlights some research results that have been achieved by the group in that direction. It is based on joint works of Dirk Peschka (04/2017–09/2023, now RG 1 *Partial Differential Equations*) and Marita Thomas (04/2017–06/2023, now Freie Universität (FU) Berlin and RG 1) with the former group members Mohammad Hassan Farshbaf Shaker (01/2020–04/2022, now Hochschule für Technik und Wirtschaft Berlin), Xin Liu (01/2021–12/2021, now Texas A&M University), Sven Tornquist (07/2018–09/2022, now FU Berlin), Andrea Zafferi (07/2018–12/2022, now FU Berlin), and many collaborators.

Variational modeling of bulk-interface systems using GENERIC

The variational modeling framework of GENERIC, the acronym for General Equation of Non-Equilibrium Reversible Irreversible Coupling, was originally introduced by Miroslav Grmela and Hans Christian Öttinger in 1997 for thermodynamically closed systems with applications in fluid dynamics. In recent years, its versatility has been proved by different authors also for many other applications such as dissipative solids, complex and reactive fluids, semiconductors and electro-chemistry, quantum mechanics, and thermodynamical multiscale processes. In addition to its physical relevance for thermodynamically consistent modeling, GENERIC is beneficial for mathematicians due to its formulation using abstract operators, function spaces, and functionals. This establishes a sound foundation for mathematical analysis, facilitates the application of multiscale methods, and provides an effective framework to develop structure-preserving numerical solution strategies, particularly in the context of systems of nonlinearly coupled partial differential equations. A GENERIC system is characterized by a quintuple $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ consisting of a state space $\mathcal{Q}$, the two driving potentials: $\mathcal{E}$ the total energy and $\mathcal{S}$ the entropy, and two geometric structures: $\mathbb{J}$ a Poisson operator and $\mathbb{K}$ an Onsager operator. Simple structural properties and variants of GENERIC are illustrated schematically below.



Herein, the triple $(\mathcal{Q}, \mathcal{E}, \mathbb{J})$ forms a Hamiltonian system characterizing the reversible contributions to the dynamics, and the triple $(\mathcal{Q}, \mathcal{S}, \mathbb{K})$ forms a gradient system accounting for the irreversible, dissipative contributions. Both triples are coupled in a GENERIC system, constrained by the additional non-interaction conditions NIC. In thermodynamically closed systems, the NIC automatically ensures conservation of energy and positivity of the entropy production, i.e., the corresponding systems of equations are thermodynamically consistent by construction. The GENERIC evolution equation clearly displays the coupling of reversible and dissipative contributions. The thermodynamical driving forces are the functional derivatives $\mathrm{D}\mathcal{E}(q)$ for reversible dynamics and $\mathrm{D}\mathcal{S}(q)$ for dissipative dynamics. GENERIC for thermodynamically closed systems generalizes related concepts for energy-driven evolution, e.g., gradient flows for overdamped systems, Hamiltonian dynamics (symplectic flows) for reversible systems, or damped Hamiltonian dynamics for isothermal systems with temperature θ^*. For bulk-interface GENERIC forces $\mathrm{D}\mathcal{E}, \mathrm{D}\mathcal{S}$, and states q need to be divided into bulk and surface terms.

Bulk-interface GENERIC. One general aim of the WG BIP was to extend the GENERIC framework to systems with bulk-interface interaction. These are systems composed of two (or more) subsystems $\Omega_\pm \subset \mathbb{R}^d$, coupled with each other along a joint interface $\Gamma = \overline{\Omega}_+ \cap \overline{\Omega}_-$ through which they exchange quantities like heat, stresses, mass, etc. Along Γ, also additional processes may take

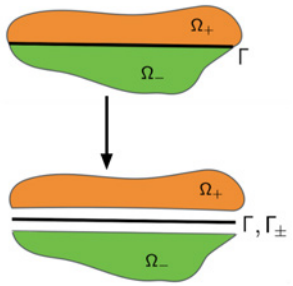


Fig. 3: *Bulk-interface system; derivatives of bulk functionals may produce interface contributions on Γ in terms of the traces on $\Gamma_\pm$ being part of the boundary of $\Omega_\pm$*

place that are modeled by additional state variables solely defined on Γ with individual evolution laws on Γ, but also driven by the interaction with the quantities from the bulk subdomains $\Omega_\pm$. While the compound $\Omega = \mathrm{int}(\overline{\Omega}_+ \cup \overline{\Omega}_-)$ can be assumed to form a thermodynamically closed system, none of the two individual subsystems $\Omega_\pm$ nor the interface Γ do so. Each of these components alone is an open system. A first approach to the GENERIC framework for thermodynamically open systems was proposed by Öttinger in 2006 using driving functionals and geometric structures for the bulk and the boundary components. Following this idea and, based on the definition of functional derivatives for integral functionals with bulk and interfacial contributions, it was proposed in [1] to regard the GENERIC formulation for bulk-interface processes in terms of a weak formulation:

$$\langle q^*, \partial_t q \rangle_{\mathcal{Q}} = \langle q_{\mathrm{B}}^*, \mathbb{J}_{\mathrm{B}} \mathrm{D}\mathcal{E}_{\mathrm{B}}(q) + \mathbb{K}_{\mathrm{B}} \mathrm{D}\mathcal{S}_{\mathrm{B}}(q) \rangle_{\mathrm{B}} + \langle q_{\Gamma\gamma}^*, \mathbb{J}_\Gamma \mathrm{D}\mathcal{E}_\Gamma(q) + \mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma(q) \rangle_\Gamma \tag{1}$$

for all suitable test functions $q^* = (q_{\mathrm{B}}^*, q_{\Gamma\gamma}^*)$. Above, $\langle \cdot, \cdot \rangle_{\mathrm{B}}$, $\langle \cdot, \cdot \rangle_\Gamma$ denote suitable dual pairings related to the function spaces on the bulk domain $\Omega \backslash \Gamma = \Omega_+ \cup \Omega_-$ and on the interface, where both trace spaces induced from the bulk and function spaces for the surface variables are involved. The state vector $q = (q_{\mathrm{B}}, q_\Gamma)$ now consists of variables q_{B} defined on $\Omega \backslash \Gamma$ and of surface variables q_Γ defined on Γ. Similarly, also the integral functionals representing energy, entropy, or (dual) dissipation of the bulk-interface system have bulk and surface contributions. More precisely, for $\Phi = \Phi_{\mathrm{B}} + \Phi_\Gamma$ as a placeholder for one of these integral functionals, we find that Φ is of the following form

$$\Phi(q) = \Phi_{\mathrm{B}}(q) + \Phi_\Gamma(q) := \int_{\Omega \backslash \Gamma} \phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) \, \mathrm{d}x + \int_\Gamma \phi_\Gamma(q_{\Gamma\gamma}) \, \mathrm{d}s \quad \text{with} \quad q_{\Gamma\gamma} := (\gamma_+ q_+, \gamma_- q_-, q_\Gamma),$$

where $q_\pm$ denotes the restriction of q_{B} to $\Omega_\pm$ and $\gamma_\pm q_\pm$ its trace on $\Gamma_\pm = \partial\Omega_\pm \cap \Gamma$ the part of the boundary of $\Omega_\pm$ that belongs to Γ. Accordingly, the functional derivative reads

$$\begin{aligned} \mathrm{D}\Phi(q)[\tilde{q}] = &\int_{\Omega \backslash \Gamma} \big(\partial_{q_{\mathrm{B}}} \phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) - \mathrm{div}\, \partial_{\nabla q_{\mathrm{B}}} \phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) \big) \tilde{q}_{\mathrm{B}} \, \mathrm{d}x \\ &+ \sum_{i \in \{+,-\}} \int_\Gamma \big(\partial_{\nabla q_i} \phi_{\mathrm{B}}(\gamma_i q_i, \gamma_i \nabla q_i) \mathrm{n}_i + \partial_{q_i} \phi_\Gamma(\gamma_+ q_+, \gamma_- q_-, q_\Gamma) \big) \gamma_i \tilde{q}_i \, \mathrm{d}s \\ &+ \int_\Gamma \partial_{q_\Gamma} \phi_\Gamma(\gamma_+ q_+, \gamma_- q_-, q_\Gamma) \tilde{q}_\Gamma \, \mathrm{d}s \end{aligned} \tag{2}$$

for all suitable test functions $\tilde{q}$. Regarding $\mathrm{D}\Phi(q)$ as a force acting on $\tilde{q}$, (2) states its split into bulk and interface forces. Similarly, also the Poisson and Onsager operators $\mathbb{J}$ and $\mathbb{K}$ are composed by a bulk and a surface contribution, which can only act on the corresponding bulk and surface terms of the driving forces $\mathrm{D}\mathcal{E}(q)$ and $\mathrm{D}\mathcal{S}(q)$. In view of (2), interfacial coupling conditions are thus displayed in the weak form of GENERIC (1) as a natural outcome.

Heat conduction as an example for bulk-interface GENERIC. As an example, we discuss here the Onsager structure for heat conduction taking into account different interfacial Onsager operators along Γ and thus resulting in different coupling conditions. The state vector $q_{\Gamma\gamma} = (\gamma_+ q_+, \gamma_- q_-)^\top$ here only accounts for the traces of the bulk variables, since there are no additional interfacial variables q_Γ with an evolution law described on the interface.

Heat conduction in the bulk $\Omega_+ \cup \Omega_-$ *:* The dual dissipation potential in the bulk is defined as

$$\Psi_{\mathrm{B}}^*(\theta;\cdot) : \mathcal{Q}^* \to \mathbb{R},\ \Psi_{\mathrm{B}}^*(\theta;\xi) := \sum_{i\in\{+,-\}} \int_{\Omega_i} \tfrac{\theta^2\kappa(\theta)}{2} \left|\nabla\left(\tfrac{\xi}{\mathrm{D}_\theta E}\right)\right|^2 \mathrm{d}x\,,$$

where $\mathcal{Q}^*$ denotes the dual space of a suitable Banach space $\mathcal{Q}$ and where the temperature θ is related to the energy and entropy densities E, S through the Gibbs relation $\theta = \frac{\mathrm{D}_\theta E}{\mathrm{D}_\theta S}$. Its functional derivative generates the bulk Onsager operator $\mathbb{K}_{\mathrm{B}}$, and it reads

$$\begin{aligned}\mathrm{D}_\xi \Psi_{\mathrm{B}}^*(\theta;\xi)[\tilde\xi] &= \sum_{i\in\{+,-\}} \int_{\Omega_i} -\operatorname{div}\left(\theta^2\kappa(\theta)\nabla\left(\tfrac{\xi}{\mathrm{D}_\theta E}\right)\right)\tfrac{\tilde\xi}{\mathrm{D}_\theta E}\mathrm{d}x + \int_{\Gamma_i} \gamma_i\left(\theta_i^2\kappa(\theta_i)\nabla\left(\tfrac{\xi_i}{\mathrm{D}_\theta E_i}\right)\right)\cdot \mathrm{n}_i\,\gamma_i\left(\tfrac{\tilde\xi_i}{\mathrm{D}_\theta E_i}\right)\mathrm{d}s \\ &=: \langle \mathbb{K}_{\mathrm{B}}(\theta)\,\xi, \tilde\xi\rangle_{\mathcal{Q}}\,.\end{aligned}$$

Here, $\gamma_i a_i$ denotes the trace of the function $a_i = a|_{\Omega_i}$ on the interface $\Gamma_i = \Gamma \cap \bar\Omega_i$ for $i \in \{+,-\}$.

Ideal heat transfer across the perfectly conducting interface Γ *:* At the perfectly conducting interface Γ, all quantities are continuous, which implies $\gamma_+\tilde\xi_+ = \gamma_-\tilde\xi_-$ for the test functions, and

$$\gamma_+\left(\tfrac{\theta_+^2\kappa_+(\theta_+)}{\mathrm{D}_\theta E_+}\nabla\left(\tfrac{\xi_+}{\mathrm{D}_\theta E_+}\right)\right)\cdot \mathrm{n}_+ = -\gamma_-\left(\tfrac{\theta_-^2\kappa_-(\theta_-)}{\mathrm{D}_\theta E_-}\nabla\left(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\right)\right)\cdot \mathrm{n}_-\,.$$

he first condition then is encoded in a suitable choice of the function space $\mathcal{Q}^*$. Integration by parts in $\langle \mathbb{K}_{\mathrm{B}}(\theta)\,\xi, \tilde\xi\rangle_{\mathcal{Q}}$ shows that the Onsager operator $\mathbb{K}_{\mathrm{B}}$ is symmetric and positively definite. Applying it to $\xi = \mathrm{D}E$ shows that also the non-interaction conditions are satisfied.

Heat transfer across the imperfect interface Γ *:* We assume that the heat transfer through Γ is regulated by the heat transfer coefficient $\hat\kappa_\Gamma(\gamma_+\theta_+, \gamma_-\theta_-)$. In this spirit, we introduce the quadratic dual dissipation potential along Γ, for every suitable $\xi_\gamma = (\xi_+, \xi_-)^\top$

$$\Psi_\Gamma^*(\theta_\gamma\,;\xi_\gamma) := \int_\Gamma \tfrac{\hat\kappa_\Gamma(\gamma_+\theta_+,\gamma_-\theta_-)}{2}\left|\gamma_+\left(\tfrac{\xi_+}{\mathrm{D}_\theta E_+}\right) - \gamma_-\left(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\right)\right|^2 \mathrm{d}s\,,$$

and we find for all suitable $\xi_\gamma\,, \tilde\xi_\gamma$ that

$$\begin{aligned}\mathrm{D}_{\xi_\gamma}\,\Psi_\Gamma^*(\theta_\gamma\,;\xi_\gamma)[\tilde\xi_\gamma] &= \int_\Gamma \hat\kappa_\Gamma(\theta_\gamma)\left(\gamma_+\left(\tfrac{\xi_+}{\mathrm{D}_\theta E_+}\right) - \gamma_-\left(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\right)\right)\left(\gamma_+\left(\tfrac{\tilde\xi_+}{\mathrm{D}_\theta E_+}\right) - \gamma_-\left(\tfrac{\tilde\xi_-}{\mathrm{D}_\theta E_-}\right)\right)\mathrm{d}s \\ &=: \langle\, \mathbb{K}_\Gamma(\theta_\gamma)\xi_\gamma\,, \tilde\xi_\gamma\,\rangle_{\tilde{\mathcal{Q}}_\Gamma}\,.\end{aligned}$$

Clearly, $\mathbb{K}_\Gamma(\theta_\gamma)$ is symmetric and positively semidefinite provided that $\hat\kappa_\Gamma(\theta_\Gamma) \geq 0$. Choosing $\xi_\gamma = (\mathrm{D}_\theta E_+, \mathrm{D}_\theta E_-)^\top$ above shows that also the non-interaction condition holds true. Thus, also the Onsager operator of the full system $\mathbb{K}(\theta) = \mathbb{K}_{\mathrm{B}}(\theta) + \mathbb{K}_\Gamma(\theta_\gamma)$ is symmetric, positively semidefinite, and satisfies the non-interaction conditions.

Now, the evolution equation of the system can be understood in a weak form (1), such that for a.a. $t \in (0,T)$ and for all $\tilde\xi \in \tilde{\mathcal{Q}} = H^1(\Omega\backslash\Gamma)$ there holds

$$\langle \dot\theta, \tilde\xi\rangle_{\tilde{\mathcal{Q}}} = \langle \mathbb{K}(\theta)\mathrm{D}_\theta\mathcal{S}(\theta), \tilde\xi\rangle_{\tilde{\mathcal{Q}}} = \langle \mathbb{K}_{\mathrm{B}}(\theta)\mathrm{D}_\theta\mathcal{S}(\theta), \tilde\xi\rangle_{H^1(\Omega\backslash\Gamma)} + \langle \mathbb{K}_\Gamma(\theta_\Gamma)\mathrm{D}_\theta\mathcal{S}_\Gamma(\theta), \tilde\xi_\Gamma\rangle_{H^{1/2}(\Gamma)}\,.$$

For a closed system, the heat flux through the boundary vanishes, i.e., $\theta^2\kappa(\theta)\nabla\left(\frac{\mathrm{D}_\theta S}{\mathrm{D}_\theta E}\right)\frac{1}{\mathrm{D}_\theta E}\cdot \mathrm{n}_{\partial\Omega} = 0$ on $\partial\Omega$. Hence, choosing test functions $\tilde\xi = \mathrm{D}_\theta E\,\hat\xi$ with $\hat\xi \in \tilde{\mathcal{Q}}$ and using the Gibbs relation, there

holds in a weak sense

$$\mathrm{D}_\theta E\,\dot\theta = -\operatorname{div}\left(\theta^2\kappa(\theta)\nabla\tfrac{1}{\theta}\right) \quad \text{in } \Omega\backslash\Gamma$$

for a.a. $t \in (0,T)$, together with the following transmission conditions along Γ

$$\begin{aligned}\gamma_+\Big(\tfrac{\theta_+^2\kappa_+(\theta_+)}{\mathrm{D}_\theta E_+}\nabla\big(\tfrac{1}{\theta_+}\big)\Big)\cdot \mathrm{n}_+ &= -\gamma_-\Big(\tfrac{\theta_-^2\kappa_-(\theta_-)}{\mathrm{D}_\theta E_-}\nabla\big(\tfrac{1}{\theta_-}\big)\Big)\cdot \mathrm{n}_-\,,\\ \gamma_+\Big(\tfrac{\theta_+^2\kappa_+(\theta_+)}{\mathrm{D}_\theta E_+}\nabla\big(\tfrac{1}{\theta_+}\big)\Big)\cdot \mathrm{n}_+ &= -\hat\kappa_\Gamma(\theta_\gamma)\big(\tfrac{1}{\gamma_+\theta_+}-\tfrac{1}{\gamma_-\theta_-}\big) = \tfrac{\hat\kappa_\Gamma(\theta_\gamma)}{\gamma_+\theta_+\gamma_-\theta_-}(\gamma_+\theta_+-\gamma_-\theta_-)\,,\end{aligned}$$

complemented by the above homogeneous boundary condition along $\partial\Omega$ and by an initial condition.

Heat conduction provides a simple example to illustrate how different phenomena of bulk-interface interaction can be described with the aid of the weak form of GENERIC and how interfacial coupling conditions arise as a natural outcome of this formulation. This framework also applies to more complex systems with bulk-interface coupling, as we further address below.

Fluid-structure interaction. Fluid-structure interaction (FSI) is another example of a larger class of bulk-interface systems that do not need additional state variables to be defined on interfaces, but rather require the systematic decomposition of driving forces from different types of physics in different subdomains of the system into contributions from the bulk and from the interface. Then, the operators acting on these contributions need to be defined consistently with the GENERIC formalism shown schematically above. In [2], the GENERIC formalism is applied to deduce a weak form of a damped Hamiltonian system describing FSI using a representation $\boldsymbol{\xi} = (\xi_\mathrm{B}, \xi_\Gamma)$ of bulk forces ξ_B and interface forces ξ_Γ via a decomposition

$$\langle \mathrm{D}\mathcal{E}(q), v\rangle = \int_\Omega \xi_\mathrm{B}\cdot v\,\mathrm{d}x + \int_\Gamma \xi_\Gamma\cdot v|_\Gamma\,\mathrm{d}s = b(\boldsymbol{\xi}, v)\,, \tag{3}$$

where the energy $\mathcal{E}(q) = \int_{\Omega\backslash\Gamma} E(q,\nabla q)\,\mathrm{d}x$ has a density E that has only a bulk part and only depends on the bulk state and its gradient without distinguished contributions on the interface. However, the dependence on ∇q generates mechanical contributions in the Piola–Kirchhoff stress in the bulk and on the interface that need to be properly transmitted through a solid-fluid interface. This was achieved in [2] with the ansatz described in the previous paragraphs and by making use of a general formalism for Lagrangian-Eulerian coordinate transformations within GENERIC that was established in [3]. In particular, it was shown in this work that such transformations preserve the structural properties of a GENERIC system. Typical Lagrangian contributions to E include kinetic energy $\frac{p^2}{2\varrho}$, hyperelastic energy $E_\mathrm{elast}(F)$ with deformation gradient $F = \nabla\chi$, or an internal energy $E_\mathrm{int}(\frac{\varrho}{\det F})$ for a compressible fluid. One key observation in [2] is that the weak form (1) of the FSI system can be rewritten as a nonlinear saddle-point problem for $q(t), \boldsymbol{\xi}(t)$

$$\begin{aligned} a(\boldsymbol{\xi}(t),\boldsymbol{\eta}) - b(\boldsymbol{\eta}, \partial_t q(t)) &= 0\,, &\text{(4a)}\\ b(\boldsymbol{\xi}(t), v) &= \langle \mathrm{D}\mathcal{E}\big(q(t)\big), v\rangle &\text{(4b)}\end{aligned}$$

to be satisfied for all suitable test functions $v, \boldsymbol{\eta}$. Here, for this damped Hamiltonian system, the bilinear form $a = j - k$ is the difference of a skew-symmetric part j and a positive definite, symmetric part k, induced by the Poisson operator $\mathbb{J}_\mathrm{B}$ and the Onsager operator $\mathbb{K}_\mathrm{B}$ comprising

Fig. 4: *Discretization of nonlinear elastodynamics (4) implemented in the open-source computing platform FEniCS, see* *github.com/dpeschka/tvtower.git*

the bulk contributions of the fluid and the solid in the weak form (1).

The saddle-point formulation (4) is a useful approach for numerical implementation. Figure 4 shows a snapshot of a corresponding nonlinear elastodynamics modeled by (4). These and similar mathematical modeling approaches were investigated within the Thematic Einstein Semester *Energy-based mathematical methods for reactive multiphase flows*, co-organized by members of WG BIP in 2020/21.

Moving contact lines. Free boundary problems with moving contact lines are one important class of problems that require a force decomposition (3) and that were investigated in WG BIP. One main feature of this particular type of problem is that domains evolve over time $\Omega = \Omega(t)$. Therefore, derivatives $\mathrm{D}\mathcal{E}(q)$ need to incorporate appropriate shape derivatives of the time-dependent domains. Surface energies of the form $\mathcal{E}_\Gamma = \int_\Gamma \mathrm{d}s$ then produce forces proportional to mean curvature on interfaces $\Gamma(t)$ and conditions for contact angles on $\partial\Gamma(t)$. The strategy is to reformulate these problems in the form of (4) to provide a GENERIC framework that can be discretized in time using time-incremental schemes and in space using finite elements.

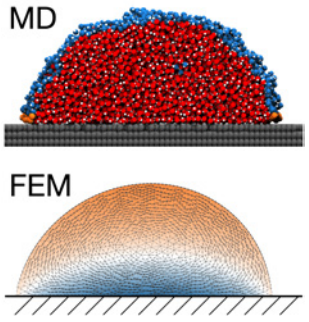


Fig. 5: *Comparison of MD water molecule configuration and FEM simulation of viscous liquid droplet showing the internal flow field*

Corresponding higher-order space and time discretizations for thin-film type models with dynamic contact angles are developed jointly with Luca Heltai, cf. 10.1016/j.jcp.2022.111325, and self-similar solutions are studied in [4]. The main challenge of these higher-order parabolic equations $\partial_t h - \nabla \cdot \big(m(h)\nabla\xi\big) = 0$ for the film height h is the degeneracy in the mobility $m(h) \to 0$ as $h \to 0$. This makes the evolution of the support set $\Omega(t) = \{x : h(x,t) > 0\}$ a free boundary problem that requires appropriate bulk-interface coupling techniques on $\partial\Omega(t)$. There it turned out, with suitable choices of the bilinear forms a, b in (4) and corresponding function spaces for q and ξ, that the mixed formulation is also suitable to study model hierarchies for vanishing dissipation or mobility and develop efficient discretization schemes for the emerging free boundary problems.

In [5], molecular dynamics (MD) predictions for droplets moving over rough surfaces were compared with continuum hydrodynamic models based on finite element method (FEM) computations; cf. Figure 5. The goal of this interdisciplinary research is to identify scaling regimes, where surface roughness leads to enhanced or reduced energy dissipation and, therefore, can be effectively treated using bulk-interface coupling techniques. For that reason, the gradient system contains dissipation potentials contributing in the bulk (3D), on interfaces (2D), and at contact lines (1D) and was combined with suitable arbitrary Lagrangian-Eulerian (ALE) techniques to efficiently treat the motion of moving meshes.

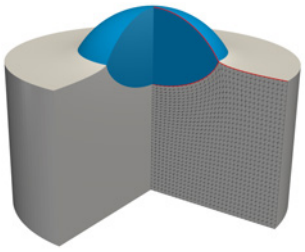


Fig. 6: *FSI for liquid droplet (blue) on elastic substrate (gray) connected by interfaces (thin red lines)*

Similar axisymmetric models are also developed to investigate sharp-interface limits of phase field models for FSI with moving contact lines. One of the main observations is that scaling limits $\varepsilon \to 0$ for coupled Navier–Stokes–Cahn–Hilliard systems depend on the scaling of the Cahn–Hilliard mobility $m_\varepsilon = m_0 \varepsilon^\alpha$ and are valid in a certain range $\underline{\alpha} < \alpha < \overline{\alpha}$ only. Depending on the norm for the sharp-interface limit, this range narrows down for multiphase systems with contact lines; cf. Figure 6.

Propagation of delamination and fracture. Models to describe the propagation of delamination, i.e., crack growth along prescribed interfaces, provide an example for bulk-interface GENERIC where the evolution law of an additional variable q_Γ is prescribed on the interface. This delamination

variable q_Γ characterizes the state of the material along the interface and evolves from the unbroken state $q_\Gamma(0,x) = 1$ to the fully broken state $q_\Gamma(t,x) = 0$ in a material point $x \in \Gamma$. A typical evolution law for q_Γ is given in terms of a subdifferential inclusion

$$-\mathrm{D}_{q_\Gamma}\mathcal{E}_\Gamma(q_\mathrm{B}, q_\Gamma) \in \partial\Psi(q;\dot{q}_\Gamma)\,.$$

This inclusion stems from the fact that for fracture problems the dissipation potential $\Psi(q;\cdot)$ is typical nonsmooth with $\Psi(q;v_\Gamma) = \infty$ if $v_\Gamma > 0$ in order to exclude the healing of the material in the model. Typical interfacial energy densities $E_\Gamma(q_\mathrm{B}, q_\Gamma)$ depend on q_Γ and on functions of the jump of the displacement field across Γ and thus result by means of (1) in coupling conditions between the normal stresses from the bulk and the interfacial stresses. It was shown in [1] that typical delamination models, as they are used in engineering literature and as they have been investigated analytically, e.g., in [6], can be understood in a weak form of GENERIC (1). In particular, the analysis in a series of works on delamination related to [6] already makes use of this structure and provides structure-preserving approximations for different types of delamination models by means of suitable discretization schemes and variational convergence methods.

Conclusions and outlook

The weak form of GENERIC (1) and the weak saddle-point structure (4) for damped Hamiltonian systems have proven a versatile modeling framework for systems with bulk-interface interaction, which naturally takes into account interfacial coupling conditions between the different subsystems. These structures have been used as a basis for mathematical analysis and numerical implementations for models from different applications with the benefit that the structure can be preserved during approximation. Future investigations will be devoted, amongst others, to geophysical and biological applications such as FSI related to sea ice dynamics and biological hydrogels.

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1.2 Phase Transitions in Random Graphs

Tejas Iyer, Lukas Lüchtrath, and Elena Magnanini

Many complex systems, in areas as diverse as biology, sociology, and computer science, can be represented as *networks*. That is, the system can be modeled by *nodes* and interactions between them, represented by *edges*. Such systems include, for example, the internet, where nodes are webpages that are connected by hyperlinks (Figure 1), networks in molecular biology (Figure 2), social networks, and communication networks. More generally, large sets of correlated data are represented by networks.

Fig. 1: *Visualization of the internet by Barrett Lyon, Opte project (2003)*

In order to gain a better understanding of certain network effects, for instance the fast spread of news through social media, it is of great importance to identify and study typical structures and features of networks arising in the real world. One easily observable property is the *degree distribution*. Here, the *degree* of a node is the number of other nodes that it is connected to, and the degree distribution then gives the probability of observing a certain degree when picking a node randomly from the network. Interestingly, it has been observed that in many real-world networks, the probability of choosing a node of degree k behaves roughly like $k^{-\tau}$ for some $\tau > 2$, a property known as being *scale free*. This property indicates the existence of exceptionally high degree nodes, thus, informally, indicating that there is no characteristic "scale" in the degrees (Figure 3). Another structural property of many networks is that they tend to display a high degree of *clustering*. Clustering refers to the feature that two nodes connected to a common node are more likely to be connected to each other, and is often measured in terms of the number of *triangles* in the network. Another property of interest is the existence of a connected component that contains a fraction of all the nodes, a *macroscopic connected component*.

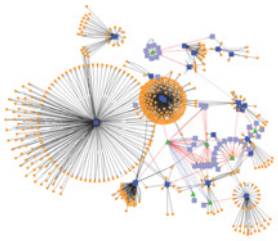

Fig. 2: *Visualization of a biological network by Fozail Ahmad, Bioinformatics Review (2016)*

Appropriate mathematical models, for which the emergence of the properties described above are proven rigorously, can be used as null models or benchmarks when it comes to testing algorithms and statistical methods for real-world applications. Moreover, these mathematical proofs can often provide insights into the reasons underlying the emergence of such properties.

Phase transitions in random graphs. In order to incorporate the uncertainties arising in real-world applications, networks are generally modeled mathematically as *random graphs*. Here, the edges and sometimes also the nodes are *random*. Of particular interest is whether or not changing certain parameters leads to dramatic changes in the graph structure, a phenomenon usually referred to as a *phase transition*. This is important since parameters associated with these networks may fluctuate (due to, for example, phenomena such as epidemics arising on these networks), and we want to know under what circumstances these fluctuations will have dramatic consequences.

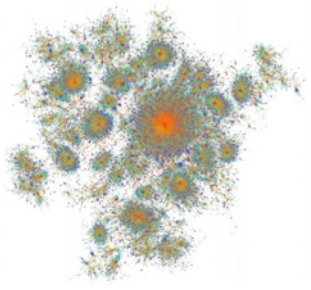

Fig. 3: *Visualization of a scale-free network by Pim van der Hoorn, Networkpages (2020)*

Our research. Our research in Research Group RG 5 *Interacting Random Systems* and the Leibniz Group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks* investigates the emergence and nature of phase transitions in multiple contexts. The first part reports on the emergence of *condensation* in inhomogeneous *preferential attachment models* (popular time-evolving models producing scale-free random graphs), where a positive proportion of the edges in

the network may accumulate around nodes of large degree. The second part highlights work related to the presence or absence of macroscopic connected components in *spatial* models, a property that is particularly interesting in the context of wireless telecommunication. The third part is related to work regarding phase transitions in the edge density of exponential random graphs. The latter arise as models incorporating clustering in diverse contexts.

Inhomogeneous preferential attachment models

A popular class of models that displays some of the features associated with complex networks, in particular the property of being *scale free*, is known as *preferential attachment*. Informally, these are sequences of graphs evolving in discrete time, where nodes arrive at discrete time-steps and connect to existing nodes with probability proportional to their degree. Models of this type date back to Yule, 1924, but were popularized in the context of random networks by Barabási and Albert, 1999.

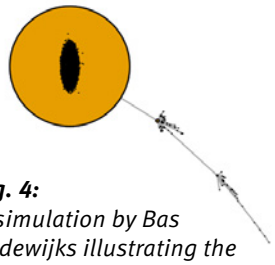

Fig. 4:
A simulation by Bas Lodewijks illustrating the extreme-condensation phase, when $f(i,w) = i^p + w$, $p > 1$. *The parameter regime simulated corresponds to that when there is a single node of infinite degree, which may be the large orange node.*

Despite their success, a shortcoming of the classical preferential attachment models is that they fail to encapsulate the inherent *inhomogeneities* arising in real-world networks. For example, in the classical models the oldest nodes will tend to have the largest degrees, whilst on the other hand, in contexts such as the internet, one may expect newer nodes to compete with older ones. Extensions and newer variants have addressed this issue by assigning positive weights to nodes, so that newer nodes attach to previous ones according to a function of their degree and their weight. If this function is monotone increasing in the weight variable, one may regard the weight as the attractiveness of a node. When this function is given by the product of the degree and weight, this model is known as *preferential attachment with multiplicative fitness*, or the *Bianconi–Barabási* model (Bianconi and Barabási, 2001). Here, researchers observed that, when nodes are assigned *independent, identically distributed* (i.i.d.) weights, there is a critical condition on the weight distribution leading to a *condensation* phase transition. In this context, condensation means that a positive fraction of edges in the network accumulates around nodes of maximum weight. This observation was first proved mathematically in Borgs et al., 2007.

Often, due to simplicity, one considers evolving tree models since one expects many properties, such as the degree distribution, to be similar to models involving evolving graphs. A natural framework of evolving trees, which encompasses and generalizes many of the existing models above, posits that nodes v arrive one at a time and are assigned a random i.i.d. *weight* W_v. These weights may take values in an arbitrary measure space $(S, \mathcal{S})$. Newly arriving nodes then connect to a single existing node with probability proportional to a general, measurable fitness function $f : \mathbb{N}_0 \times S \to [0, \infty)$ that incorporates information about the current degree of the target node, and its weight. This model class possesses a rather rich structure. The condensation behavior may roughly be classified according to the following conjectured phases [3]:

1. *Non-condensation phase:* There exists $\lambda > 0$ such that $\sum_{j=1}^{\infty} \mathbb{E}\left[\prod_{i=0}^{j-1} \frac{f(i,W)}{f(i,W)+\lambda}\right] = 1$.
2. *Condensation phase:* For any $\lambda > 0$ such that the sum converges $\sum_{j=1}^{\infty} \mathbb{E}\left[\prod_{i=0}^{j-1} \frac{f(i,W)}{f(i,W)+\lambda}\right] < 1$.
3. *Extreme-condensation phase:* For any $\lambda > 0$, $\sum_{j=1}^{\infty} \mathbb{E}\left[\prod_{i=0}^{j-1} \frac{f(i,W)}{f(i,W)+\lambda}\right] = \infty$.

This conjecture is proved in a number of specific cases in [3]. Both the second and third phase are of particular interest in exploring more detailed properties of the process. In the third phase, all of the mass of edges concentrates on a *sub-linear* number of nodes of large weight and degree. Ongoing work in exploring this phase has led to some more interesting results concerning the limiting infinite tree associated with the model, roughly establishing two other phases:

1. The *no-sideways explosion* phase: For *almost all* W, $\sum_{i=0}^{\infty} \frac{1}{f(i,W)} = \infty$. In this case, under another critical condition, there is either a single infinite path in the associated infinite tree, with every node having finite degree, or, when $f(i, W) > 0$ for all $i \in \mathbb{N}$, there exist infinitely many nodes of infinite degree and uncountably many infinite paths. The former phase may be regarded as an extreme effect of competition on the structure of the infinite tree, making everyone poor in the sense that their degree is finite rather than infinite. In [5], we derived sufficient criteria for either case.
2. The *certain-sideways explosion* phase: For almost all W, $\sum_{i=0}^{\infty} \frac{1}{f(i,W)} < \infty$. In this case, there are precisely two scenarios: Either the infinite tree contains exactly one node of infinite degree or exactly one infinite path (but not both!); see Figures 4 and 5. We also derived sufficient conditions for either scenario, proving a phase transition in many particular instances of the model [4].

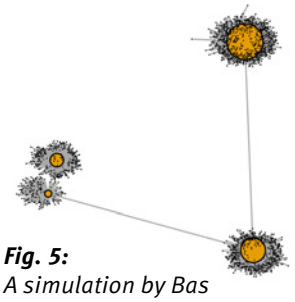

Fig. 5: *A simulation by Bas Lodewijks illustrating the "extreme condensation" phase, when $f(i, w) = i^p + w$, $p > 1$. In the parameter regime shown, there is a single infinite path.*

Work on this problem is closely related to so-called *Crump–Mode–Jagers branching processes*, which model the size and structures of populations in continuous times (for example, the number of species of a biological entity) and are thus of interest in regards to other potential applications outside network science.

Percolation phase transition in the weight-dependent random connection model

The models described in the previous part can produce scale-free networks. By further embedding the nodes into *space*, in addition to assigning them weights, we can also incorporate clustering. More precisely, in the models we consider in this part, pairs of nodes that are located *closer* to each other are more likely to connect, in addition to pairs where one node has a high weight. A well-known example is the *Boolean model*, where the weights are random radii, and two vertices are connected when the associated balls centered at the nodes intersect (Figure 6). Unlike the model of the previous part, this model has no time parameter and consists of infinitely many nodes homogeneously distributed in the entire Euclidean space. A main interest of DYCOMNET lies in finding criteria for the presence or absence of infinite connected components. For communication applications, the components are the parts of the network through which messages can be exchanged. Hence, the existence of infinitely large components is of fundamental importance. We say that a graph with an infinite component *percolates*. Originally, *percolation* was introduced by Broadbent and Hammersley (1957). The idea was to model a porous medium as a random graph, and an infinite component is interpreted as a fluid being able to percolate through the medium.

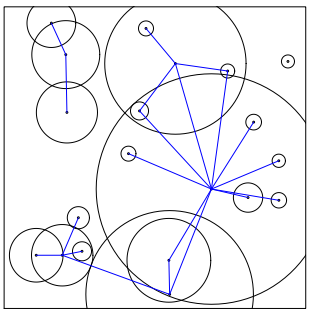

Fig. 6: *Realization of the Boolean model based on a Poisson point cloud*

A key quantity in our setting is the amount of long edges as a measure of what different regions a vertex can reach. Formally, the nodes are embedded into d-dimensional Euclidean space through a standard *Poisson point process* and additionally assigned an independent *mark* distributed uniformly on $(0, 1)$ representing its *inverse weight*. Any pair of nodes x and y with marks u_x

and u_y then independently forms an edge with probability $\rho(\beta^{-1}g(u_x,u_y)|x-y|^d)$. Here, ρ is a non-increasing function and, hence, short distances lead to larger probabilities. The function g is assumed to be non-increasing such that smaller marks (i.e., larger weights) lead to higher connection probabilities. Additionally, $\beta > 0$ is an intensity parameter scaling the expected degree. Many established models belong to the presented class. For instance, the aforementioned Boolean model is given by the choice $\rho = \mathbf{1}_{[0,1]}$ and $g(u_x,u_y) = (u_x^{-\gamma/d} + u_y^{-\gamma/d})^{-d}$ for some $\gamma \in (0,1)$.

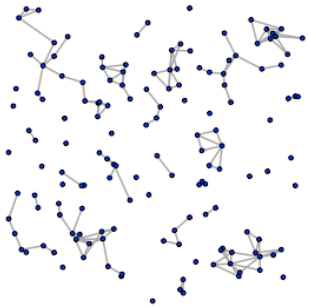

Fig. 7: *Snapshot of a weight-dependent random connection model with $\delta_{eff} > 2$ and small β*

As it is well known that for $d \geq 2$ graphs of this class contain an infinite connected component for large values of β, we are interested in whether there is a phase transition such that an infinite component no longer exists when β is small. The key to answering this question is to quantify the occurrence of long edges on various scales via the *effective decay exponent* defined as

$$\delta_{\text{eff}} := -\lim_{n\to\infty} \frac{\log \int_{1/n}^1 \int_{1/n}^1 \rho(\beta^{-1}g(s,t)n)\,\mathrm{d}s\,\mathrm{d}t}{\log n}.$$

It turns out that $\delta_{\text{eff}} > 2$ is a sufficient condition for the absence of percolation for small enough β (Figure 7). Additionally, one can express in terms of δ_{eff} the decay of the probability that the cardinality and/or the spatial extension of a typical component in the non-percolation regime exceed a certain size [6]. The situation in dimension $d = 1$ is different. Here, the existence of an infinite component is rather hard to achieve. Nevertheless, it turns out that $\delta_{\text{eff}} < 2$ implies the presence for large β and conversely $\delta_{\text{eff}} > 2$ implies the absence of an infinite component for all β. We also show the existence of a largest component of linear size in larger and larger snapshots of the graph [2]. The idea behind the results is that $n^{-\delta_{\text{eff}}}$ approximates the probability of an edge between two vertices chosen uniformly among two sets of n vertices at distance roughly $n^{1/d}$ when n is large. Ignoring correlations, there are n^2 trials to form an edge between those sets and, therefore, the probability of connecting two distant sets of nodes increases for $\delta_{\text{eff}} < 2$, but decreases for $\delta_{\text{eff}} > 2$.

Limit theorems for exponential random graphs

Fig. 8: *Snapshot of a weight-dependent random connection model with $\delta_{eff} < 2$ and small β*

Exponential random graphs are another ubiquitous class of models that can incorporate clustering amongst other network tendencies. From the point of view of sociology, one of the main desires is to understand how the connectivity in local communities can influence the overall network structure. This can be modeled by considering a probability distribution that biases the occurrence of certain features, such as the number of edges or *triangles*, and then analyzing the large-scale properties of random networks sampled according to this distribution. Mathematically, if this bias is introduced by means of an exponential term, such a distribution is called a *Gibbs measure*, and the function that encodes this biasing is called a *Hamiltonian*. For instance, for a simple graph G on n labeled vertices with $E(G)$ edges and $T(G)$ triangles, we define the Hamiltonian

$$\mathcal{H}_{n;\alpha,h}(G) := \frac{\alpha}{n}T(G) + hE(G), \quad \text{with } \alpha, h \in \mathbb{R}. \tag{1}$$

As a probability measure on the space $\mathcal{G}_n$ of simple graphs with n vertices, we take the following

Gibbs probability

$$\mu_{n;\alpha,h}(G) := \frac{\exp\left(\mathcal{H}_{n;\alpha,h}(G)\right)}{Z_{n;\alpha,h}}, \quad \text{with} \quad Z_{n;\alpha,h} := \sum_{G\in\mathcal{G}_n} \exp\left(\mathcal{H}_{n;\alpha,h}(G)\right), \tag{2}$$

where the normalizing constant $Z_{n;\alpha,h}$ is called *partition function*. Random graphs whose distribution is a Gibbs measure of the form (2) are called *exponential random graphs*. When the Hamiltonian is of the form (1), we speak of the *edge-triangle* model; the well-known *Erdős–Rényi random graph* is given by the special case $\alpha = 0$ and $h = \log \frac{p}{1-p}$. A crucial characteristic of the model is the so-called *limiting free energy* associated with (2), which is defined as

$$f_{\alpha,h} := \lim_{n\to+\infty} \frac{1}{n^2} \ln Z_{n;\alpha,h}.$$

A lack of analyticity in this function characterizes the presence of a phase transition. An explicit expression of $f_{\alpha,h}$ has been obtained in Chatterjee and Diaconis, 2013, when the parameters (α, h) lie in a specific region called the *replica-symmetric regime*, corresponding to $\alpha > -2$, $h \in \mathbb{R}$. This term is borrowed from *spin glass* theory and is related to the fact that, in the limit, the model behaves like a mean-field model. In particular, it has been proved (Radin and Yin, 2013) that the replica symmetric region includes a (non-explicit) continuous and strictly decreasing curve $\mathcal{M}^{\mathrm{rs}}$ at which a first-order phase transition in the limiting edge density $u^*(\alpha, h)$ occurs, and the first-order partial derivatives of $f_{\alpha,h}$ have jump discontinuities. At the critical point $(\alpha_c, h_c) = (27/8, \log 2 - 3/2)$, the phase transition is of second order, and the second-order partial derivatives of $f_{\alpha,h}$ diverge (see Figure 9 for a qualitative representation of the phase diagram).

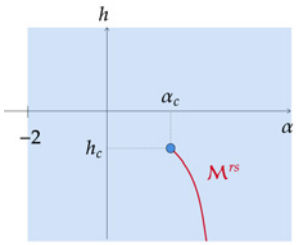

Fig. 9: *Illustration of the phase space (α, h) for the edge-triangle model (1) in the replica-symmetric regime*

One of the key results of our paper [1] is the determination of the asymptotic distribution of the edge density $\frac{2E(G)}{n^2}$ (as the graph size n tends to infinity) within the replica-symmetric regime. Our analysis provides a *strong law of large numbers* whenever the parameters (α, h) are taken outside the critical curve and proves that the edge density concentrates with high probability in a neighborhood of the *free energy maximizers* on the critical curve. Fluctuations of the edge density are also investigated, and a *central limit theorem* is derived for parameters outside the critical curve and away from the critical point (α_c, h_c). These results are extended to a general family of exponential random graphs where the Hamiltonian involves various sub-graphs counts. A predominant part of our results includes the exploration of a simplified model, the *mean-field* approximation of the edge-triangle model. A major advantage of this approximation is that the Hamiltonian can be expressed as a function of the edge density, and exact computations are possible (like in the *Curie–Weiss model*). In this setting, we can prove the analogous of the results derived for the edge-triangle model (partially in a stronger form), and we can go further, in particular, we are able to characterize the fluctuations at the critical point, presenting a *non-standard central limit theorem* with scaling exponent $3/2$.

Some heuristic computations based on *large deviation* estimates suggest that the edge-triangle model may exhibit the same behavior as the mean-field approximation when the parameters vary in the phase space. We then formulate conjectures about fluctuations at the critical point and about the behavior of the edge-triangle model on the critical curve.

Conclusion and outlook

Our work deals with phase transitions arising from random graphs occurring in diverse contexts. The models we consider reflect many real-world properties, such as clustering and being scale free, and often exhibit important features associated with the networks: the distribution of edges amongst nodes of certain weights, crucial connectivity properties, or the edge density. We therefore believe that this is an important, rich area with interesting problems both in the context of new applications, and mathematically. There are many more results in the pipeline!

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1.3 Spin-Qubit Shuttles for Scalable Semiconductor Quantum Computers: Modeling, Simulation and Optimal Control

Lasse Ermoneit, Burkhard Schmidt, Jürgen Fuhrmann, Thomas Koprucki, and Markus Kantner

Quantum computers harness the principles of quantum mechanics to outperform classical computers in tackling certain mathematical problem classes. These problems encompass various tasks such as, e.g., integer factorization, searches in large unsorted databases, solving huge linear systems of equations and combinatorial optimization problems. Furthermore, a particular type of quantum computer—the quantum simulator—holds the potential for efficient simulations of large-scale quantum many-body systems, which are ubiquitous in materials research (e.g., high-temperature superconductors, catalysts, etc.) or pharmaceutical drug development.

In contrast to classical digital computers, where information is encoded in bits that can be either in the state 0 or 1, the information in quantum computers is encoded in so-called *quantum bits*, or *qubits* for short. These qubits represent abstract quantum mechanical two-level systems that are not limited to reside in one of the basis states[1] $|0\rangle$ or $|1\rangle$, but can also exist in any continuous superposition $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$. The information is encoded in the complex amplitudes $\alpha, \beta \in \mathbb{C}$, which describe a point on the unit sphere, the so-called *Bloch sphere*; see Figure 1. Accordingly, a quantum computer is more similar to an analog classical computer than to a digital one. The ability of a quantum system to be in a coherent superposition of different states simultaneously is a fundamentally non-classical property of the system that, however, requires careful shielding from its environment. Otherwise, coupling to external reservoirs might lead to uncontrolled disturbances or even to a "collapse of the wave function" into one of the two basis states when observing the qubit with a macroscopic measurement apparatus.

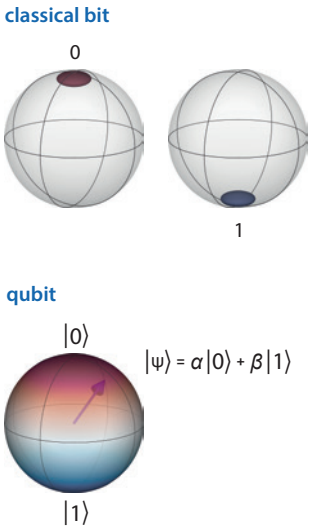

Fig. 1: *Bits in classical computers encode only digital information (state 0 or 1) whereas a qubit can be in a superposition of both states simultaneously (visualized as a point on the Bloch sphere)*

The true potential of quantum computers unfolds when a large number of qubits is considered. A system of N qubits can be in a superposition of up to 2^N states simultaneously, which means that a correspondingly large amount of information can be encoded in the associated 2^N amplitudes. The information stored in a qubit register thus scales exponentially with the system size, so that when a single new qubit is added, the size of the underlying state space doubles (and not just increases by +1 as with classical bits). It is this scaling behavior that limits the feasibility of simulating large quantum many-body systems on classical computers that inspired Richard Feynman in 1982 to the idea of using artificial quantum systems as novel type of computers. This led to the emergence of the new field of *quantum information theory* in the late 1980s and early 1990s, which quickly spawned several new algorithms such as the Shor algorithm for integer factorization (1994) that received enormous attention because of its potential to break widely used encryption methods.

The actual implementation of quantum algorithms requires new hardware realizations that have to meet very demanding and partly even complementary requirements. In 2000, David DiVincenzo published a list of criteria that potential hardware platforms for quantum computing must fulfill. This includes the ability to, e.g., initialize the qubit register with high precision in a specific state, control the system in a targeted manner to execute the actual computing steps (quantum gate operations) and to precisely measure the system in order to extract the results. Although each of

[1] Here, we use Dirac's notation, where $|\cdot\rangle$ denotes a Hilbert space vector.

these tasks requires a specific interaction of the qubits with the environment (preparation, manipulation, measurement), the register must be almost perfectly shielded from any other environmental influences, as otherwise the many-body wave function would dissipate into a classical mixture of states (known as *decoherence*), and the information encoded in the amplitudes would be lost.

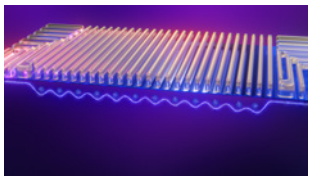

Fig. 2: *Schematic illustration of Intel's 12-qubit silicon quantum processor "Tunnel Falls" © Intel Corporation*

Electron spins in semiconductor nanostructures are among the most promising hardware platforms for the realization of universal quantum computers. In this technology, electrons are trapped in electrostatically defined quantum dots (QDs) resulting from a combination of epitaxial confinement in the vertical direction (a quantum well) and in-plane confinement generated by an electrostatic potential landscape shaped by gate electrodes on the top surface. Electrons bound in such QDs can reside only in discrete states, which can be selectively manipulated by adjusting the electrode voltages. In order to realize universal quantum algorithms, it is necessary to implement arbitrary one-qubit gates and a specific two-qubit gate. The former correspond to arbitrary rotations of the qubit on the Bloch sphere and can be realized via micromagnets or all-electrically using alternating current pulses to trigger the electron spin resonance. For the realization of two-qubit gates, the exchange interaction between electrons in neighboring QDs is used to build up non-classical correlations between them (known as *entanglement*). Both types of operations as well as initialization and readout have already been demonstrated with high fidelity exceeding 99% [1]. A key factor for the quality of these qubits is the use of isotopically purified ^{28}Si in the quantum well, which enables very long coherence times. The great prospect of this technology is its compatibility with industrial fabrication techniques that should enable scaling to a very large number of qubits just as it has been achieved with silicon transistors in classical computers. As a landmark step in this direction, Intel unveiled its first 12-qubit silicon quantum processor *Tunnel Falls* in June 2023; see Figure 2.

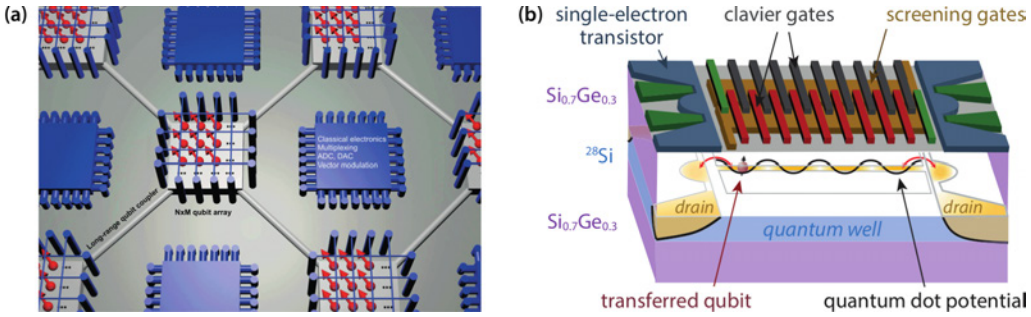

Fig. 3: *(a) Small-scale qubit arrays interconnected by links for coherent exchange of quantum information as a concept for a scalable quantum computing architecture [2]. (b) Concept for a spin-qubit shuttling device developed at RWTH Aachen/ FZ Jülich [3].*

Wiring of a large number of QDs on a chip, however, is a great challenge, as each QD requires several contact lines for confinement, readout, and signaling that must be stacked in multiple layers. This results in geometric limitations as well as the risk of unintentional self-heating due to high current densities. A potential remedy is a modular design with rather small qubit arrays that are interconnected by so-called *quantum links* [2]; see Figure 3 (a). These quantum links serve—in analogy to the bus system in classical computers—to exchange quantum information between qubit arrays, whereby even spatially far separated qubits can become entangled. One possible realization of such a quantum link is the quantum bus [3] that is currently being developed at Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen and Forschungszentrum (FZ) Jülich; see Figure 3 (b). The WIAS Focus Platform SemQuTech *Simulation of Semiconductor Devices for Quantum Technologies* supports this development with mathematical modeling and numerical

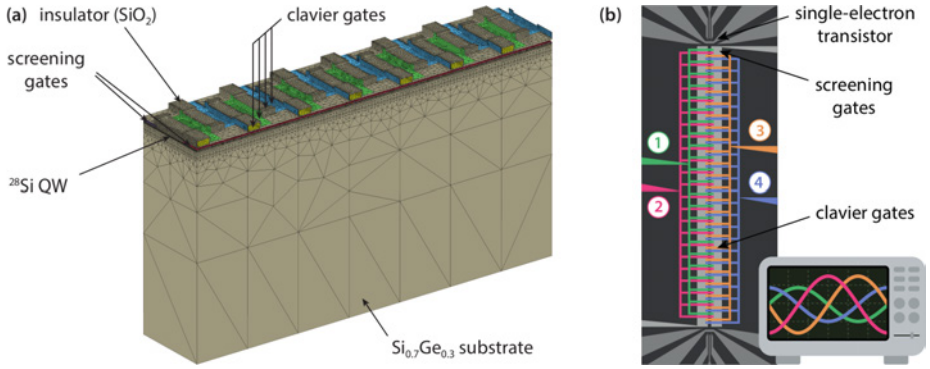

Fig. 4: *(a) Delaunay mesh of the Si-Qubus device with indicated gate electrodes, insulators, and ^{28}Si quantum well (QW). The computational mesh has about 20 million nodes and was generated using* `TetGen`*. (b) Top view on the quantum bus shown in Figure 3 (b), adapted from [3]. The four different clavier gate sets are indicated by color.*

simulation. The collaboration interlinks the two Clusters of Excellence *Matter and Light for Quantum Computing* (ML4Q) and *MATH+*.

Modeling and simulation of spin-qubit shuttling

The quantum bus shown in Figure 4 (a) forms a moving chain of QDs that can be propagated by suitable pulsing of the clavier gates like a conveyor belt. This enables shuttling of electrons inbetween qubit arrays. A key feature of the device concept is that there are only four different clavier gate sets, with every fourth being electrostatically connected to all the others in the chain; see Figure 4 (b). Hence, the number of required control signals is independent of the length of the shuttle, making the technology scalable. Moreover, the required classical control electronics can be integrated directly on the chip; see Figure 3 (a). Next to the clavier gates, there are two screening gates at the sides that can be used for lateral control of the shuttling trajectory; see Figure 4.

The starting point for numerical device simulation is the computation of the electrostatic potential distribution Φ to generate the QDs. The potential is given as the solution of the Poisson problem

$$\begin{aligned} -\nabla \cdot (\varepsilon(\mathbf{r}) \nabla \Phi(\mathbf{r},t)) = 0, \qquad & \Phi(\mathbf{r},t)|_{\Gamma_{D_k}} = U_k(t), \\ \mathbf{n} \cdot \nabla \Phi(\mathbf{r},t)|_{\Gamma_N} = 0, \quad & \Phi(\mathbf{r},t)|_{\Gamma_{\text{period}}} = \Phi(\mathbf{r}+\mathbf{e}_x L_x, t), \end{aligned} \tag{1}$$

with Dirichlet (at the gate contacts Γ_{D_k}), Neumann, and periodic (in propagation direction) boundary conditions. By exploiting the linearity of the problem, the system (1) can be reduced via

$$\Phi(\mathbf{r},t) = \sum_k U_k(t)\,\phi_k(\mathbf{r}) \tag{2}$$

to a stationary Poisson problem for each of the six independent electrode potentials ϕ_k; see Figure 5. The clavier gate voltage sequence for conveyor-mode qubit shuttling is

$$U_k(t) = U_k^{\text{DC}} + U_k^{\text{AC}} \sin\left(\frac{\pi}{2}k + 2\pi f_s t\right), \qquad k = 1 \ldots 4, \tag{3}$$

where f_s is the shuttling frequency. The problem (1) is discretized using a finite volume method and solved by Conjugate Gradient (CG) iteration. The numerical computation is based on the Julia package `VoronoiFVM.jl` [4].

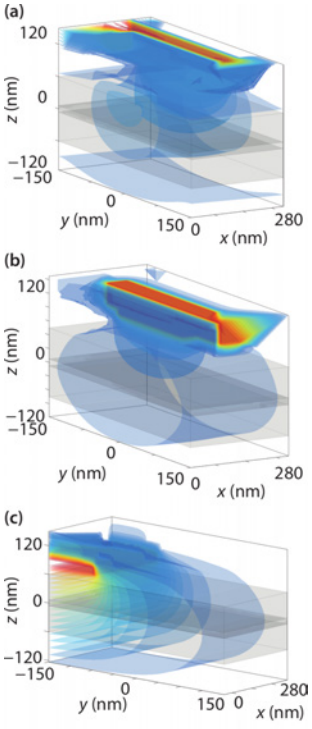

Fig. 5: *Normalized gate electrode potentials ϕ_k of the (a) upper clavier gates, (b) lower clavier gates, and (c) screening gates*

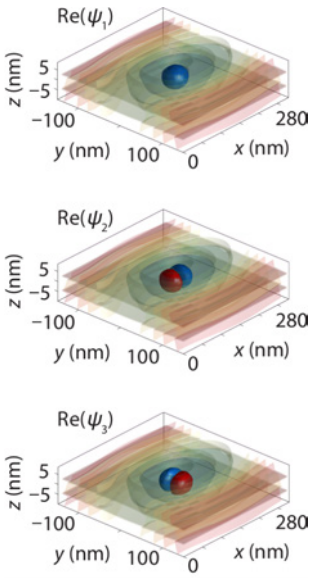

Fig. 6: *Isosurface plots of the three lowest energy quantum dot orbital eigenstates and the confinement potential*

Having the electrostatic potential generating the QDs at our disposal, we can turn to electron wave packet propagation that is described by the time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = H(\mathbf{r},t,\mathbf{u}(t))\,\Psi(\mathbf{r},t) = \left(H_0(\mathbf{r},t) - e_0\sum_k u_k(t)\,\phi_k(\mathbf{r})\right)\Psi(\mathbf{r},t)\,, \tag{4}$$

where Ψ is the wave function. The reference Hamiltonian

$$H_0(\mathbf{r},t) = -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*(\mathbf{r})}\nabla\right) - e_0\Phi(\mathbf{r},t) + V_{\mathrm{QW}}(\mathbf{r}) + V_{\mathrm{defect}}(\mathbf{r}) \tag{5}$$

describes the kinetic energy of the electron (with effective mass m^*), the electric potential of the gate electrodes, the quantum well confinement potential V_{QW} and the potential V_{defect} of charged defects. Because of the pulse sequence (3), the Hamiltonian H_0 is also time dependent. In addition, the full Hamiltonian in (4) includes an extra control part that describes a correction $u_k(t)$ to the nominal pulse sequence $U_k(t)$. A direct simulation of (4) by spectral and split-step methods is computationally expensive due to a large time-scale separation: While the envelope of the wave packet evolves only slowly during shuttling (typical time scale is tens of ns), the phase undergoes rapid oscillations that are several orders of magnitude faster. Therefore, an alternative approach is pursued that is based on an expansion of the wave function in instantaneous eigenfunctions ψ_n of H_0 (see Figure 6)

$$\Psi(\mathbf{r},t) = \sum_n c_n(t)\,\psi_n(\mathbf{r},t)\,.$$

With the help of the Hellmann–Feynman theorem, the TDSE (4) can be reduced to a system for the complex amplitudes $c_n(t)$, which has several advantages: It is directly interpretable, provides a dramatic reduction of the dynamical state space and, furthermore, allows to eliminate the rapid phase oscillations [5]. This approach, however, requires the (partial) eigendecomposition of H_0 for any point in time (and a suitable strategy for adaptive refinement) in a pre-processing step. Figure 7 shows the eigenvalue curves as a function of the shuttling phase featuring numerous avoided crossings, each of which can give rise to complex dynamics. Note that the spectrum can be strongly modified in the presence of a charged defect; see Figure 7 (b). Forward simulations of conveyor-mode shuttling depicted in Figure 8 show the impact of a charged defect within the channel that triggers undesired population transfer to excited states in a sequence of Landau–Zener transitions. Since the coupling of the spin to the external magnetic field is modified for excited states, this will lead to a randomization of the accumulated spin phase that must be avoided.

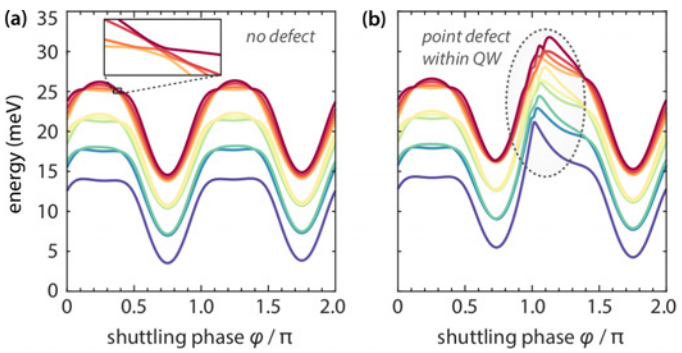

Fig. 7: *Eigenvalue branches as a function of the shuttling phase $\varphi = 2\pi f_s t$, cf. (3), (a) without a defect and (b) with a charged point defect in the QW center*

Quantum optimal control

Pontryagin's maximum principle [6] is employed to engineer control pulse sequences $u_k(t)$ to counteract the impact of charged material defects. This is achieved by minimizing a cost functional

$$J(\Psi, \mathbf{u}) \propto \int_{t_0}^{T} \mathrm{d}t \left(\langle \Psi(t) | \hat{H}^2(t, \mathbf{u}(t)) | \Psi(t) \rangle - \left(\langle \Psi(t) | \hat{H}(t, \mathbf{u}(t)) | \Psi(t) \rangle \right)^2 \right) \tag{6}$$

that penalizes the accumulated energy uncertainty of the electron during shuttling, which is proportional to the infidelity due to spin dephasing. The functional (6) is supplemented with the TDSE (4) as a dynamical constraint using the Lagrange multiplier method. Variation of the augmented functional yields evolution equations for the state and co-state that allow to construct gradients of the functional with respect to the controls. These equations are solved using structure-preserving propagation schemes to preserve the norm of the wave function. Functional minimization is carried out using a quasi-Newton method (L-BFGS) in a collaboration with Technische Universität Berlin (MATH+ project AA2-17). The controls obtained this way enable an almost deterministic passage of the electron through the channel without reducing the shuttling velocity [5].

Conclusions and outlook

Electron shuttling devices are new functional elements in modular concepts for spin-qubit based quantum computers that have promising prospects for scalability due to direct compatibility with industrial fabrication techniques. Numerical device simulation is crucial for understanding the limiting factors and performance bottlenecks of such devices and provides a means for further optimization. Quantum optimal control theory can be used to engineer pulse sequences that enable a high transfer fidelity of the qubit even in the presence of charged impurities and other defects. In the future, the model will be extended by further important aspects such as mechanical deformations (strain) and random alloy fluctuations at the Si/SiGe heterostructure interface.

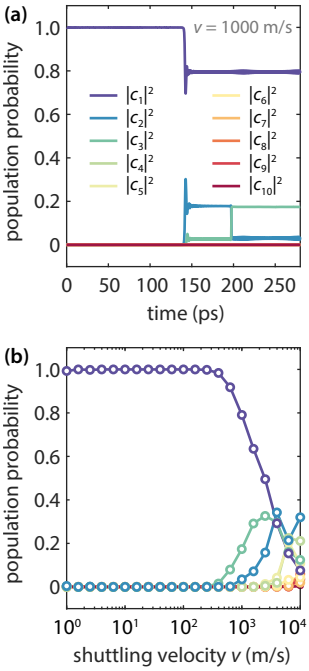

Fig. 8: *(a) Population dynamics of a qubit swept through a sequence of avoided crossings showing several Landau–Zener transitions. (b) Final state population probability vs. shuttling velocity $v = L_x f_s$ after propagation over one unit cell (four clavier gates).*

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1.4 Symmetrization in Cross-diffusions

Katharina Hopf

Introduction

The term *diffusion* stems from the Latin word *diffundere*, which means *to spread*.

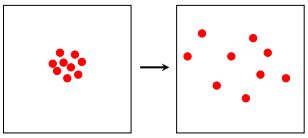


Fig. 1: *Diffusing particles*

Diffusion is an irreversible process governing the movement of particles from regions of higher to regions of lower concentration. The phenomenon of diffusion is ubiquitous in nature and can be observed in gas, liquids, and even in solids. Everyday examples include the spread of perfume, smoke, and other airborne particles through the surrounding air, and the dispersion of a droplet of ink in a glass of water until the solution becomes uniformly colored. The continuum approach, which treats diffusion as a continuous process rather than focusing on individual particles, traces back to Fick's laws in the 19th century. This approach, which we adopt in this article, is well-suited for studying physical systems from a macroscopic viewpoint.

In systems with multiple components, diffusive processes can become intricate, and the flux of a species S_1 may be influenced by the density gradient of a second species S_2. This is when cross-diffusion occurs. Physical systems that can exhibit cross-diffusive behavior comprise electrolytes, temperature-responsive materials, and thermoelectric materials where a temperature gradient may induce an electric current.

The mathematical concept of cross-diffusion also encompasses certain biological processes, including chemotaxis and cross-effects arising in predator-prey systems. Cross-diffusion may induce intriguing patterns in reaction–diffusion systems. It may lead to the surprising phenomenon of uphill diffusion, which in contrast to the classical Fickian diffusion downhill, i.e., in the direction of the negative density gradient, describes a movement uphill, towards higher density. For an illustration in one space dimension we refer to Figure 2, where, loosely speaking, in the region $x \approx 0.5$ the red species gets pushed away uphill by the blue species. (Detailed descriptions of the numerical experiments will be omitted in this short highlight article.)

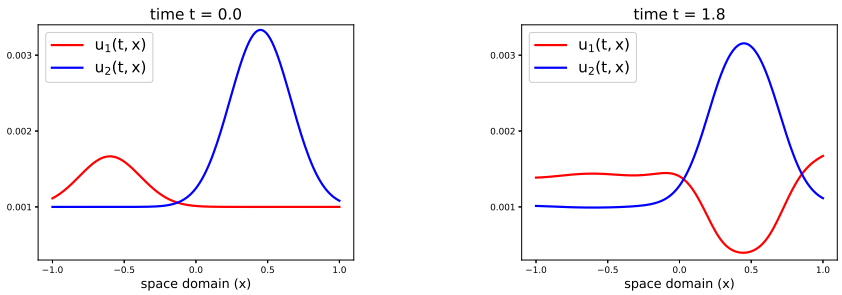


Fig. 2: *Uphill diffusion in the segregation cross-diffusion system (6) (n=2, k_1=17, k_2=1 & no-flux boundary c)*

(a) Density profiles at initial time

(b) Effect of uphill diffusion in u_1

Cross-diffusion systems are challenging to analyze mathematically, and explicit solution formulas are rarely available. Effective methods for their analysis often rely on specific structural conditions. In this article, we outline our recent results on the analysis of cross-diffusion systems enjoying a structure motivated by thermodynamics: the systems considered are driven by an entropy, and

dissipative effects are induced by a symmetric and positive semidefinite tensor acting on the driving forces. The symmetry of the dissipation tensor is linked to the famous *reciprocal relations*, also called *Onsager symmetry*—a concept attributed to the Nobel Prize laureate Lars Onsager that expresses a symmetry property of the transport coefficients in nonequilibrium systems modeling an irreversible thermodynamic process.

In the next section, we introduce key notions with a focus on parabolic cross-diffusion and briefly discuss the example in [2, 3]. Subsequently, we focus on a cross-diffusion system of hyperbolic–parabolic type, which arises in mathematical biology, and describe our approach in [1] towards its analysis. Certain types of symmetry properties turn out to be useful if not indispensable when it comes to deriving *a priori* estimates.

Entropy structure and Onsager symmetry

Consider a quasilinear second-order system of partial differential equations (PDEs) of the form

$$\frac{\partial u}{\partial t} = \nabla \cdot (\mathbb{A}(u)\nabla u), \quad \text{where } u = (u_1, \dots, u_n)^T,\ \mathbb{A}(u) \in \mathbb{R}^{n\times n}. \tag{1}$$

Formally, cross-diffusion is characterized by the presence of a non-vanishing off-diagonal term in the so-called *diffusion matrix* $\mathbb{A}(u)$. A fundamental question in the mathematical analysis of PDEs such as (1) concerns their well-posedness, which comprises three properties: the existence of a solution, its uniqueness, and the continuous dependence of the solution on the data. In order for system (1) to be well posed for suitable initial and boundary conditions, it is necessary to impose a structural condition on the matrix $\mathbb{A}$. Sufficient for the well-posedness on a short time interval is the spectral condition $\sigma(\mathbb{A}(u)) \subset \{z \in \mathbb{C} : \Re(z) > 0\}$, in which case the system is *parabolic* (in the sense of Petrovskii). For understanding the global well-posedness, spectral properties alone are insufficient.

Diffusive systems arising in thermodynamics often exhibit a formal gradient-flow structure, expressed as (cf. [6])

$$\dot{u} = -\mathcal{K}(u)D\mathcal{H}(u), \tag{2}$$

where $\dot{u} = \frac{\mathrm{d}}{\mathrm{d}t}u$, $\mathcal{H}$ denotes a (differentiable) driving functional and $\mathcal{K}$ the Onsager operator, a symmetric and positive semidefinite linear operator, whose symmetry property reflects the Onsager principle. In this article, we focus on systems (2) with $u = u(t,x) \in [0,\infty)^n, t > 0, x \in \mathbb{T}^d, n, d \in \mathbb{N}$, where $\mathcal{H}$ is given by an integral functional $\mathcal{H}(u) = \int_{\mathbb{T}^d} h(u)$ with $h \in C^2$ strictly convex and where the Onsager operator takes the form $\mathcal{K}(u)\xi = -\nabla \cdot (\mathbb{M}(u)\nabla\xi)$ with $\mathbb{M}(u) \in \mathbb{R}^{n\times n}$ symmetric and positive semidefinite. Inserting these choices into (2) yields (1) with

$$\mathbb{A}(u) = \mathbb{M}(u)D^2h(u). \tag{3}$$

Observe that the matrix $\mathbb{A}(u)$ need not be symmetric. But identity (3) implies that $\mathbb{A}(u)$ is diagonalizable over $\mathbb{R}$ and all its eigenvalues are nonnegative. Thus, if in addition $\operatorname{rank}\mathbb{A}(u) = n$, the PDE system (1) is parabolic. For parabolic cross-diffusion systems, the structure (3) is very useful in the construction of global-in-time weak solutions.

Entropy variables and symmetrization

Given an entropy function h on a convex domain $\widehat{\mathcal{D}} \subseteq (0,\infty)^n$, the so-called *entropy variable* $v := Dh(u)$ plays an important role in the construction of global (weak) solutions and the design of suitable approximation schemes. Notice that for h strongly convex and smooth, the differential Dh is a diffeomorphism onto its image. Recovering u from v via $u = (Dh)^{-1}(v) = Dh^*(v)$, where h^* is the Legendre transform of h, we deduce $u \in \widehat{\mathcal{D}}$ and thus $u_i \geq 0$ for all $i = 1,\dots,n$—a conclusion that can be seen as a substitute for a weak form of the maximum principle. Importantly, the change to entropy variables brings the PDE system (1), (3) in a symmetric form

$$D^2h^*(v)\partial_t v = \nabla\cdot(\mathbb{M}(u)\nabla v), \tag{4}$$

in which the entropy estimate is derived by taking as a test function the unknown v itself.

Example: Soret and Dufour effect

The Soret effect, also called *thermodiffusion*, refers to the occurrence of a diffusion flux caused by a thermal gradient. Its counterpart, according to Onsager symmetry, is the Dufour effect—a heat flux induced by a density gradient. In the joint paper [2], we established a global existence result for nonisothermal reaction–diffusion systems accounting for cross-effects of Soret and Dufour type. The approximation scheme in [2] is based on a variant of (4) including a higher-order elliptic regularization term. The usefulness of the thermodynamic structure for establishing weak–strong uniqueness of nonisothermal reaction–diffusion systems has been observed in [3] (see also [4]).

Cross-diffusion with incomplete diffusion

The condition $\operatorname{rank}\mathbb{A}(u) = n$ is not satisfied in all applications. For instance, biological tissue tends to separate into distinct regions, a behavior known as segregation, which is incompatible with complete diffusive mixing. In this context, we considered in [1, 5] the following cross-diffusion system

$$\partial_t u_i = \nabla\cdot(u_i\nabla(\mathbb{B}u)_i), \qquad i = 1,\dots,n, \tag{5}$$

where $\mathbb{B} \in \mathbb{R}^{n\times n}$ is such that $\mathbb{B}\mathbb{D}(\lambda) \in \mathbb{R}^{n\times n}$ is symmetric and positive semidefinite for some $\lambda \in (0,\infty)^n$, where $\mathbb{D}(\lambda) := \operatorname{diag}(\lambda_1,\dots,\lambda_n)$. This system generalizes the equations

$$\partial_t u_i = \nabla\cdot(k_i u_i \nabla p), \quad i = 1,\dots,n, \qquad \text{where } p = \sum_{i=1}^n u_i,\ k_i > 0, \tag{6}$$

obtained by the choice $\mathbb{B} = \mathbf{k}\otimes\mathbf{1}$, $\mathbf{1} := (1,\dots,1)^T$, $\mathbf{k} := (k_1,\dots,k_n)^T$, which is admissible with $\lambda = \mathbf{k}$. Equations (6) have been proposed in the mathematical biology literature and describe the mass-preserving transport of a system of n species with densities u_i, $i = 1,\dots,n$, along the velocity fields $-k_i\nabla p$, each of which points in the direction of fastest spatial decay of the total density p. Thus, the equations model species undergoing a directed motion in order to avoid spatial crowding.

System (5) has a gradient-flow structure of the form (3). Indeed, letting

$$h(u) = \sum_{i=1}^{n} \frac{1}{\lambda_i}(u_i \log u_i - u_i) \quad \text{and} \quad \mathbb{M}(u) = \mathbb{D}(u)\mathbb{B}\mathbb{D}(\lambda)\mathbb{D}(u),$$

we recognize in the product $\mathbb{M}(u)D^2h(u)$ the diffusion matrix $\mathbb{A}(u) = \mathbb{D}(u)\mathbb{B}$. Notice that $\operatorname{rank}\mathbb{A}(u) = \operatorname{rank}\mathbb{B}$ for all $u \in (0,\infty)^n$. Hence, if $r := \operatorname{rank}\mathbb{B} < n$, the PDE system is not parabolic, and we are faced with a borderline case, where local well-posedness cannot directly be inferred from classical literature, but may still be expected given the nonnegativity of all eigenvalues of $\mathbb{A}(u)$.

Normal form

To analyze the local well-posedness of (5), we introduced in [1] a change of variables that brings the system in a more canonical form, a so-called *normal form*.

Change of variables. Let $\Phi : (0,\infty)^n \to \mathcal{D} \subseteq \mathbb{R}^n$ be a diffeomorphism with inverse Ψ, and define $w := \Phi(u)$. Then, the equation for w takes the form

$$\partial_t w = \nabla \cdot (\hat{\mathbb{A}}(w)\nabla w) - (\nabla D\Psi(w)^{-1}) \cdot \mathbb{A}(\Psi(w))D\Psi(w)\nabla w, \tag{7}$$

where the diffusion matrix $\hat{\mathbb{A}}(w) := D\Psi(w)^{-1}\mathbb{A}(\Psi(w))D\Psi(w)$ is conjugate to $\mathbb{A}(\Psi(w))$. In particular, the two matrices share their spectrum and rank, which implies that $\operatorname{rank}\hat{\mathbb{A}}(\Phi(u)) = \operatorname{rank}\mathbb{A}(u) = r$ for $u \in (0,\infty)^n$.

A key point of the normal form is to choose Φ in such a way that $\hat{\mathbb{A}}(w)$ has a block structure

$$\hat{\mathbb{A}}(w) = \begin{pmatrix} \mathbf{0}_{(n-r)\times(n-r)} & \mathbf{0}_{(n-r)\times r} \\ \mathbf{0}_{r\times(n-r)} & \mathbb{A}_*^{\mathrm{II}}(w) \end{pmatrix}, \text{ where } \mathbb{A}_*^{\mathrm{II}}(w) \in \mathbb{R}^{r\times r} \text{ has full rank.} \tag{8}$$

In this case, the last r components $w_{\mathrm{II}} := (w_{n-r+1},\dots,w_n)$ satisfy a parabolic subsystem, and it remains to understand the structure of the $(n-r)\times(n-r)$ first-order subsystem that governs the evolution of $w_{\mathrm{I}} := (w_1,\dots,w_{n-r})$.

Symmetrization of first-order subsystem. If $r < n-1$, the quasilinear first-order subsystem of (7) satisfied by w_{I} is nonscalar, in which case its local well-posedness, for w_{II} fixed, becomes nontrivial. Crucial for the derivation of *a priori* bounds from energy estimates is *symmetrizability* (in a sense different from the Onsager principle). A first-order PDE system of the form

$$\mathbb{A}_0\partial_t v + \sum_{j=1}^{d} \mathbb{A}_j\partial_{x_j} v + F = 0, \tag{9}$$

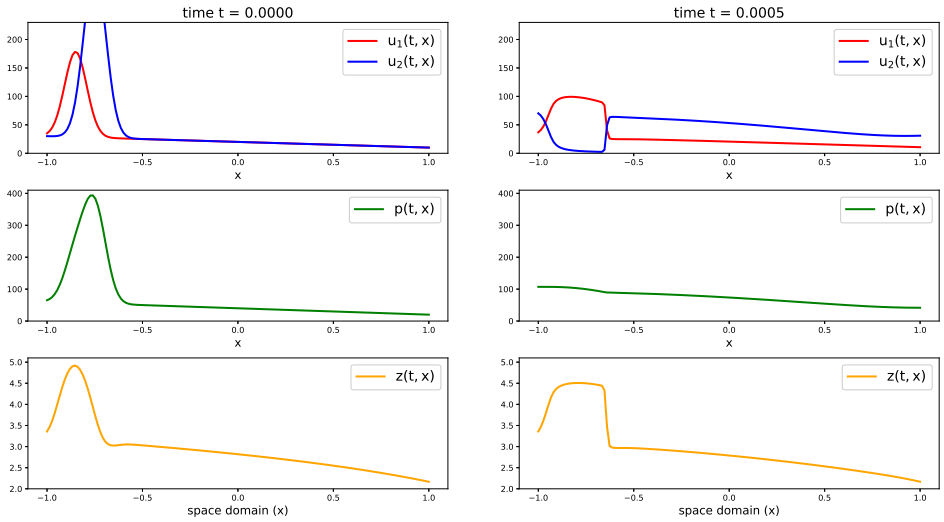
where $v = (v_1,\dots,v_m)$, $\mathbb{A}_j = \mathbb{A}_j(t,x) \in \mathbb{R}^{m\times m}$, $F = F(t,x) \in \mathbb{R}^m$, is called *symmetric hyperbolic* if the matrices $\mathbb{A}_j$, $j = 0,\dots,m$, are symmetric and if $\mathbb{A}_0$ is positive definite. System (9) is called *symmetrizable* if it can be cast in a symmetric hyperbolic form upon left-multiplication by a nonsingular matrix $\widetilde{\mathbb{A}}_0(t,x)$. Symmetrizability is classical for hyperbolic systems of conservation

laws with an entropy structure. However, the symmetrizability of the first-order subsystem in (7) (assuming (8)) is not immediate. In [1], we have established it by an explicit calculation for a (nonlinear) change of variables Φ based on an eigenbasis of the symmetric matrix $\mathbb{BD}(\lambda)$. As a matter of fact, in the new variables $w = \Phi(u)$ we obtained in [1] a system in normal form of symmetric hyperbolic–parabolic type, which reads as

$$\mathbb{A}_0^{\mathrm{I}}(w)\partial_t w_{\mathrm{I}} + \sum_{j=1}^{d} \mathbb{A}_1^{\mathrm{I}}(w, \partial_{x_j} w_{\mathrm{II}})\partial_{x_j} w_{\mathrm{I}} = f_{\mathrm{I}}(w, \nabla w_{\mathrm{II}}),$$
$$\mathbb{A}_0^{\mathrm{II}}\,\partial_t w_{\mathrm{II}} - \nabla \cdot \left(\mathbb{A}_*^{\mathrm{II}}(w)\nabla w_{\mathrm{II}}\right) = 0,$$

where $\mathbb{A}_0^{\mathrm{I}} : \mathcal{D} \longrightarrow \mathbb{R}^{(n-r)\times(n-r)}_{\mathrm{spd}}$, where $\mathbb{A}_1^{\mathrm{I}} : \mathcal{D} \times \mathbb{R}^r \longrightarrow \mathbb{R}^{(n-r)\times(n-r)}_{\mathrm{sym}}$ is linear in its second argument, and where $f_{\mathrm{I}} : \mathcal{D} \times \mathbb{R}^{dr} \longrightarrow \mathbb{R}^{n-r}$ is quadratic in its second argument. Furthermore, $\mathbb{A}_0^{\mathrm{II}} \in \mathbb{R}^{r\times r}_{\mathrm{spd}}$ is constant, and $\mathbb{A}_*^{\mathrm{II}} : \mathcal{D} \longrightarrow \mathbb{R}^{r\times r}_{\mathrm{spd}}$. By $\mathbb{R}^{m\times m}_{\mathrm{spd}}$, we denote the cone of symmetric positive definite real $m\times m$ matrices.

This normal form allowed us to apply existing methods for symmetric hyperbolic systems and (symmetric) parabolic systems separately to the respective subsystem. A short-time classical solution to the coupled hyperbolic–parabolic system, and thus also to (5), was then obtained by a contraction mapping argument.



(a) Profiles at initial time

(b) Shock in z at a later time

Fig. 3: *Parabolic (middle) & hyperbolic (bottom) part of normal form (11), and densities u_1, u_2 (top) (k_1=1, k_2=17)*

Example

For system (6) with $n = 2$, the change of variables introduced in [1] takes the form

$$w = (z, p) := (\Phi_{\mathrm{I}}(u), \Phi_{\mathrm{II}}(u)) = \left(\log(u_1^{1/k_1}/u_2^{1/k_2}), u_1+u_2\right), \tag{10}$$

and the PDE system in the new variables becomes an inhomogeneous quasilinear transport equation coupled to a quasilinear parabolic equation:

$$\begin{aligned} \partial_t z - c(w)\nabla p \cdot \nabla z &= f(w, \nabla p), \\ \partial_t p &= \nabla \cdot (a(w)\nabla p), \end{aligned} \tag{11}$$

where (with $u = \Phi^{-1}(w)$)

$$c(w) = k_1 + (k_2 - k_1)\frac{k_1 u_1}{a(w)} > 0, \quad f(w, \nabla p) = -\frac{(k_2 - k_1)}{a(w)}|\nabla p|^2, \quad a(w) = \sum_{i=1}^{2} k_i u_i.$$

Figure 3 illustrates the change of variables (10) leading to the normal form. The hyperbolic character of the z-evolution becomes apparent through the shock-type singularity that emerges when passing from Figure 3 (a) to (b).

Conclusion and outlook

Thermodynamic structures give rise to effective methods to analyze cross-diffusion, including change to entropy variables and symmetrization. For cross-diffusion with incomplete diffusion, local-in-time well-posedness in spaces of smooth functions relies on a change of variables that brings the underlying PDE system in a normal form. In this context, it would be interesting to identify, in more generality, the relevant structural properties that ensure symmetrizability of the resulting first-order subsystem. Another challenging question concerns the possibility of a finite-time breakdown of the local classical solution to (6), which we have only captured numerically so far (cf. Figure 3). Concerning the important questions of a global-in-time analysis of (5) for large data based on generalized solution concepts as well as numerical approximations preserving the thermodynamic structure, we refer to our recent preprint [5].

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1.5 Solving Parametric PDEs with Neural Networks

Martin Eigel and Janina Schütte

Deutsche Forschungsgemeinschaft

Fig. 1: *Deutsche Forschungsgemeinschaft*

FoDL priority program

Fig. 2: *SPP 2298 Theoretical Foundations of Deep Learning*

Deep learning has emerged as a versatile numerical tool in many application areas, recently extending its reach beyond natural language processing, image recognition and generation also into the realms of solving *partial differential equations* (PDEs). PDEs are mathematical models for a wide range of physical phenomena used in science and engineering, ranging from heat conduction, electrostatics, and (quantum) mechanics to fluid dynamics. Parametric PDEs (pPDEs) generalize the concept by adding (possibly infinitely many) parameters describing the data of the models. The significance of solving pPDEs lies in their crucial role for practical problems where uncertainties or a large set of data realizations have to be taken into account. Understanding the impact of varying model parameters, determined by prescribed probability distributions, is essential for predicting outcome statistics and for making reliable simulation-driven decisions. Deep learning offers a modern approach to tackle the high complexity of pPDEs. By training deep neural networks on appropriate data sets, these models learn intricate relationships between parameters and the corresponding system behavior. This expedites the solution process and, therefore, enables one to observe different states of the system under the influence of very many different parameters and efficiently evaluate statistical properties.

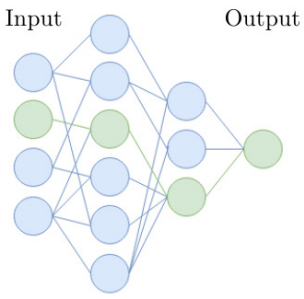

Fig. 3: *Visualization of a generic NN architecture*

Deep learning. Deep learning evolves around training *neural networks* (NNs), a class of function representations loosely inspired by the interconnections of neurons in a human brain. There are two main challenges when utilizing NNs for a problem at hand. First, the *architecture* of the NN has to be decided upon. This includes the number of neurons and the assumed connections between them. Second, the weights in the network, i.e., the strengths of the connections, need to be *learned*. The depth in deep learning comes from the way neurons are organized in an NN. It corresponds to the number of layers that an input passes through, as depicted in Figure 3. To solve pPDEs, it is possible to employ a special network architecture, called *convolutional neural networks* (CNNs), which are typically used for image data. It can be proven that the number weights and their values can be chosen such that the parameter-to-solution map is approximated arbitrarily well. To find these weights, the network has to be trained with many data points, consisting of pairs of parameters and corresponding solutions of the pPDE at hand. Since computing high resolution solutions with classical algorithms for given parameters as training data is expensive, we proposed a multilevel decomposition of the solutions, which works efficiently with a combination of a large set of computationally inexpensive coarse resolution data and a small set of expensive high resolution data.

Deep learning framework

Different deep learning methods have been proposed to tackle the task of finding a functional representation of the parameter-to-solution map. This can, e.g., be based on a reduced basis method [5], deep operator networks [6], Fourier neural operators [7], and physics-informed NNs (PINNs) [8]. Despite their large expressivity, these architectures have difficulties to live up to the

promising theoretical results in practical experiments, which is largely due to the challenging training process. In this article, a neural network architecture based on CNNs is constructed that can be trained efficiently in practice, reaching state-of-the-art accuracy for a class of pPDEs. Moreover, theoretical guarantees can be shown for the existence of CNNs that are able to approximate the solution operator arbitrarily well.

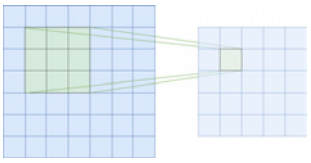

Fig. 4: *Visualization of the application of a kernel in a CNN architecture*

CNNs are a special class of neural networks designed for tasks involving visual data such as image recognition and computer vision. Applying the action of a network on an image involves the application of local kernels. Here, a kernel (equivalent to a small image) is multiplied to regions of the input image and summed over to yield an entry of the output image as illustrated in Figure 4. Furthermore, a nonlinear activation function, which decides how important a neuron is, such as the rectified linear unit function, or pooling operators are usually applied. An efficient architecture of CNNs is the U-Net, originally developed for biomedical image segmentation. It gets its name from the shape of its visualization as shown in Figure 5. By first contracting the input resolution to capture context of the input image and then expanding it to allow for localization, U-Nets are able to capture fine-scale as well as coarse-scale features of an image. Skip connections incorporate earlier computed results in later steps on each resolution level of the images, which gives the architecture the power to combine the information of different scales.

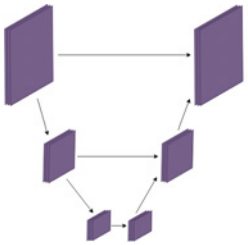

Fig. 5: *Visualization of a U-Net architecture*

When applied to solving pPDEs on a uniform grid, we have shown that the U-Net is able to approximate one step in a classical multigrid solver as used in finite element (FE) simulations; see [1]. Multigrid solvers leverage a hierarchical discretization of the problem to achieve fast convergence, combining coarse-scale solutions with smoothing and fine-scale corrections. When multiplying a $0-1$ mask to each image in the U-Net, we have shown that successive subspace algorithms can be approximated by the NN architecture; see [2]. This is required when the pPDE should be solved on an adaptively refined grid instead of a uniform grid, leading to more efficient approximations of the solution operator.

Parametric partial differential equations

There exist well-developed numerical methods to solve partial differential equations, specifically FE and finite volume methods. These methods can be extended to accommodate the setting of pPDEs. Prominent examples are, e.g., adaptive stochastic Galerkin FEM [4] or the variational Monte Carlo method [3], which are based on a polynomial chaos expansion and low-rank tensor approximations. The newly introduced NN-based methods are sample based and can be applied to data generated with a large class of linear and nonlinear pPDEs. In the analysis, the focus lies on the parametric (stationary diffusion) *Darcy problem*, which is also used as a benchmark problem in the numerical experiments and in many papers on uncertainty quantification. We define the problem in the following: Let $D \subset \mathbb{R}^d$ be a sufficiently smooth physical domain, here $\bar{D} = [0,1]^2$ is considered. Let $\Gamma \subset \mathbb{R}^{\mathbb{N}}$ be a possibly countable infinite-dimensional parameter space and $f : D \to \mathbb{R}$. We aim to approximate the map $u : \Gamma \times D \to \mathbb{R}$, which satisfies

$$\begin{cases} \nabla_x \cdot (\kappa(y,x)\nabla_x u(y,x)) = f(x) & \text{for } x \in D, \\ u(x) = 0 & \text{for } x \in \partial D \end{cases} \tag{1}$$

for the coefficient field $\kappa : \Gamma \times D \to \mathbb{R}$ and with derivatives with respect to the variable $x \in D$. The dependence of the parameter field on the parameter vector y is often characterized by a truncated *Karhunen–Loéve expansion* (KLE) for some $p \in \mathbb{N}$ given by

$$\kappa(y, x) = a_0(x) + \sum_{k=1}^{p} y_k a_k(x),$$

with $a_k : D \to \mathbb{R}$ for $k = 0, \dots, p$. We consider two problem settings, determined by the structure of κ. First, the *cookie problem* is defined for $\Gamma = [0, 1]^p$, $y \in \Gamma$ with uniformly distributed $y_k \sim U[0, 1]$ for $k = 1, \dots, p$, $a_0 = 0.1$, and $a_k = \chi_{D_k}$ indicator functions equal to 1 in D_k and 0 otherwise, where D_k are disks with fixed centers. Second, the *log-normal Gaussian coefficient* is defined for $\Gamma = \mathbb{R}^p$, normally distributed $y_k \sim \mathcal{N}(0, 1)$, and $\kappa(y, x) = \exp(\tilde{\kappa}(y, x))$, where $\tilde{\kappa}$ is defined by the KLE with $a_0 = 0$ and $\|a_k\|_\infty = 0.1k^{-2}$ for $k = 1, \dots, p$. A visualization of the cookie parameters, the log-normal coefficients, and the corresponding FE solutions can be seen in Figure 6 in the top and bottom row, respectively.

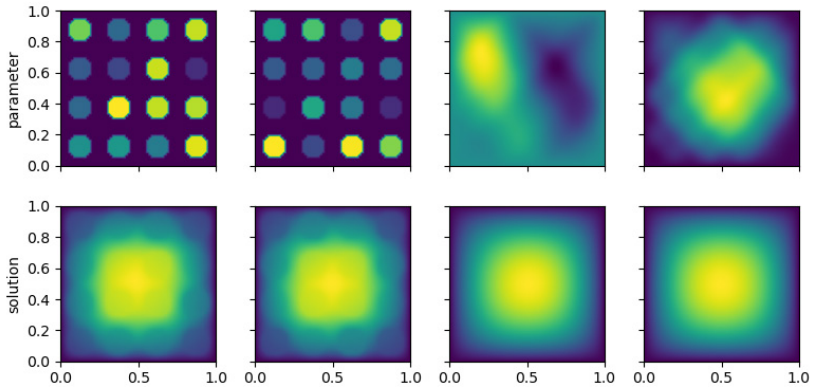

Fig. 6: *Realizations of parameter fields for the cookie problem (first two columns), the log-normal coefficient (last two columns), and the corresponding solutions of the parametric Darcy problem*

Solving parametric PDEs with neural networks

Multilevel decomposition. Training large NNs with many parameters is a key challenge in deep learning due to the nonlinearity and nonconvexity of the model class. Many aspects of the learning algorithm, such as the chosen optimizer, the learning rate, the batch sizes, and several more have to be considered. To circumvent the handling of large intractable NNs, we propose a multilevel decomposition of the data as depicted in Figure 7 and described in the following.

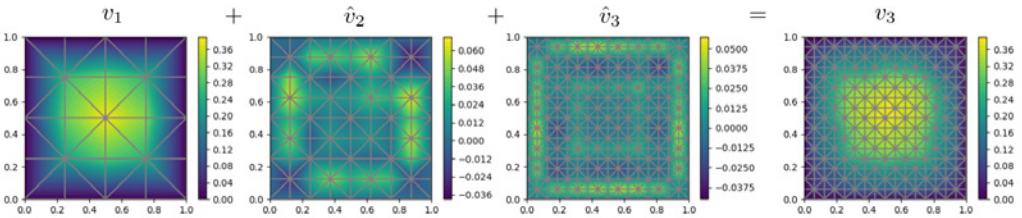

Fig. 7: *Visualization of the multilevel decomposition*

Let $V_1 \subset H_0^1(D)$ be a conforming piecewise linear (P_1) FE space on a uniform grid and let V_ℓ be the space on the uniformly refined grid of $V_{\ell-1}$ for $\ell = 2, \dots, L$, where $L \in \mathbb{N}$ is the number of levels. For the Galerkin projection v_ℓ of the solution of the PDE (1) for a fixed parameter $y \in \Gamma$ onto the space V_ℓ, let $\hat{v}_\ell := v_\ell - v_{\ell-1}$ be the correction of $v_{\ell-1}$ to the solution on the finer grid for $\ell = 2, \dots, L$. Then, individual CNNs can be trained to approximate the solution on the coarse grid v_1 and the corrections on the finer grids $\hat{v}_\ell$ for $\ell = 2, \dots L$. Due to solution smoothness, the entries of the corrections decrease exponentially over the levels. This yields a rapid decrease of importance and, therefore, of required accuracy in the fine grid-corrections, which can be translated to a reduced number of parameters in the CNN and a small number of expensive fine-grid training samples. In contrast, on coarse grids the accuracy has to be high, but only few FE coefficients have to be approximated, by which the network sizes can be controlled. Therefore, the decomposition leads to two advantages. On the one hand, the CNNs to be trained do not consist of a large amount of parameters. On the other hand, a small set of expensive-to-compute solutions on a fine grid suffices for training.

Network architecture. We derived a CNN architecture that can provably approximate the solution of the parametric Darcy problem in the conforming P_1 FE function space V_L on a uniformly refined square grid in the following sense: Denote by f_L and $\kappa_L(y)$ the coefficients of the interpolation of f and $\kappa(y, \cdot)$ in V_L, respectively. Assume that $\kappa_L(y)$ is uniformly bounded for all $y \in \Gamma$. We have shown that there exists a constant $C > 0$ such that for any $\varepsilon > 0$ there exists a CNN $\Psi : \mathbb{R}^{2\times \dim V_L} \to \mathbb{R}^{\dim V_L}$ with the number of parameters bounded by $CL\log(\varepsilon^{-1}) + CL^2$ such that

$$\|\Psi(\kappa_L, f_L) - v_L^c(y)\|_{H^1(D)} \leq \varepsilon \|f\|_*,$$

where $v_L^c(y)$ denotes the coefficients $v_L(y)$ with parameter field $\kappa_L(y, \cdot)$. The architecture of the considered CNN is depicted in Figure 8. Here, the first two yellow images depict the input containing the coefficients of the interpolated parameter field and the right-hand side in V_L. The orange outputs of the network correspond to the solution and corrections of the solution $v_1, \hat{v}_2, \dots, \hat{v}_L$. The different colored U-Nets have been shown to approximate multigrid solvers in the spaces $V_1, \dots, V_L$.

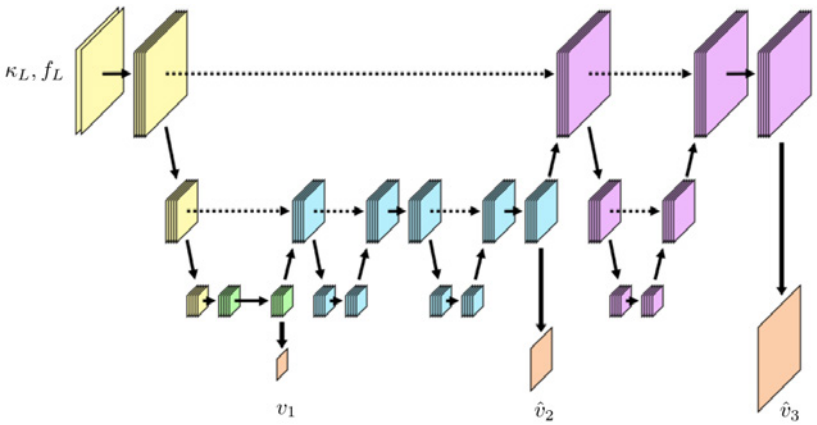

Fig. 8: *Example architecture of our multilevel CNN approximating the solution on $L = 3$ levels*

Numerical results. In the experiments, the overall error $\mathcal{E}^{\text{ref}}$ and the network error $\mathcal{E}^{\text{net}}$ are considered separately, where $\mathcal{E}^{\text{ref}}$ is the average $H^1(D)$ distance of the network output to a reference solution on a twice-uniformly refined grid, and $\mathcal{E}^{\text{net}}$ is the average $H^1(D)$ error of the network output to the Galerkin solution on the same grid.

problem	parameter dimension p	$\mathcal{E}^{\text{ref}}$	$\mathcal{E}^{\text{net}}$
cookie	16	7.09e−2 ± 1.87e−5	9.41e−4 ± 1.12e−4
	64	9.73e−2 ± 1.16e−5	1.85e−3 ± 1.38e−4
log-normal	10	5.33e−3 ± 2.93e−6	2.15e−4 ± 6.18e−5
	200	5.34e−3 ± 3.03e−6	3.00e−4 ± 1.43e−5

Table 1: *Multilevel CNN evaluated on test sets to solve the parametric Darcy problem*

In the experiments, it is evident that the network error is at least one magnitude smaller than the reference error, which implies that the reduction of the overall error can only be achieved by considering finer resolutions or better-suited FE discretization spaces. Uniformly refining the spaces quickly leads to an infeasible computational complexity as the number of parameters grows exponentially in the number of levels.

Adaptive refinement. Efficient discretization spaces V_h can be built iteratively to control the overall error $\mathcal{E} = \|u(y,\cdot) - u_h(y,\cdot)\|_{H^1_0(D)}$ for any $y \in \Gamma$, where u is the solution of (1) in $H^1_0(D)$ and u_h is its Galerkin projection onto V_h. The space is built in an adaptive way by starting with a coarse space V_1 and repeating the procedure:

$$\text{Solve on current space} \to \text{Estimate } \mathcal{E} \text{ locally} \to \text{Mark large error regions} \to \text{Refine marked regions.}$$

The resulting meshes for the cookie problem are visualized in Figure 9. A CNN architecture can be derived that approximates every step of the above iteration. Let $\mathcal{F} : \mathbb{R}^{\sum_{\ell=1}^{L} \dim V_\ell} \to V_L$ map coefficients to the corresponding FE function. Then, there exists a constant $C > 0$ such that for any $\varepsilon > 0$, number of iterations $K \in \mathbb{N}$, and local refinements $L \in \mathbb{N}$, there exists a CNN $\Psi : \mathbb{R}^{2\times \dim V_L} \to \mathbb{R}^{\sum_{\ell=1}^{L} \dim V_\ell}$ with at most $CLK \log(\varepsilon^{-1})$ parameters such that

$$\|u(y,\cdot) - \mathcal{F}(\Psi(\kappa_L(y), f_L))\|_{H^1(D)} \le \|u(y,\cdot) - u_h(y,\cdot)\|_{H^1(D)} + \varepsilon.$$

Conclusions and outlook

Convolutional neural networks are an efficient tool to solve pPDEs and are amenable to a thorough mathematical analysis. Theoretically, small approximation errors can be achieved with network sizes growing only logarithmically with the inverse of the required error bound. Numerically, the multilevel decomposition of the data allows for efficient training of small networks and with only few expensive and many cheap data samples. Solving a pPDE for a given parameter with the trained neural network only takes one forward pass of the network, which can be evaluated quickly to obtain statistical estimates of the solution. Interesting directions for future research are the application of this network architecture to more challenging (nonlinear, instationary) PDEs and using it in the context of statistical inverse problems.

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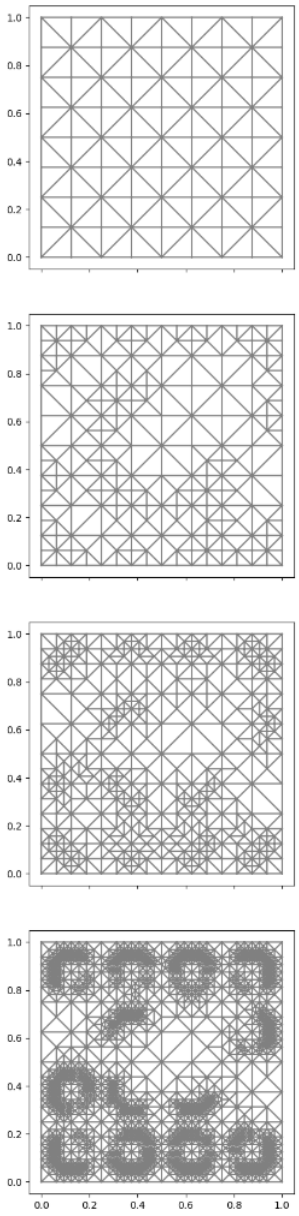

Fig. 9: *Adaptively refined meshes for the cookie problem with* $p = 16$ *inclusions*

1.6 Data-driven Regularization and Quantitative Imaging

Moritz Flaschel, Michael Hintermüller, Clemens Sirotenko, and Karsten Tabelow

Inverse problems are ubiquitous in all areas of science where measurements and data play a role. Numerous examples can be found in physics, economics, engineering, or medical imaging, which is the particular subject of this article. In general, inverse problems focus on the reconstruction of quantities $u_{true} \in X$ from measured noisy and degraded data $f \in Y$. Here, X, Y are typically normed vector spaces. It is often assumed that the process that generates the data is at least partially known a priory and can be described by a possibly nonlinear function $A : X \to Y$ called *forward mapping*. In the case of image reconstruction, we often consider an image domain $\Omega \subset \mathbf{R}^d$, e.g., a rectangle in $\mathbf{R}^2$. A continuous image on this domain is a function $u : \Omega \to \mathbf{R}^m$ where $u(x)$ describes, for instance, the image intensity or the color at the location $x \in \Omega$. To account for unknown errors in the data, we introduce the variable $\eta \in Y$. While in the field of nonparametric statistics, this error is modeled as a random variable following some known distribution $\eta \sim \mathbf{P}^Y$ on Y, the deterministic viewpoint assumes η just to be a norm-bounded highly oscillating function in Y. The overall data-generating process can eventually be described by the equation

$$f = A(u_{true}) + \eta \tag{1}$$

with f being either a Y-valued random variable or simply an element of Y, when the noise distribution is not modeled explicitly.

Model-based reconstruction. A natural approach to recovering u_{true} from measured data f could be to solve the least-squares problem

$$A^\dagger(f) = \operatorname*{argmin}_{u \in X} \frac{1}{2}\|A(u) - f\|_Y^2, \tag{2}$$

which defines an operator called *pseudo-inverse* $A^\dagger : R(A) \to X$ on the range $R(A)$ of the operator A. However, it is well known that this operator can be set valued, and even for bounded and linear A, the pseudo-inverse $A^\dagger$ is known to be discontinuous in many applications. This results in amplified errors and unstable reconstruction processes. The classical way to overcome these problems is to regularize the problem. Regularization generally describes the process of using prior knowledge about the appearance of the true solution. These are often properties like sparsity or additional smoothness. This approach leads to optimization problems of the type

$$\operatorname*{minimize}_{u \in X} D(A(u), f) + \mathcal{R}(\alpha, u). \tag{3}$$

Here, $D : Y \times Y \to \mathbf{R}$ denotes a distance-like function on Y, also called *data fidelity*, which is chosen depending on the noise distribution. The term $\mathcal{R}(\alpha, u)$ is used to penalize undesired behavior of the solution, e.g., fast oscillations. The parameter $\alpha \in U$ balances the influence of the regularizer $\mathcal{R}(\alpha, u)$ and the data-fidelity term $D(A(u), f)$. Often, $\alpha > 0$ is chosen to be scalar, but in order to account also for different regularization in different parts of the image domain, we allow that α lies in some general vector space U. The approach of representing estimators of clean images as minimization problems of type (3) is often called *variational* or *model-based approach*.

For a comparison of the least-squares and a regularized solution using a total variation (TV) penalty with scalar parameter; see Figure 1.

Weighted magnetic resonance imaging. The main examples that we want to focus on are weighted magnetic resonance imaging (MRI) and quantitative MRI (qMRI). The reconstruction of sensor data for complex weighted MRI can be mathematically described by the continuous Fourier transform. The forward operator reads in this case $A : L^2(\Omega, \mathbf{C}) \to L^2(\Omega_k, \mathbf{C})$ defined as $Au = P \circ \mathcal{F}u$ where $\mathcal{F}$ denotes the continuous Fourier transform, and P is a projection-type linear operator that selects a set of frequencies $\Omega_k \subset \mathbf{R}^2$ in the space of possible all frequencies, also called k*-space*. In Figure 1, a prototypical MRI setup and two reconstructions are depicted. A sampling mask is shown on the right-hand side, in which the white lines represent the frequencies in Ω_k that are actually sampled. If there are only a few white lines, this is referred to as *highly under-sampled* images. A practical disadvantage of classical weighted MRI is that the images depend on acquisition parameters that are not comparable across time and site. This problem will be addressed later by qMRI.

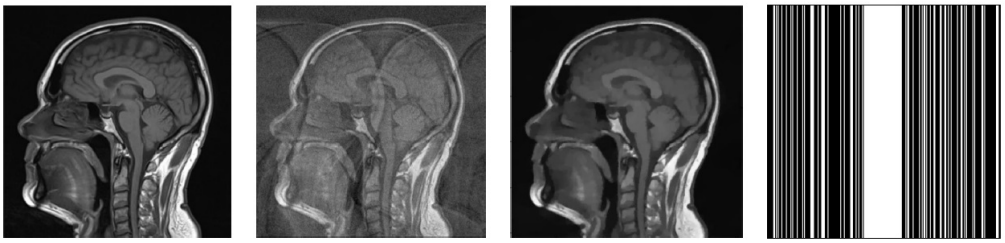

Fig. 1: *Different solutions of the MRI inverse problem. From left to right: Clean image u_{true}, least-squares solution $A^\dagger f$, total variation regularization, sampling mask.*

Data-driven regularization

While the model-based approach features nice theoretical properties, there might be some underlying structure in the data that is not captured by these handcrafted regularizers. One possible approach to incorporate additional knowledge, which is hidden in the data, is proposed in [2] where the classical TV minimization and its second-order extension, the total generalized variation (TGV), are combined with spatial adaptive regularization parameter choice; see also Figure 1 for an example of TV reconstruction with scalar parameters. In fact, we consider for the linear forward operator $A : X \to Y$ the problem

$$\underset{u \in X}{\text{minimize}} \quad \frac{1}{2}\|Au - f\|_Y^2 + \int_\Omega \alpha(x)\, \mathrm{d}|Du|\,. \tag{4}$$

Recall that $|Du|$ denotes the total variation of the measure-valued distributional derivative Du of u. For the sake of simplicity, we will concentrate here on TV only. The idea is to choose the spatially-dependent regularization parameter $\alpha \in C(\overline{\Omega})_{>0}$ adapted to the data f. In [2], the following unsupervised loss function is proposed:

$$L_{k,\sigma}(u, f) = \int_\Omega \max(k * (Au - f)^2 - \overline{\sigma}^2, 0) + \min(k * (Au - f)^2 - \underline{\sigma}^2, 0)\, \mathrm{d}x. \tag{5}$$

Here, the true variance $\sigma^2 > 0$ of $\eta \in Y$ must be known in advance, and $k : \mathbf{R}^n \to \mathbf{R}$ denotes a suitable L^1-normalized kernel with small support including zero. The function $L_{k,\sigma}(u, f)$ locally penalizes deviations of the averaged squared residual $(Au - f)^2$ from a small neighborhood $(\underline{\sigma}^2, \overline{\sigma}^2)$ around the known true variance $\sigma^2 > 0$. The approach results in the bilevel optimization problem

$$\begin{cases} \underset{u \in X, \alpha \in U_{ad}}{\text{minimize}} & L_{k,\sigma}(u, f) + r(\alpha) \\ \text{s.t.} & u = u(\alpha, f) \in \underset{u \in X}{\text{argmin}} \ \frac{1}{2}\|Au - f\|_Y^2 + \int_\Omega \alpha(x)\, \mathrm{d}|Du|, \end{cases} \tag{6}$$

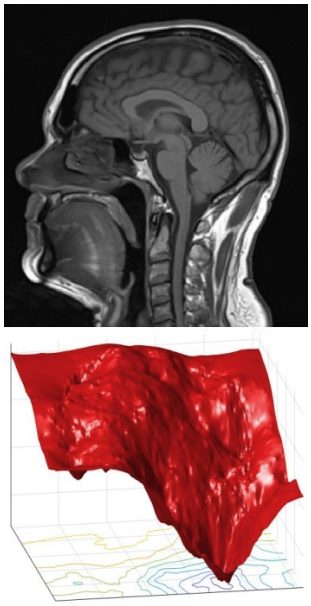

Fig. 2: *Spatially-dependent parameter for TGV regularization, which is found using the approach in [2]*

where $r : U \to \mathbf{R}$ enforces additional smoothness on α, and $U_{ad} \subset U$ is the set of admissible parameters. While this approach does not require training data, we still face a nonconvex, non-differentiable bilevel problem with solution in a nonreflexive Banach space. This problem class is notoriously difficult to solve due to the lack of standard constraint qualifications. To overcome these issues, additional smoothing techniques are presented in [2], which are known from optimal control theory to eventually find stationary points of an optimization problem where the constraints are given by a quasi-linear elliptic partial differential equation (PDE). These stationary points are found by utilizing a projected gradient descent approach, whose analysis is presented in an infinite-dimensional setup. The results of the proposed method are presented in Figure 2. Note that the regularization parameter, found by (6), is low in areas around the neck, where fine structures must be preserved, and high in smoother areas of the image. A natural extension of this work is presented in [3]. Here, the lower-level problem is approximated by k steps of an iterative solver that is known to converge to a solution of (4). Let the k-th step of this solver be denoted by $S_k(\alpha, f, u_0)$ when initialized at u_0. The spatially-adaptive regularization parameter $\alpha \in C(\overline{\Omega})$ is then replaced by a learnable structure, e.g., a neural network $\alpha_\theta : X \to C(\overline{\Omega})$ with parameters $\theta \in \Theta$. The resulting learning problem then reads

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \frac{1}{2M} \sum_{i=1}^{M} \|u_i^\dagger - u_i\|_X^2 + \frac{1}{2}\|\theta\|^2 \quad \text{s.t. } u_i = S_k(\alpha_\theta(A^\dagger f_i), f_i, A^\dagger f_i)\,, \tag{7}$$

where training pairs $(u_i^\dagger, f_i)_{i=1}^M$ are used that are generated according to $f_i = Au_i^\dagger + \eta_i$. The overall unrolled optimization algorithm has the structure of a multi-layer neural network, and (7) is a classical supervised learning problem whose solution can be approximated by using of the shelf stochastic optimizers like Adam (Kingma & Ba, 2014) alongside techniques from automatic differentiation. The setup is analyzed in [3] in finite dimensions for an unrolled primal-dual splitting algorithm (PDHG), and the convergence of the solutions of (7) to solutions of a suitable bilevel problem is addressed for $k \to \infty$.

Quantitative imaging

In contrast to weighted MRI, the goal of qMRI is the voxel-wise reconstruction of tissue parameters such as proton-spin density ρ and relaxation times T_1, T_2. These are sensitive to the biological tissue properties, allow for a quantitative comparison across different scanners and can be used as non-invasive disease markers. The general idea is to collect not only one, but multiple highly

under-sampled Fourier images $f_i = P_i \mathcal{F} u_i, i = 1, \dots L$ at subsequent time points $t_1 < \dots < t_L$. The images $u = (u_1, \dots, u_L)$ are implicitly connected to the physical quantity q by an equation $e(u, q) = 0$, where $e : X \times Q \to Z$ is an operator describing some physical law, and $q \in Q$ denotes the physical quantity of interest. In many cases, $e(u, q) = 0$ consists of partial or ordinary differential equations. This type of problem setting particularly fits for qMRI, which has been intensively investigated recently in [1]. Here, $u_i(x) = \rho(x)[m_1(x, t_i) + i m_2(x, t_i)] \in \mathbf{C}$, where $\rho(x)$ is the proton-spin density, and $m(x, t) = (m_1, m_2, m_3)(x, t)$ denotes the average magnetization of the hydrogen protons located at x at time t under the influence of some externally controlled magnetic field $B(x, t)$. The differential equation that describes this process is called Bloch equation:

$$\partial_t m(x,t) = m(x,t) \times \gamma B(x,t) - \left(\frac{m_1(x,t)}{T_2(x)}, \frac{m_2(x,t)}{T_2(x)}, \frac{m_3(x,t) - m_{eq}}{T_1(x)} \right)^\top . \qquad \text{(Bloch)}$$

Here $q = (\rho, T_1, T_2)(x)^\top$ denotes the physical quantity of interest. In [1] and forthcoming articles, a series of problems is analyzed that aim at extracting $q \in Q$ from the measurements f. Starting from the smooth constrained optimization problem

$$\underset{q \in \mathcal{C}_{ad}}{\text{minimize}} \quad \frac{1}{2} \| A\Pi(q) - f \|_Y^2 + \frac{\alpha}{2} \| q \|_Q^2 , \qquad (8)$$

fast solvers are developed and analyzed in function space using a smooth solution operator $\Pi : Q \to X$ of the equation $e(u, q) = 0$. However, this assumption is only rarely met in practice, where not every Bloch equation has an explicit solution operator. Moreover, the Bloch equation is only a mathematical model that uses simplified experimental assumptions that are far more complicated in reality. In order to account for this model uncertainty, the equation $e(u, q) = 0$ is replaced by some learned equation $e_\theta(u, y) = 0$ in which some parts or even the whole operator $e_\theta(\cdot, \cdot)$ is learned a priori from training data using a neural network with weights θ. The resulting optimization problem eventually reads in this case

$$\underset{u \in X, q \in Q}{\text{minimize}} \quad \frac{1}{2} \| Au - f \|_Y^2 + \frac{\alpha}{2} \| q \|_Q^2 \quad \text{subject to} \quad e_\theta(u, q) = 0 \text{ and } q \in \mathcal{C}_{ad}. \qquad (9)$$

As above, $\mathcal{C}_{ad} \subset Q$ denotes a convex, closed set of admissible parameters. This problem is much more involved than (8), due to the nondifferentiability that is introduced by using typical non-smooth activation functions of the neural network. In [1], stationarity concepts for these types of problems in infinite dimensions are developed and a sequential quadratic programming-type descent algorithm is proposed. One set of recovered physical parameters from noisy data is depicted in Figure 3.

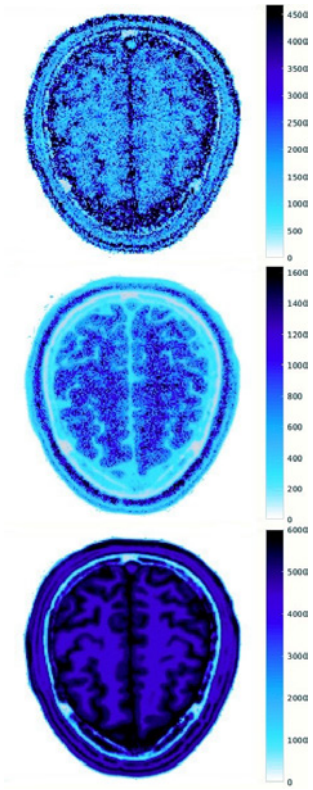

Fig. 3: *The results from the work [1]. The parameters $T1, T2$, and ρ are presented from top to bottom.*

Estimation bias

Even if we know the operator A from physics exactly or are convinced that it describes an appropriate model for the observed data f, the noise distribution η and the operator A do influence whether the estimates of u_{true} using, e.g., Eq. (2), are biased due to some nonlinearity of A or the noise η being non-Gaussian. As a real-world example, we consider measurements S from

diffusion-weigthed MRI (dMRI) which can be modeled by a diffusion kurtosis model (DKI):

$$S_{b,\vec{g}} = S_0 \cdot \exp\left(-bD + \frac{b^2}{6}\left(\frac{\mathrm{Tr}(D)}{3}\right)^2 W\right) + \eta\,, \tag{10}$$

where $D = \sum_{i,j=1}^{3} g_i g_j D^{ij}$, $W = \sum_{i,j,k,l=1}^{3} g_i g_j g_k g_l W^{ijkl}$, and acquisition parameters $b, \vec{g}$. Here, $u = (D^{ij}, W^{ijkl})$ are the components of the diffusion and kurtosis tensor and form the basic parameters of interest. This general DKI model can be simplified assuming a symmetry that can be justified by biophysical considerations. Moreover, the noise η is not Gaussian but Rician or, more generally, noncentral χ distributed as it refers to magnitude data from complex Gaussian noise. The resulting estimation bias has been examined in [4, 5], which shows different severity for different parameters from u due to the non-Gaussian noise, the nonlinearity of the operator, and the violation of assumptions for real data. Consequently, for parameter estimation not only noise reduction, e.g., through regularization, is important, but also appropriate bias reduction; see, e.g., Polzehl and Tabelow, *Low SNR in diffusion MRI models*, J. Amer. Statist. Assoc., **111** (2016), pp. 1480–1490.

Conclusions and outlook

The development and mathematical analysis of quantitative imaging methodologies is still at the beginning stage. Relevant topics for the application of qMRI range from the development of more sophisticated physical models encoded in the equation $e(u, q) = 0$ to the usage of modern data-driven regularization techniques, such as (coupled) dictionary learning or plug-and-play methods, that are able to incorporate prior knowledge from data while retaining interpretability and which can also be combined with handcrafted regularization techniques. Usually, these regularizers lead to high-dimensional nonconvex and nondifferentiable optimization problems for which the analysis is delicate. Current mathematical research focuses on the development and analysis of fast solvers for such problems and on the analysis of their regularization properties in dependence of the sampling methodology. Moreover, algorithms involving learned structures often are used in a finite-dimensional context. However, an infinite-dimensional setup is particularly important in physical imaging. Not only because the algorithms should work resolution-independently, but also because the physical models are provided in the continuous regime. For this reason, there is a natural demand to extend these data-driven regularization techniques to an infinite-dimensional setup. This topic is also of particular relevance in the current work.

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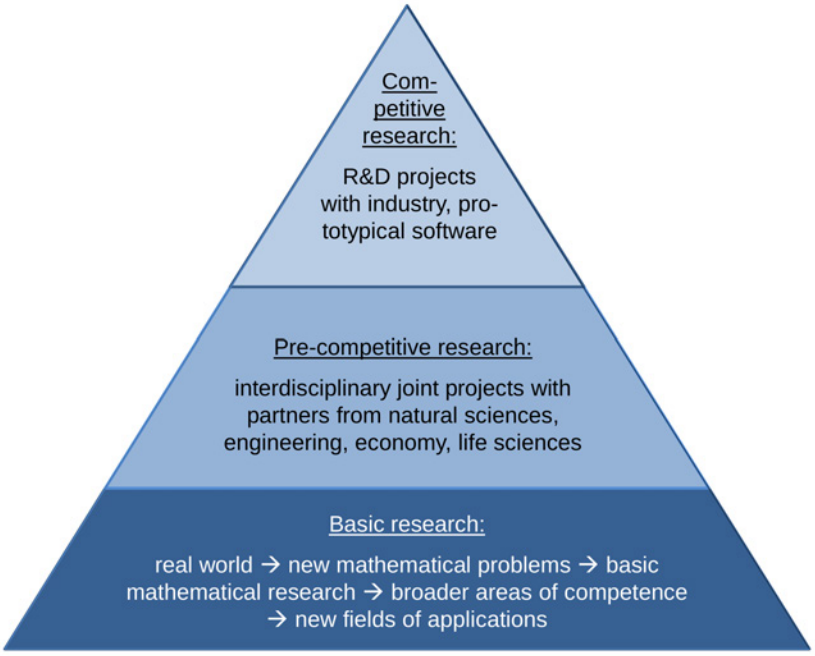
2 WIAS in 2023

2.1 Profile

The *Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Leibniz Institute in Forschungsverbund Berlin e. V. (FVB)* is one of seven scientifically independent institutes forming the legal entity FVB. All the institutes of FVB belong individually to the *Leibniz Association (WGL)*. The *Director of WIAS* is responsible for the scientific work at WIAS, the *Managing Director* of the 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 multidisciplinary 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 Berlin universities and the supervision of theses to the mentoring of postdoctoral researchers and to the preparation of, currently, three trainees to become "mathematical technical software developers."

WIAS promotes 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. WIAS coordinates the **Leibniz Research Network "Mathematical Modeling and Simulation (MMS)"** connecting 36 partners from all sections of the Leibniz Association. Modern methods of MMS are imperative for progress in science and technology in many research areas. The activities of the network are supported by a grant from the Strategic Fund of the Leibniz Association. The Leibniz MMS Days 2023 took place from April 17 to 19 at the Leibniz Institute for Agricultural Engineering and Bioeconomy (ATB) in Potsdam. It was attended by 61 scientists from 21 institutions. A Leibniz MMS AI (Artificial Intelligence) School took place from October 16 to 19, 2023, at the Leibniz Institute of Surface Engineering e.V. in Leipzig together with experts from the Center for Scalable Data Analytics and Artificial Intelligence. 40 participants had the opportunity to learn the basics of machine learning and gain practical experience in using common tools.

The **Mathematical Research Data Initiative (MaRDI)**, funded for five years since Oct. 1, 2021, (http://www.mardi4nfdi.de/) is the mathematical consortium within the German *Nationale Forschungsdateninfrastruktur (NFDI)*. WIAS's role within MaRDI is twofold: It coordinates the consortium, and it performs part of its work program in two areas of specific expertise, namely statistics and machine learning and interdisciplinary mathematics. The goal of MaRDI is to build an infrastructure for mathematical research data and knowledge that adheres to the FAIR principles, i.e., to make data findable, accessible, interoperable, and re-useable. Thereby, data will be better documented, potential re-invention of the wheel can be avoided, and reproducibility of research results can be improved. However, FAIR data does not automatically imply open data, rather accessibility can be regulated by suitable licences. This is especially important in interdisciplinary mathematical research where data access might be restricted due to requirements by law or the cooperation partners.

MaRDI is currently working in its third year and has been actively developing services for the community. MaRDI has successfully launched the initial version of the Portal https://portal.mardi4nfdi.de importing metadata from several sources like the Digital Library of Mathematical Functions (DLMF), arXiv, CRAN, and many more into the MaRDI knowledge graph. Other services have already been prototyped, like the knowledge graph on mathematical algorithms (https://algodata.mardi4nfdi.de) or the knowledge graph on mathematical models. These and other services will be integrated into

the MaRDI Portal making it a central one-stop point of access. The broad availability of the services and their development closely with researchers from disciplines other than mathematics support the overall goal of building one NFDI.

Another important line of work is the assistance of researchers in their research data management (RDM) planning. A common tool is RDMO, where MaRDI provides a plugin MaRDMO tailor-made for mathematical projects. Currently, the plugin is rolled out in several institutions and excellence clusters for further refinement. In 2023, the consortium published a white paper on RDM for grant proposals and research projects that researchers can use when writing proposals or creating data management plans for their project, supplementing the existing DFG checklists.

MaRDI has a general outreach program, including a 4-issue Newsletter focusing on specific topics related to research data and its management (https://www.mardi4nfdi.de/community/newsletter; subscribe), a MaRDI station including a game on research data and the FAIR principles that will be part of the exhibition on the ship MS Wissenschaft later in 2024. In addition, lectures, workshops, and mini-symposia in the areas of discrete mathematics, scientific computing, and computer algebra, or for a broader audience have been organized.

How WIAS is handling its own research data is one focus of the **research data management (RDM) / library department**. It aims to provide researchers with services, recommendations for action and operational support for research data management. The specifics of the software and data strategy are also accompanied by the Commission for Software and Research Data Management, which is developing concepts for software and research data in a common structure.

MATH+

WIAS has a number of cooperation agreements with universities. The main joint project with the Berlin universities is **the 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), which has been funded since January 2019. The WIAS Director, Michael Hintermüller, is a founding member (PI) of MATH+ and since November 2022 Chair of the center. 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.

BR50

Berlin's non-university research institutions launched a joint initiative in 2020 to strengthen the capital's role as an international science hub. They have formed **BR50 (Berlin Research 50)**. The WIAS Director Michael Hintermüller was one of the four founding coordinators and is now the spokesperson for Unit 4 (Technology and Engineering).

2.2 Structure and Scientific Organization

2.2.1 Structure

From a mathematical point of view, the institute is divided into research groups that each have special strengths and work on cooperative problem-solving. If there is a current demand, due to certain problem areas and topics arising, additional temporary and short-term groups are set up in a Flexible Research Platform. In 2023, WIAS was organized into the following divisions for fulfilling its mission: Eight research groups, two Leibniz groups (funded by the Leibniz Association), two Weierstrass groups (funded by WIAS), and two Focus Platforms[1] (also funded by WIAS) form the scientific body of the institute. In their mission, they are supported by the departments for technical and administrative services.

The Secretariat of the International Mathematical Union (IMU, see page 64), hosted by WIAS, is a supportive institution for the international mathematical community. Moreover, WIAS hosts the German Mathematics Association DMV and the Society of Didactics of Mathematics GDM.

Research Groups:

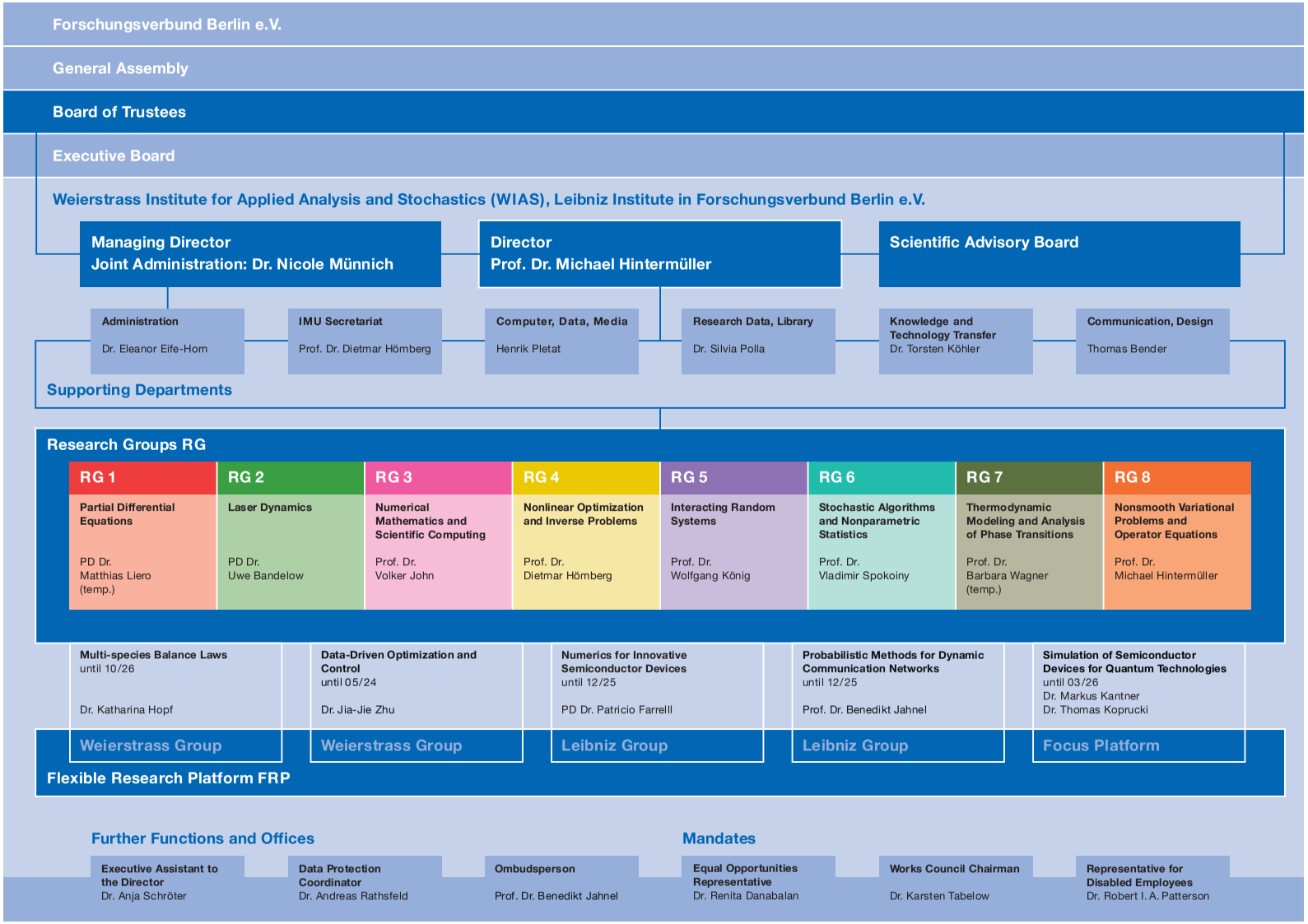
RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing
RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase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

Flexible Research Platform:

LG NUMSEMIC. Numerical Methods for Innovative Semiconductor Devices
LG DYCOMNET. Probabilistic Methods for Dynamic Communication Networks
WG BIP. Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes (until June 30, 2023)
WG DOC. Data-driven Optimization and Control
WG MBaL. Multi-species Balance Laws (from November 1, 2023)
FP 1. Quantitative Analysis of Stochastic and Rough Systems
FP 2. Simulation of Semiconductor Devices for Quantum Technologies

The organization chart on page 52 gives an overview of the organizational structure of WIAS in 2023 (as of Dec. 31, 2023).

[1] In the following, the terms “research group” will often be abbreviated by “RG,” “Leibniz group” by “LG,” Weierstrass group by “WG,” and Focus Platform by “FP.”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RG 8
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Prof. Dr. Michael Hintermüller
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Dr. Robert I. A. Patterson

2.2.2 Main Application Areas

The research at WIAS focused in 2023 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

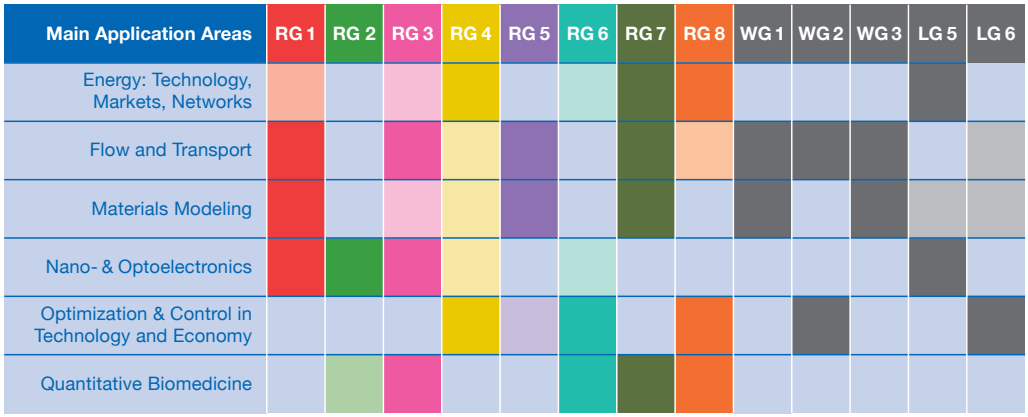
- **Energy: Technology, Markets, Networks**
- **Flow and Transport**
- **Materials Modeling**
- **Nano- and Optoelectronics**
- **Optimization and Control in Technology and Economy**
- **Quantitative Biomedicine**

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

2.2.3 Contributions of the Groups

The eight research groups, the Leibniz groups, and the Weierstrass groups 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 2023 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).



Here, WG BIP is called WG 1, WG DOC becomes WG 2, WG MBaL WG 3, LG NUMSEMIC LG 5, and LG DYCOMNET LG 6 (the latter are the groups no. 5 and 6 that were/are supported until now by the Leibniz Association at the WIAS).

In the following, special research topics are listed that were addressed in 2023 within the general framework of the main application areas.

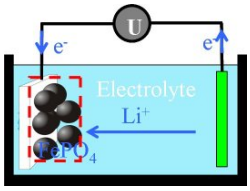


Fig. 1: *Sketch of a lithium-ion battery (LiFePO4)*

Energy: Technology, Markets, Networks

This main application area takes account of an economic use of energy 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. Furthermore, RG 4 and RG 8 investigate aspects of uncertainty in energy management via stochastic optimization or uncertainty quantification. 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 3)
- Modeling of experimental electrochemical cells for the investigation of catalytic reaction kinetics (in RG 3)
- Lithium-ion batteries (in RG 1, 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 PDE systems (in RG 8)
- Modeling and simulation of charge transport in perovskite solar cells (in LG NUMSEMIC)
- Modeling and optimization of weakly coupled minigrids under uncertainty (in RG 4)
- Modeling of gas/power markets using physics of gas transport under uncertainty (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 or interacting random systems. 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 have become important in the research of the institute.

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 and LG NUMSEMIC)
- Modeling and numerical methods for particle systems (in RG 1, RG 5, and WG DOC)
- 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 LG DYCOMNET)
- Thermomechanical modeling, analysis, and simulation of multiphase flows (with free boundaries; in RG 1, RG 7, and WG BIP)
- Theoretical analysis of intermittent mass flow through random media (in RG 5)
- Gradient flow and optimal transport applications to machine learning and data-driven optimization (in WG DOC)
- Analysis, simulation, and optimal control of nonlinear electrokinetics in anisotropic microfluids (in RG 4)

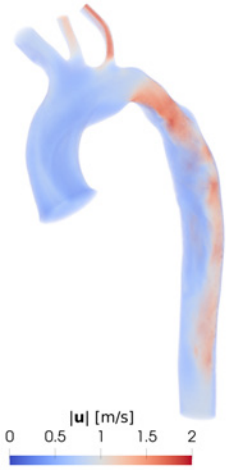


Fig. 2: *Simulation of pulsatile blood flow in an aortic coarctation, snapshot of the velocity field*

Materials Modeling

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.

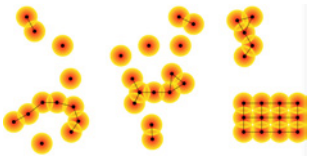


Fig. 3: *A realization of a many-body system showing a small crystal in the lower right corner*

Core areas:

- Homogenization and localization in random media (in RG 1, RG 5, and LG DYCOMNET)
- Stochastic and thermodynamic modeling and analysis of phase transitions, e.g., of condensation, crystallization, or gelation type (in RG 1, RG 4, RG 5, and LG DYCOMNET)
- Asymptotic analysis of nano- and micro-structured interfaces, including their interaction with volume effects (in RG 7 and WG BIP)
- Dynamical processes in nonhomogeneous media (in WG BIP, RG 1, RG 5, RG 6, and RG 7)
- Material models with stochastic coefficients (in RG 1, RG 4, RG 5, RG 7, and LG DYCOMNET)

- Modeling and analysis of complex fluids including suspensions, hydrogels, polyelectrolytes, proteins (in RG 1, RG 7, and WG BIP)
- Thermodynamically consistent electrochemical models of lithium-ion batteries, fuel cells, and solid oxide electrolytes (in RG 3 and RG 7)
- Hysteresis effects, e.g., in electro/magneto-mechanical components, elastoplasticity, lithium batteries (in RG 1, RG 7, and WG BIP)
- Modeling of elastoplastic and phase-separating materials including damage and fracture processes (in RG 1, RG 7, and WG BIP)
- Derivation and analysis of local and nonlocal phase field models and their sharp-interface limits (in RG 7 and WG BIP)
- Modeling and simulation of electronic properties of perovskites (in LG NUMSEMIC)

Nano- and Optoelectronics

Optical technologies are among the key technologies of the 21st century as they enable innovative infrastructures that are essential for the further digitalization of industry, science, and society. Currently emerging quantum technologies are expected to provide tap-proof communication networks, fast information processing devices, and extremely sensitive sensors in the future.

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.

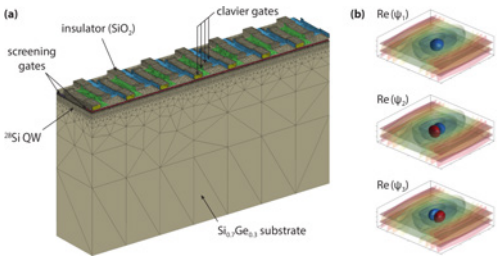


Fig. 4: *(a) Quantum bus for coherent transfer of quantum information in semiconductor quantum processors based on gate-defined quantum dots in Si/SiGe heterostructures. (b) Snapshots of low-energy electronic orbitals of the transported electron spin-qubit in the quantum bus; see also Scientific Highlights article on page 23.*

Core areas:

- Microelectronic devices (simulation of semiconductor devices; in RG 1, RG 2, RG 3, and LG NUMSEMIC)
- Mathematical modeling of semiconductor heterostructures (in RG 1 and LG NUMSEMIC)
- 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, RG 2, and FP 2)
- Laser structures and their dynamics (high-power lasers, photonic crystal surface emitting lasers, ultra-narrow linewidth lasers, UV-C lasers; in RG 1, RG 2, RG 3, and FP 2)

- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in RG 2)
- Photovoltaics, OLED lighting, and organic transistors (in RG 1 and RG 3)
- Electronic properties of semiconductor nanostructures such as nanowires and quantum dots (in RG 1, RG 2, LG NUMSEMIC, and FP 2)
- Simulation of semiconductor devices for quantum technologies (in RG 1, RG 2, and FP 2)

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 or telecommunication systems, 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.

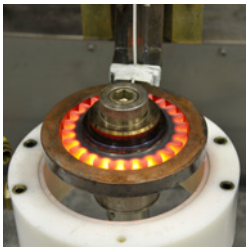


Fig. 5: *Induction heat treatment of a gear*

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, and mobile device-to-device communication systems.

Core areas:

- Simulation and control in process engineering (in RG 4, RG 6, and WG DOC)
- Problems of optimal shape and topology design (in RG 4 and RG 8)
- Optimal control of multi-field problems in continuum mechanics and biology (in RG 3, RG 4, and RG 7)
- Analysis of the spread of malware through a spatial ad-hoc telecommunication system and of the influence of random countermeasures (in LG DYCOMNET)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6 and WG DOC)
- Optimal control of multiphase fluids and droplets (in RG 8)
- Optimization for machine learning and data-driven applications (in WG DOC)

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 neuro-sciences are considered. They include classical tasks like registration, denoising, equalization, and

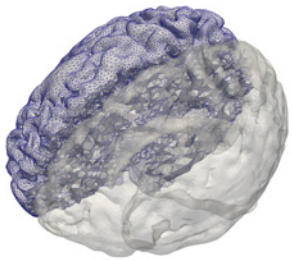


Fig. 6: *Computational model of brain tissue obtained from 3D MRI images*

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 and numerical models for a better understanding of hemodynamic processes are developed and investigated. 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 or 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 Activities in Equal Opportunities and Work-Life Issues

WIAS is committed to diversity, equity, and inclusion. In particular, the active promotion of equal opportunities, including gender equality and persons with disabilities, is an important management task at WIAS that is firmly anchored in the institute's mission. This aim is to be achieved both by creating a family-friendly environment and by the equal opportunities officers' involvement in staffing procedures.

A decision taken by the WIAS scientific management sees one of its members taking charge of equal opportunities issues for a period of three years each. This is a rotational appointment, and Dietmar Hömberg, head of Research Group 4 *Nonlinear Optimization and Inverse Problems*, is designated as the person in charge from 2023 to 2025.

Renita Danabalan as the Equal Opportunities Officer and Andrea Eismann as her deputy have been active in the recruitment process at WIAS. This includes reading applications and participating in job interviews to ensure that in the case of equal qualifications and suitability, persons of the underrepresented gender be given preferential consideration.

Aside from recruitment, they were part of the writing team for the WIAS Equal Opportunities Plan 2024–2027. One of the new measures in the plan is targeted to promote female postdocs. This was launched in 2023 as a part of the **Iris Runge Program (IRP)**, so named after a female German applied mathematician and physicist. This is an open call to early-stage female postdoctoral researchers (up to three years after completion of Ph.D.) to apply for a position at WIAS. Successful candidates will be integrated into a Research Group of their choice for a duration of 2–3 years. Long-term appointments

will be possible. The IRP will be open to both internal and external applicants. Additionally, Renita Danabalan was also a part of the team to implement institute-wide measures based on the outcome of the Employee Satisfaction survey.

In 2023, two new female master's degree candidates were recruited as student assistants at WIAS in the WIAS Female Master Students Program. Three former graduates of the program started their doctorate at WIAS.

For the first time in late 2022, the bi-annual employee survey was carried out by a professional institute, which organized also the evaluation and consulted the institute in various ways. Afterwards, a committee was founded that discussed concrete wishes and desires for measures to the benefit of the daily work life with the status groups. As a consequence, a number of measures were examined and finally realized, like a buddy system, a mentoring system, and regular social activities, and the intranet information was greatly expanded. Further measures are to follow.

audit berufundfamilie. Since 2013, WIAS has been certified and re-certified as a family-friendly employer by the "audit berufundfamilie." The certificate demonstrates the Institute's ongoing commitment to a sustainable personnel policy that cares about the needs of employees in different life phases and family situations. In March 2023, following the successful fourth re-certification, the dialogue process for the audit was completed. WIAS was awarded the certificate with distinction, which now has a permanent character. The certificate was presented to the Director of WIAS (in the middle of the group on the photo) at a festive ceremony held in June in the presence of the Federal Minister for Family Affairs.

The implementation and continuation of the family-friendly measures is monitored and supported by the work-and-family team. In March, the team's project management was transferred from Olaf Klein to Pia Pfau. The role of management representative was taken over by Dietmar Hömberg, who will assume this task until the end of 2025. Veronica Bove assists the team as secretary. The

team kept employees regularly informed about issues and events such as webinars and online talks, e.g., on parenting, care, health, and resilience. On November 26, 2023, a workshop for employees was conducted in German and English on the topic of stress management and burnout prevention. The event was held in collaboration with benefit@work, which presented its support services at an information stand after the workshop. The family service agency benefit@work is available for employees to offer support in balancing work and private life. In difficult life and work situations, staff members additionally have the option of contacting a qualified therapist and receive free individual coaching. On December 8, 2023, the work-and-family team organized a children's Christmas party for the employees' younger children, with stories and activities about the Christmas elves and a visit by Father Christmas.

The bi-lingual intranet pages on work-life balance were completely revised in 2023. Employees find comprehensive information on the options and benefits available, as well as documentation on the progress and future goals of the Institute's family- and life-phase-conscious personnel policy. The already high standards established in the "Company agreement regarding the compatibility of career and family" are being continuously improved and strengthened. Options such as flexible working hours and mobile working are highly valued. They enable to balance work and private life – an important part of today's world of work with advancing technological developments and demographic change.

2.4 Grants

The successful acquisition of third-party funded projects in 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 2023, having raised a total of 3.62 million euros, from which 53 additional researchers [2] (plus 14.5 outside WIAS; Dec. 31, 2023) were financed. In total in 2023, 25 percent of the total budget of WIAS and 44.9 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 132ff.

2.5 Participation in Structured Graduation Programs

Graduate School *Berlin Mathematical School (BMS)*

Berlin Mathematical School

Berlin's mathematicians were 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.

[2] Including scholarship holders.

International Research Training Group (IRTG) 2544 *Stochastic Analysis in Interaction* of the DFG

In 2020, this International Research Training Group was installed for 4.5 years at the Technische Universität Berlin; it is run jointly by about 15 researchers in probability from Humboldt-Universität zu Berlin, Freie Universität Berlin, the WIAS (RG 5 and RG 6), and the University of Oxford. It is a particularly visible activity of the Oxford–Berlin Research Partnership, which has been launched by a Memorandum of Understanding in December 2017.
For more information see https://www3.math.tu-berlin.de/stoch/IRTG/ and https://www.berlin-university-alliance.de/commitments/international/oxford/index.html.

Within this IRTG, in 2023, the WIAS participated with two Ph.D. projects running in RG 5 on “Phase transitions in random loop models” (until Sept. 2023) and “Large deviations for spatial dense random graphs” (since April 2023) and with one Ph.D. project running in RG 6 on “Numerics for rough paths and SPDEs” (until April 2024).

Interdisciplinary Research Training Group (RTG) 2433 *Differential Equation- and Data-driven Models in Life Sciences and Fluid Dynamics (DAEDALUS)* of the DFG

DAEDALUS
RTG 2433

The main goal of DAEDALUS, based at the Technische Universität Berlin, consists in studying the interplay between data-based and differential equation-based modeling. DAEDALUS focuses on applications in life sciences as well as in fluid dynamics. A WIAS-supervised project (in RG 3) for a student from the second cohort, which started in 2021, studies data-driven methods for the non-invasive estimation of blood flow biomarkers from phase-contrast MRI data.

2.6 Scientific 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 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 195ff. 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

3.1 The Secretariat of the International Mathematical Union (IMU)

Since January 2011, the Secretariat of the International Mathematical Union (IMU) has been permanently based in Berlin, Germany, at WIAS. Under the supervision of the IMU Executive Committee (EC), 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 between WIAS and the 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 enter into a new and unlimited Cooperation Agreement, which was signed immediately after the General Assembly.

The offices of the IMU Secretariat are located on the fourth floor of Hausvogteiplatz 11A, close to the main building of WIAS.

Staff members

Dietmar Hömberg *Head of the IMU Secretariat and IMU Treasurer*. D. Hömberg is a professor at Technische Universität Berlin, and head of Research Group 4 at WIAS. He has been Head of the Secretariat and IMU Treasurer since July 2020. In his function as the Head of the Secretariat, he is responsible for the IMU Secretariat as a separate unit within WIAS. As IMU Treasurer he reports to the IMU EC and is responsible for all financial aspects, including collecting dues, financial reports, and drafting the budget of the IMU.

Scott Jung, *Manager of the IMU Secretariat*. S. Jung's responsibilities include heading and supervising the administrative operations of the Secretariat and actively supporting the IMU Secretary General in the implementation of the decisions and duties of the IMU EC and the IMU General Assembly. He communicates with IMU members, drafts written materials, writes minutes and reports, and supervises the IMU website. His tasks include steering and overseeing the Secretariat's operations and IMU finances, and also deadline monitoring.

Lena Koch, *ICMI and CDC Administrative Manager*. L. Koch's responsibilities include administratively supporting the activities of CDC and ICMI. This refers, in particular, to promoting the work of both commissions, managing their web presence—including public relations and communications—and handling grant applications and support programs.

Mariusz Szmerlo, *IMU Accountant*. M. Szmerlo is, under the supervision of the IMU Treasurer, in charge of executing the financial decisions of the IMU, which includes 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 preserving and making paper documents, photos, pictures, and IMU artifacts accessible, as well as supporting the decision process concerning the electronic archiving of IMU documentation. She also provided additional administrative support to CWM in 2023.

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 facilitating various IT services for IMU members, commissions, and committees.

Vanessa Chung, *Project Assistant*. V. Chung joined the IMU Secretariat in January 2021. Her primary 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.

IMU Secretary General

Christoph Sorger is the IMU Secretary General for the 2023–2026 term. He is Professor of Mathematics at Université de Nantes in France. He maintains regular contact with the IMU Secretariat via electronic communication and frequently visits the office.

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

3.2 A New Term: 2023–2026

A new term of office began on January 1, 2023, with the newly-elected IMU office holders taking up their respective roles for the 2023–2026 term. The IMU Secretariat provided support for the induction of the new office holders and hosted the first meeting of the newly-elected IMU EC at the Secretariat's premises in Berlin in March 2023. At this meeting, a number of important tasks were completed, in particular, the selection of the new ICM Program Committee and Fields Medal Committee, so that these committees could already begin their work in preparation for the next International Congress of Mathematicians (ICM) in 2026.

Following the vote of the 19th IMU General Assembly in Helsinki in 2022 to accept the bid from the United States of America to host ICM 2026 and the 20th IMU General Assembly, the IMU announced in August 2023 that

Fig. 1: *ICM 2026 Logo*

ICM 2026 will take place over July 23–30, 2026, in Philadelphia, USA.

The 20th IMU General Assembly will be held in New York City, USA, on July 20–21, 2026.

These are the final, confirmed dates of ICM 2026 and the 20th IMU General Assembly. The official website of the Congress is www.icm2026.org.

The ICM 2026 Program Committee Chair is Claire Voisin, CNRS, Institut de Mathématiques de Jussieu-Paris Rive Gauche, France. Preparations for ICM 2026 in Philadelphia have thus already begun, and will continue to shape the Secretariat's work over the coming period, as will the organization of the 20th IMU General Assembly.

3.3 Commission for Developing Countries

Andrea Solotar, CDC President (2023–2026) and Ludovic Rifford, CDC Secretary for Policy (2023–2026)

The IMU hosts several commissions dedicated to addressing the diverse challenges faced by the mathematical community. Among these, the Commission for Developing Countries (CDC) focuses its attention on providing assistance and resources to mathematicians in economically disadvantaged countries. Established in 2010, the Commission inherits the legacy of earlier IMU structures that have consistently engaged in international solidarity activities throughout its century-long existence. Its mission is to manage and promote various IMU programs for developing countries, seek funding for them, and establish partnerships with other scientific organizations with common objectives.

Following the established four-year cycle pattern of the International Congresses of Mathematicians, the newly elected Commission, chaired by the Argentinian mathematician Andrea Solotar from the University of Buenos Aires, began its term in early 2023. Comprising 11 members, the Commission held its first meeting at the IMU Secretariat in Berlin on March 12–14, 2023. This gathering allowed for a thorough assessment of all funding programs, the formation of various committees—some involving mathematicians external to the CDC—and the setting of a framework budget for the period 2023–2026. Beyond its formal agenda, the meeting also offered a valuable opportunity for CDC members and IMU staff to acquaint themselves, fostering subsequent electronic communication among them and thereby facilitating the Commission's future work.

Fig. 2: *First meeting of the 2023–2026 CDC at the IMU Secretariat (Berlin, Germany), March 2023*

Determinedly committed to its mission towards developing countries, the CDC works tirelessly to secure new funding and adapt its existing programs to an ever-changing world. With this goal in mind and to better address the needs of our colleagues worldwide, it recently redefined—in coordination with the IMU Executive Committee—its list of developing countries.

The CDC currently offers seven funding programs, categorized into grants for conferences, research visits, graduate students, and institutions. Each program is managed by an ad hoc committee, typically involving members of the CDC and members from partner institutions such as the International Center for Theoretical Physics, the American Mathematical Society, and the London Mathematical Society.

The Conference Support Program offers financial aid organizing conferences and schools in developing countries.

Fig. 3: *Conference "Applications of Mathematics to Nonlinear Sciences 2019" (Pokhara, Nepal), June 2019*

The research visit grants, including the Abel Visiting Scholar Program and the Individual Travel

Support Program, provide funding for mathematicians based in developing countries to visit an international research collaborator for a period of one month.

Fig. 4: *Nguyen Thi Van Anh (left) from Hanoi National University of Education (Vietnam) visited the Rochester Institute of Technology (USA), and Len Meas (right) from the Royal University of Phnom Penh (Cambodia) visited Linkoping University (Sweden)*

The CDC offers two types of grants for graduate students, the IMU Breakout Graduate Fellowship Program and the Graduate Research Assistantships in Developing Countries (GRAID) Program. Launched in 2016 thanks to generous donations from winners of the Breakthrough Prize in Mathematics, the IMU Breakout Graduate Fellowship Program aims to support postgraduate studies, in a developing country, leading to a Ph.D. degree in the mathematical sciences. The GRAID Program, established in 2017, provides modest support for emerging research groups, working in a developing country listed in Priority 1 or 2 of the IMU Definition of Developing Countries, making it possible for them to fund their most talented students to study full-time as graduate research assistants and pursue a Master or Ph.D. graduate degree in mathematics.

Fig. 5: *Abebe Regassa Tufa from Ethiopia was the first laureate of the Breakout Graduate Fellowship Program to defend his Ph.D., at the University of Botswana in June 2018*

In terms of grants to institutions, the CDC offers two programs, the Volunteer Lecturer Program (VLP) and the Library Assistance Scheme. The purpose of the VLP is to provide funding for the organization of courses given by external lecturers for courses which are part of a regular undergraduate or master degree program, or courses at doctoral level, which can be beneficial to Ph.D. students or researchers. The Library Assistance Scheme aims to match donors of math books with libraries in developing countries, where there is a need for mathematical literature, and covers the shipment costs.

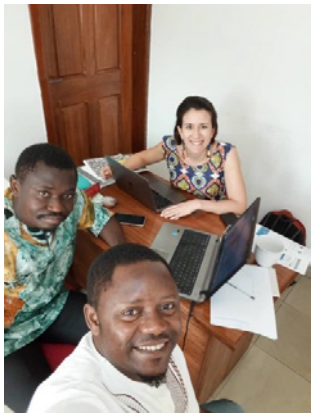


Fig. 6: *In 2020, Prof. Diletta Martinelli (Universiteit van Amsterdam, Netherlands) donated books to AIMS-Cameroon (Limbe, Cameroon)*

Finally, 2023 also saw the CDC introduce its new grant application platform, the implementation of which is supported by the IMU Secretariat. The CDC decided to take this opportunity and host two online webinars (November 30 and December 7, 2023), to promote CDC funding programs and introduce the new platform to potential applicants. The CDC hopes that these efforts will both streamline the application process and broaden the applicant pool as we move into 2024.

3.4 Overview of Meetings and Events 2023

Fig. 7: *IMU Executive Committee Meeting, Berlin, March 2023*

Meeting of the IMU EC, March 10–12, 2023. The first annual meeting of the 2023–2026 IMU EC was hosted at the IMU Secretariat in Berlin. The meeting concluded with a joint session with the 2023–2026 CDC on March 12.

Participants: Hiraku Nakajima, Christoph Sorger, Ulrike Tillmann, Tatiana Toro, Mouhamed Moustapha Fall, Nalini Joshi, JongHae Keum, Paolo Piccione, Günter M. Ziegler, Tamar Ziegler, Carlos E. Kenig, Dietmar Hömberg, Scott Jung. Guests invited for particular agenda items: Claire Voisin, Terence Tao, IMU Secretariat Staff.

Meeting of the CDC, March 12–14, 2023. The first annual meeting of the 2023–2026 CDC was hosted at the IMU Secretariat in Berlin. The meeting began with a joint session with the 2023–2026 IMU EC on March 12.

Participants: Andrea Solotar, Ludovic Rifford, Jose Maria P. Balmaceda, Mahouton Norbert Hounkonnou, Le Tuan Hoa, Mariel Saez, Dayue Chen, K.N. Raghavan, Anjum Halai, Hiraku Nakajima,Tamar Ziegler. Guests invited for particular agenda items: IMU Secretariat Staff.

ICMI Executive Committee Meeting: February 12–14, 2023. The second in-person meeting of the 2021–2024 ICMI EC took place in February 2023 in Bangkok, Thailand, supported by IMU Secretariat staff.

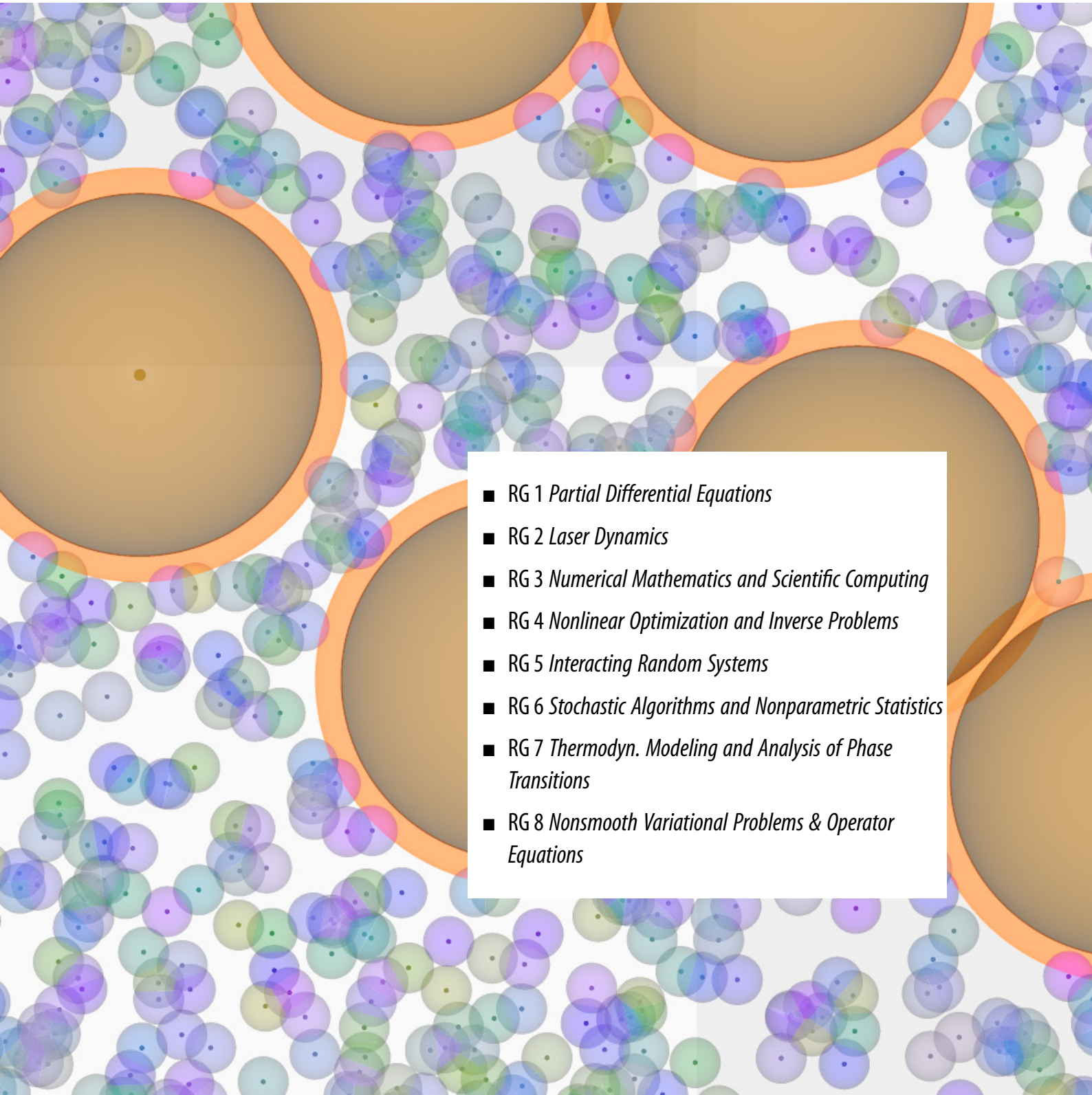
Participants: ICMI EC members, IMU EC liaison person, ICMI Administrative Manager.

Mathematics for Everyone": The International Day of Mathematics (IDM), March 14, 2023. "Mathematics for Everyone" was the theme for the IDM in 2023. The theme for IDM 2024 will be "Playing with Math."

European Consortium for Mathematics in Industry | Research and Innovation Committee: November 9–10, 2023. The IMU Secretariat hosted a meeting of the European Consortium for Mathematics in Industry and its Research and Innovation Committee, the latter chaired by the Head of the IMU Secretariat Dietmar Hömberg, followed by a board and a council meeting.

Guests at the Secretariat. Prof. Dr. Martina Brockmeier (President of Leibniz Association) received a tour of the IMU Secretariat on June 8, 2023, together with colleagues Dr. Felix Kießling and Dr. Samuel Krug. June Barrow-Green, Curator of the IMU Archive, visited the IMU Archive between June 20–22, 2023. Former IMU Secretary Generals Martin Grötschel and Helge Holden also made visits to the Secretariat in 2023, as did Robert Bryant, Member of the ICM 2026 Local Organizing Committee.

4 Research Groups' Essentials



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

4.1 Research Group 1 "Partial Differential Equations"

Head (until Sept.):	Prof. Dr. Alexander Mielke
Head (acting from Oct.):	Priv.-Doz. Dr. Matthias Liero
Team:	Dr. Thomas Eiter Priv.-Doz. Dr. Annegret Glitzky Priv.-Doz. Dr. Martin Heida Georg Heinze Dr. Katharina Hopf Dr. Michael Kniely (long-term guest) Dr. Thomas Koprucki Dr. Anieza Maltsi Dr. Michael O'Donovan Willem van Oosterhout Dr. Joachim Rehberg Dr. Dirk Peschka Stefanie Schindler Priv.-Doz. Dr. Burkhard Schmidt Leon Schütz Magdalena Śliwińska (WIAS Female Master Students Program) Dr. Artur Stephan Prof. Dr. Marita Thomas Michael Tsopanopoulos (long-term guest)
Secretary:	Andrea Eismann
Nonresident Members:	Prof. Dr. Alexander Mielke Prof. Dr. Jürgen Sprekels

The mathematical focus of this research group is on 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:

- Nonlinear material models and multiscale problems
- Modeling of semiconductors; in particular, for optoelectronic devices and quantum technologies
- Reaction-diffusion systems, also including temperature coupling

The methods involve topics from pure functional analysis, mathematical physics, pure and applied analysis, calculus of variations, and numerical analysis with special emphasis on Hamiltonian and gradient flow structures, multiscale methods for deriving effective models, as well as existence, uniqueness, and regularity theory for initial and boundary value problems in nonsmooth domains and with nonsmooth coefficients. Corresponding scientific software tools are developed in cooperation with other research groups.

Fig. 1: *Speakers, organizers, and guest of honor at the colloquium on the occasion of Alexander Mielke's retirement*

In September 2023, the head of the research group, Alexander Mielke, retired, and Matthias Liero became acting head. Alexander Mielke's retirement was celebrated at a festive colloquium at the Humboldt-Universität zu Berlin on September 6, 2023. His influence on the research group, the Weierstrass Institute, and mathematics was honored with several greetings and three invited talks by Rupert Klein (Freie Universität Berlin), Felix Otto (Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig), and Riccarda Rossi (Università di Brescia).

Katharina Hopf left the group in November 2023 to start the new Weierstrass Group WG MBaL *Multi-species Balance Laws*. This group focuses on the mathematical analysis of strongly coupled partial differential equation (PDE) systems, modeling the evolution of interacting species with different mechanical properties; see also Katharina Hopf's Scientific Highlights article "Symmetrization in Cross-diffusions" on page 28. Michael O'Donovan successfully defended his Ph.D. thesis titled "Theory of carrier transport in III-Nitride based heterostructures" at the Tyndall National Institute (Cork, Ireland) in March 2023. Funded via a BMS scholarship, Michael Tsopanopoulos started as a Ph.D. student in RG 1. Within the WIAS Female Master Students Program, Magdalena Śliwińska successfully defended her master's thesis "Analysis of a coupled biomechanical model for growth" at the Humboldt-Universität zu Berlin. Subsequently, she started as a Ph.D. student in the subproject "Analysis of energy-variational solutions for hyperbolic conservation laws" of the Priority Program 2410 *Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness*, which is a joint project of RG 1 and RG 4 *Nonlinear Optimization and Inverse Problems*.

Materials modeling and multiscale problems

The research on this topic was done in cooperation with RG 5 *Interacting Random Systems* and WG BIP *Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes* within the subprojects B09 "Materials with discontinuities on many scales" and C02 "Interface dynamics: Bridging stochastic and hydrodynamic descriptions" of the Collaborative Research Center 1114 *Scaling Cascades in Complex Systems* and within subprojects of the Priority Program 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*. RG 1 is also involved in the subproject AA4-8 "Recovery of battery aging dynamics with multiple timescales" within the Berlin Mathematics Research Center MATH+ with RG 4 and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*. Moreover, together with RG 7, the subproject "Modeling battery electrodes with mechanical interactions and multiple phase transitions upon ion insertion" was successfully acquired within MATH+.

Computation of high-dimensional Voronoi diagrams. The evolution of large molecules can be modeled using the Smoluchovski equation for the probability distribution of the conformation. While the true state space consists of the positions and velocities of all atoms of the molecule, for large molecules one can often identify several critical degrees of freedom that dominate the behavior and the state of the molecule, which can be used to reduce the dimension of the state space. However, in most situations, the dimension is still larger than three. To simulate the evolution of the system in this case, a tesselation of the state space via Voronoi partitions is a fundamental tool. In WIAS Preprint no. 3041, the Julia package *HighVoronoi.jl* along with the underlying mathematics based on geometry and set-valued analysis is introduced. The package is designed to calculate Voronoi diagrams for any given configuration of generating points, in any dimension $d \geq 2$, and on any convex polytope domain. The diagram can also be designed periodically in one or several dimensions. Its performance is of factor 2–2.5 compared to the standard Quickhull algorithm, but it has the important feature to calculate the diagram also for nodes in non-general position, e.g., if more than $d+1$ Voronoi cells share a common vertex, and with respect to (periodic) boundaries. Additionally, the package provides various tools for fast periodic mesh generation, mesh refinement,

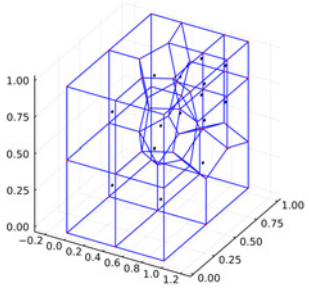


Fig. 2: *A three-dimensional example of a low- and a higher-resolution Voronoi grid glued together using the HighVoronoi "substitute!" command*

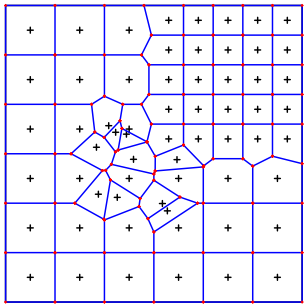


Fig. 3: *A two-dimensional sample of two rectangular Voronoi diagrams glued together and refined by some random points*

local substitution, projection operators, and three different algorithms for the numerical integration of functions over Voronoi cells and interfaces. It finally provides a backend to easily implement a finite volume discretization based on the computed data. A particular feature of *HighVoronoi.jl* is its ability to deal with vertices where more than four cells intersect and with edges where more than three cells interact.

A poro-visco-elastic model at finite strains. The coupling of the mechanical deformations of solids to other physical processes such as heat conduction or diffusion of chemical species is relevant in many applications in technology or biology. In [4], a quasi-static nonlinear model for poro-visco-elastic solids at finite strains was considered in the Lagrangian frame using the concept of second-order non-simple materials. The elastic stresses satisfy static frame-indifference, while the viscous stresses satisfy dynamic frame-indifference. The mechanical equation is coupled to a diffusion equation for a solvent or fluid content. The latter is pulled back to the reference configuration. To treat the nonlinear dependence of the mobility tensor on the deformation gradient, a result by Healey & Krömer is used to show that the determinant of the deformation gradient is bounded away from zero. Moreover, the focus is on the physically relevant case of degenerate mobilities. The existence of weak solutions was established using a staggered time-incremental scheme and suitable energy dissipation inequalities.

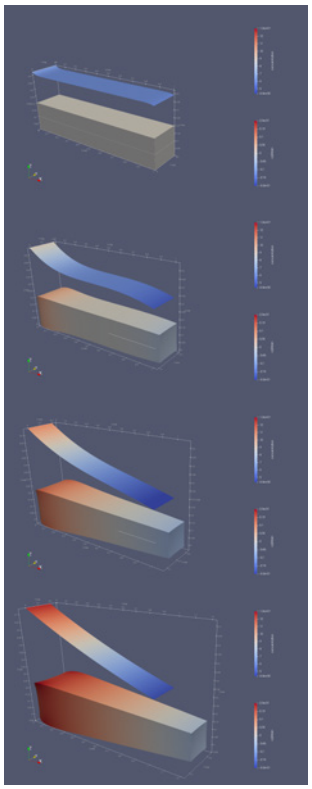


Fig. 4: *Evolution of swelling in a visco-elastic body due to diffusing species*

Mathematical methods for optoelectronic and quantum technologies

In this field, the research group benefits from a strong cooperation with RG 2 *Laser Dynamics*, RG 3 *Numerical Mathematics and Scientific Computing*, and LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*. In particular, the newly founded Focus Platform "Simulation of Semiconductor Devices for Quantum Technologies (SemQTech)" is a collaboration with these groups to contribute to the development of semiconductor quantum computers by combining the theory of open quantum systems and modeling approaches from electrical engineering with methods from applied mathematics; see also the Scientific Highlights article "Spin-qubit shuttles for scalable semiconductor quantum computers: Modeling, simulation and optimal control" on page 23. Within the UVSimTec project, funded in the framework of the Leibniz Competition 2022, the research group collaborates with the Ferdinand-Braun-Institut (FBH), the Leibniz-Institut für Kristallzüchtung (IKZ), the Research Group "Experimental Nanophysics and Photonics" at the Technische Universität Berlin, and the Institute for Optoelectronics at the Friedrich-Alexander-Universität Erlangen-Nürnberg.

Impact of alloy disorder on carrier transport in deep ultraviolet (UV) light emitters. Aluminium gallium nitride [(Al,Ga)N] is a material that—due to a direct and wide band gap—is of particular interest for optoelectronic applications in the deep ultraviolet range (‹280 nm). In collaboration with RG 3, LG NUMSEMIC, and Tyndall National Institute (Cork, Ireland), a three-dimensional multiscale framework using the WIAS software packages `pdelib` and `ddfermi` was employed to study the impact of alloy disorder on device behavior. In particular, the influence of disorder on carrier transport, radiative, and non-radiative recombination processes in an $Al_{0.7}Ga_{0.3}N/Al_{0.8}Ga_{0.2}N$ quantum well embedded in a pn junction was investigated.

The calculations revealed that alloy fluctuations can open “percolative” pathways that promote transport for the electrons and holes into the quantum well region (Figure 5) [2]. Such an effect is neglected in conventional and widely used transport simulations. Moreover, it was established that the resulting increased carrier density and alloy induced carrier localization effects significantly increase non-radiative Auger–Meitner recombination in comparison to the radiative process. Thus, to suppress such non-radiative processes and potentially related material degradation, a careful design (wider well, multi-quantum wells) of the active region is required to improve the efficiency of deep UV light emitters. This study has been carried out as a part of the project UVSimTec, which is aimed at developing (Al,Ga)N-based electrically pumped deep-UV lasers.

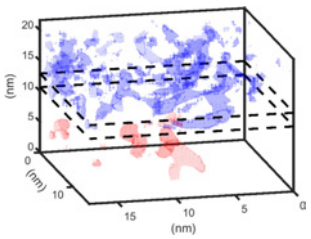


Fig. 5: *Hole (blue) and electron (red) current through an (Al,Ga)N quantum well structure. Alloy-induced percolation paths result in regions of high carrier density .*

Heat and charge-carrier flow in organic devices with thermal and electrical environment. The interplay of self-heating and the rising conductivity of organic semiconductor materials with higher temperature is crucial for the design of organic electronic devices. Therefore, a stationary model for the electrothermal behavior of organic thin-film devices including their electrical and thermal environment was derived and analytically investigated. Whereas the electrodes are modeled by Ohm’s law, the electronics of the organic device itself is described by a generalized van Roosbroeck system with temperature dependent mobilities and using Gauss–Fermi integrals for the statistical relation. The electrical currents give rise to Joule heat that together with the heat produced by the generation/recombination of electrons and holes in the organic device occur as source terms in the heat flow equation that has to be considered on the whole structure.

The crucial task is to establish that the quantities in the transfer conditions at the interfaces between electrodes and the organic semiconductor device (see blue dashed lines in Figure 6) have sufficient regularity. Working in a $W^{1,q}$ setting for some $q > 2$ and in two spatial dimensions, the existence of weak solutions is demonstrated by Schauder’s fixed point theorem and by proving a novel regularity result for strongly coupled systems with nonsmooth data and mixed boundary conditions. The latter is verified by Caccioppoli estimates and a Gehring-type lemma; see [3].

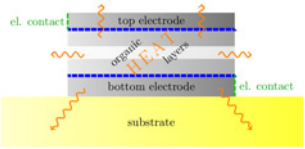


Fig. 6: *Sketch of organic thin-film device with electrical (metallic electrodes) and thermal (electrodes and substrate) environments*

Evolution equations

This field of research provides the basic research for the analytical treatment of coupled systems of nonlinear PDEs arising in different applications, e.g., in natural sciences, technology, economy, and life sciences. The results of the group include, e.g., variational methods for evolutionary systems, generalized gradient systems, entropy methods, and generalized solution concepts. The cooperation with RG 4 was intensified due to the successfully acquired joint subproject “Analysis of energy-variational solutions for hyperbolic conservation laws” within the Priority Program 2410 *Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness*.

Time-splitting methods for gradient systems. The group’s research on generalized gradient systems, which describe the evolution of a system in the direction of the steepest descent of a driving functional $\mathcal{E}$, was continued. Mathematically, gradient flow equations are given by $u'(t) \in \partial\mathcal{R}^*(-\mathrm{D}\mathcal{E}(u(t)))$, where the dissipation mechanism is encoded by the dissipation potential $\mathcal{R}^*$. There are multifaceted reasons why the complex evolution equation splits into several parts: A

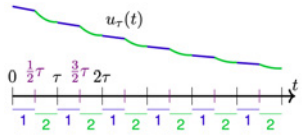


Fig. 7: *Concatenating flows of two systems (1) and (2) with small time-step τ for constructing the solution $u_\tau \approx u$*

modeling ansatz might rely on Newton's law and uses the additivity of forces; the mathematical analysis is simplified by distinguishing between dominant parts and perturbations; specified numerical routines can be used to treat the different parts individually and thus save computational costs. The so-called *split-step method*, which can be understood as a temporal discretization, provides a construction of the solution of the whole evolution by concatenating the separate flows. The mathematical convergence analysis of split-step methods for gradient flows is shown in [5] in the situation where the dissipation consists of two parts, i.e., $\mathcal{R}^* = \mathcal{R}_1^* + \mathcal{R}_2^*$. The flexible analysis is purely variational and relies on the energy dissipation balance. Moreover, it allows for different temporal discretizations and various functional analytic settings. However, it was discovered that one needs the crucial additional requirement that the (Fréchet) subdifferential of the driving functional is a singleton with counterexamples showing that convergence of the time-splitting scheme may in fact break down otherwise.

A corresponding quantitative convergence result with almost optimal convergence rate is established in WIAS Preprint no. 3030 by using methods from functional analysis and operator theory.

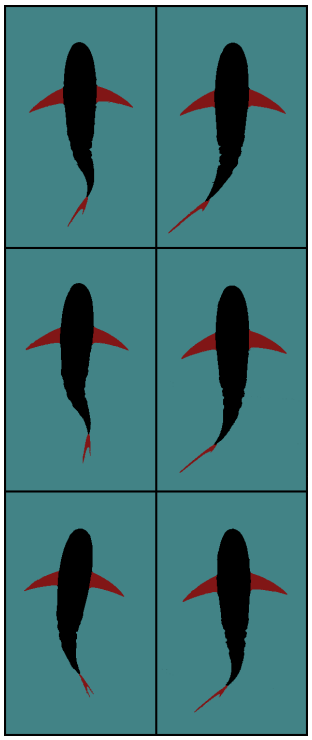


Fig. 8: *The periodic movement of a robotic fish leads to a fluid flow problem with oscillating boundary*

Fluid flow in domains with oscillating boundaries. The fluid motion around a swimming fish can be seen as an example for a flow in a container with a periodically moving boundary, see Figure 8. Existence of solutions to the corresponding Navier–Stokes equations in a bounded domain was established based on existence properties of the associated linearization in [1]. There, a novel approach towards time-periodic maximal L^p regularity for general evolution equations via suitable $\mathcal{R}$-bounds for the associated resolvent problem was developed. In the WIAS Preprint no. 3000, the above existence theory was extended to flows in unbounded domains. Here, time-periodic maximal L^p regularity can only be achieved in a framework of homogeneous Sobolev spaces. Since this is not sufficient to treat the nonlinear terms, it was combined with pointwise decay properties, which were derived from corresponding time-periodic fundamental solutions.

Organized workshops & events

The international conference "Variational and Geometric Structures for Evolution" took place in Levico Terme (Italy) from October 9 to 13. It was jointly organized by Marita Thomas (RG 1 and Freie Universität Berlin), Dorothee Knees (Universität Kassel), Riccarda Rossi (Università degli Studi di Brescia), and Giuseppe Savaré (Università Commerciale Luigi Bocconi). The scientific focus was on recent developments in the identification and analytic exploration of variational and geometric structures for evolutionary problems. With a variety of topics, ranging from multiscale problems in continuum mechanics to stochastic particle systems, the conference also marked the 65th birthday of Alexander Mielke, former head of RG 1, and honored his achievements in this field.

From December 4 to 8, the fourth workshop of the series "Variational Methods for Evolution" took place at the Mathematisches Forschungsinstitut Oberwolfach. It was co-organized by Franca Hoffmann (Universität Bonn), Alexander Mielke (WIAS and Humboldt-Universität zu Berlin), Mark Peletier (Eindhoven University of Technology), and Dejan Slepcev (University of Pittsburgh) and brought together a wide scope of mathematical researchers from calculus of variations, partial differential equations, analysis and stochastics with researchers from data science and machine

learning to exchange ideas, to foster interaction, and to develop new avenues.

From September 13 to 15, 2023, the workshop "Energetic Methods for Multi-Component Reactive Mixtures – Modelling, Stability, and Asymptotic Analysis" (EMRM) took place at WIAS. It was organized by Katharina Hopf and Michael Kniely (both RG 1) in cooperation with Ansgar Jüngel (Technische Universität Wien). The 22 talks and three poster presentations covered a variety of aspects in the modeling and analysis of reaction-diffusion systems and fluid models, including visco-elastic fluids and multiphase flows. Special emphasis was put on energy and entropy methods, which are known as a versatile tool in the context of complex systems subject to temperature effects, electrostatic forces, and compressibility.

Fig. 9: *Workshop EMRM 2023*

The Kickoff Meeting for UVSimTec (UV Lasers: From Modeling and Simulation to Technology) took place in January 2023. The project, funded by the Leibniz Competition 2022 and led by WIAS, includes collaborators from Friedrich-Alexander-Universität Erlangen-Nürnberg, Ferdinand-Braun-Institut (FBH), Leibniz-Institut für Kristallzüchtung (IKZ) and Technische Universität Berlin.

Fig. 10: *UVSimTec Kickoff Meeting*

References

[1] T. Eiter, M. Kyed, Y. Shibata, *Periodic L^p estimates by $\mathcal{R}$-boundedness: Applications to the Navier–Stokes equations*, Acta Appl. Math., **188** (2023), pp. 1/1–1/43.

[2] R. Finn, M. O'Donovan, P. Farrell, J. Moatti, T. Streckenbach, Th. Koprucki, S. Schulz, *Theoretical study of the impact of alloy disorder on carrier transport and recombination processes in deep UV (Al,Ga)N light emitters*, Appl. Phys. Lett., **122** (2023), pp. 241104/1–241104/6.

[3] A. Glitzky, M. Liero, *A drift-diffusion based electrothermal model for organic thin-film devices including electrical and thermal environment*, Z. Angew. Math. Mech., published online on 27.11.2023.

[4] W. van Oosterhout, M. Liero, *Finite-strain poro-visco-elasticity with degenerate mobility*, WIAS Preprint no. 3027, 2023.

[5] A. Mielke, R. Rossi, A. Stephan, *On time-splitting methods for gradient flows with two dissipation mechanisms*, WIAS Preprint no. 3033, 2023.

4.2 Research Group 2 "Laser Dynamics"

Head:	Priv.-Doz. Dr. Uwe Bandelow
Deputy Head:	Dr. Matthias Wolfrum
Team:	Dr. Shalva Amiranashvili Dr. Oleksandr Burylko Dr. Daria Dolinina Lasse Ermoneit Katharina Joachimsmeyer (WIAS Female Master Students Program) Dr. Markus Kantner Dr. Eduard Kuhn Lutz Mertenskötter Dr. Mindaugas Radziunas Mina Stöhr Dr. Andrei G. Vladimirov
Secretary:	Veronica Bove

The research of this group is devoted to the study of mathematical problems that appear in nonlinear optics, optoelectronics, and quantum devices. 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, mostly in the field of *dynamical systems*. The research is mainly devoted to the application-oriented research topics *dynamics of semiconductor lasers* and *pulses in nonlinear optical media* and contributes to the WIAS core-expertise in *modeling and simulation of semiconductor devices*. In 2023, the joint activities with RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, and LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices* were bundeled by introducing the new focus platform *Simulation of Semiconductor Devices for Quantum Technologies*; see also the Scientific Highlights article on page 23.

Berlin Mathematics Research Center MATH+

In 2023, external funding was received within the Cluster of Excellence MATH+: The subproject AA2-13 "Data-driven stochastic modeling of semiconductor lasers" together with the Technische Universität (TU) Berlin and the Ferdinand-Braun-Institut Berlin (FBH), and the subproject AA2-17 "Coherent transport of semiconductor spin-qubits: Modeling, simulation and optimal control" together with the TU Berlin and RG 1. Collaboration partners in AA2-17 are the Rheinisch-Westfälische Technische Hochschule Aachen, the JARA-FIT Institute for Quantum Information, the Leibniz-Institut für Kristallzüchtung (IKZ), and the Technische Universität München. Moreover, the group participates in projects within the framework of the Leibniz Competition in "Collaborative Excellence:" in the project "Excellence in Photonic Crystal Surface Emitting Lasers (PCSELence)," together with RG 3, LG NUMSEMIC, and the FBH as the coordinating partner and in the project "UV Lasers: From Modeling and Simulation to Technology (UVSimTec)," which is a joint project together with RG 1, RG 3, the TU Berlin, the Friedrich-Alexander-Universität Erlangen-Nürnberg, IKZ, and FBH. A further project of the group, "Hybrid Chip-scale Frequency Combs Combining III–V Quantum-Dash Mode-Locked Lasers and High-Q Silicon-Nitride Microresonators (HybridComb)," is a joint project with Karlsruhe Institute of Technology, Physics Institute in Nice, Telecom SudParis, and Center for Nanosciences

Leibniz Competition

and Nanotechnologies at the University of Paris-Saclay, and is funded by the German Research Foundation (DFG) and the Agence Nationale de la Recherche (ANR, France). Moreover, at the end of 2023, a license agreement with the FBH for the software BALaser (including support) concerning simulations of high-power broad-area semiconductor lasers, was extended for another two years.

The cooperation with Russia within the framework of the DFG-RSF (Russian Science Foundation) projects "Underlying nonlinear science of hybrid SOA-fiber laser systems with feedback" and "Collective dynamics of heterogeneous networks of active elements" was suspended as a reaction to the Russian invasion in Ukraine. During several months in 2023, the group was hosting Dr. O. Burylko (Institute of Mathematics of the National Academy of Sciences of Ukraine), who received a special MATH+ fellowship for mathematicians from Ukraine.

An extraordinary highlight in 2023 was the Friedrich Wilhelm Bessel Research Award of the Alexander von Humboldt Foundation awarded to Prof. Tiago Pereira from the University of São Paulo, which offered him the opportunity of extended research visits at WIAS. The research group organized two international workshops on "Nonlinear Dynamics in Semiconductor Lasers" and "Dynamics in Coupled Network Systems" gathering the international collaboration networks of the group and strengthening the exchange between mathematical theory and applications in these two fields. Moreover, the group participates in the organization of the Leibniz Research Network "Mathematical Modeling and Simulation (MMS)."

Dynamics of semiconductor lasers

Calculating optical modes in PCSELs. Photonic crystal (PC) surface-emitting lasers (SELs), as in Figure 1(a), are novel devices capable of emitting nearly perfect high-power beams. In contrast to conventional edge-emitting semiconductor lasers with comparable emission powers, PCSELs can operate on a single optical mode, guaranteeing a low beam divergence. An efficient calculation of leading optical modes in PCSELs is crucial when looking for suitable heterostructures including size and configuration of lateral photonic crystal layers. RG 2 developed efficient algorithms for the construction of model equations and corresponding spectral problems, given by two-dimensional partial differential equations (PDEs) for four counterpropagating and cross-coupled field amplitudes, red arrows in Figure 1(a) [1]. We constructed second- and higher-precision order schemes (WIAS Preprint no. 3059, 2023), analyzed calculated spectra, as in Figure 1(b), and the performance of the schemes. The newly developed solver is used to evaluate different PCSEL configurations suggested by the project partners at the FBH.

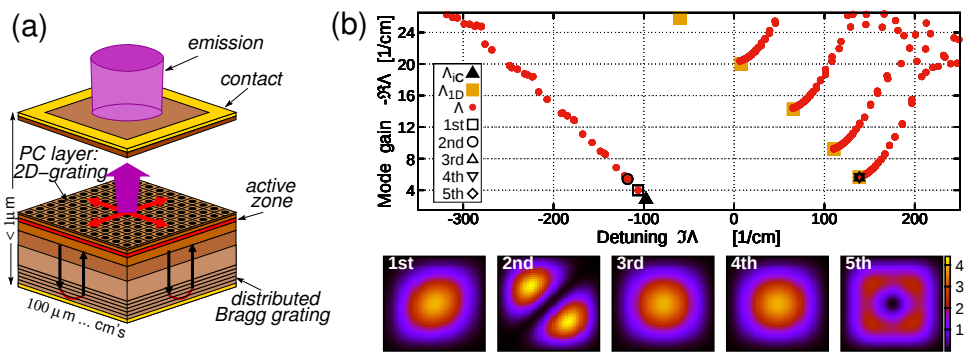


Fig. 1: *(a): Schematics of the PCSEL. (b): Eigenvalues of the spectral problem (bullets) and its two limit cases (filled triangles and squares). Five main modes are represented by empty symbols (top) and intensity distributions (bottom).*

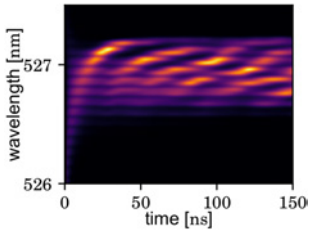


Fig. 2: *Mode dynamics in broad-ridge Fabry–Perot laser*

Mode dynamics in broad-ridge laser diodes. In Fabry–Perot-type laser diodes, various mode-competition phenomena can be observed. For example, these lasers show mode hopping, where the activity level of different longitudinal modes changes over time due to beating vibrations of the carrier densities in the active region. While simulations of the longitudinal mode dynamics in small-ridge laser diodes are well established in the literature, there is a notable gap for broad-ridge laser diodes with multiple lateral modes. We developed a model using an effective interaction term [2] in conjunction with drift-diffusion equations (WIAS Preprint no. 3061, 2023) and used it to simulate the mode dynamics in these devices; see Figure 2 for example.

Estimation of frequency noise in narrow-linewidth lasers. Self-heterodyne beat note measurements are widely used for the experimental characterization of the frequency-noise power spectral density (FN–PSD) and the spectral linewidth of lasers. The measured data, however, must be corrected for the transfer function of the experimental setup in a post-processing routine. The standard approach disregards the detector noise and thereby induces reconstruction artifacts and systematic errors in the reconstructed FN–PSD. We developed an improved post-processing routine based on a parametric Wiener filter [5], which provides an artifact-free estimate of the hidden FN–PSD, from which the laser linewidth can be extracted with high accuracy. The method requires an estimate of the frequency-dependent signal-to-noise ratio, for which we developed a Bayesian estimation approach using a Markov chain Monte Carlo method and a statistical model of the experiment.

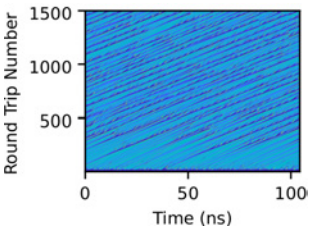


Fig. 3: *Numerical map of the laser intensity illustrating the development of power dropouts during laser turn-on*

Turn-on dynamics of an SOA fiber laser. The turn-on process in a hybrid semiconductor optical amplifier (SOA) fiber laser with the round-trip time several orders of magnitude greater than the SOA relaxation time was investigated in [6]. Theoretical analysis of the turn-on dynamics was performed with the help of a delay-differential equation (DDE) laser model and appears to be in a good agreement with the experimental data. It was shown that in the large delay limit, the evolution of the photon statistics from thermal to Poissonian distribution involves the emergence of power dropouts, which can later seed coherent structures similar to dark solitons or Nozaki–Bekki holes. The coherent structures connecting stationary laser emission domains having different optical frequencies emit intensity bursts, which travel at a different speed and may collide with other coherent structures, thus leading to an overall turbulent dynamics; see Figure 3.

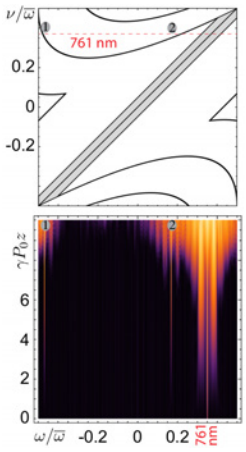


Fig. 4: *Top: Resonance curves. Bottom: Four-wave mixing spectrum is destroyed due to aliasing phenomenon.*

Pulses in nonlinear optical media

The split-step method is a simple and popular way to find numerical solutions to the pulse propagation equations in nonlinear optics. However, the method is explicit, and the resulting numerical solutions can suffer from the spurious four-wave mixing processes (Figure 4). This is particularly dangerous when considering a complex field state subject to true physical instabilities, because the true and spurious instabilities can be mixed. We studied how the nonphysical resonances appear in solutions of an extremely stiff generalized nonlinear Schrödinger equation with an arbitrary dispersion operator. Our approach is based on the consideration of simple situations where one can obtain analytical solutions both for the equation in question and for its numerical implementation (Figure 5). Using the requirement that only physically relevant instabilities develop, we determine the necessary restrictions on the temporal and spatial resolution of the splitting scheme [3]. The

restrictions are especially important to meet when an envelope equation has to be applied in a wide spectral window, e.g., because of the spectral broadening.

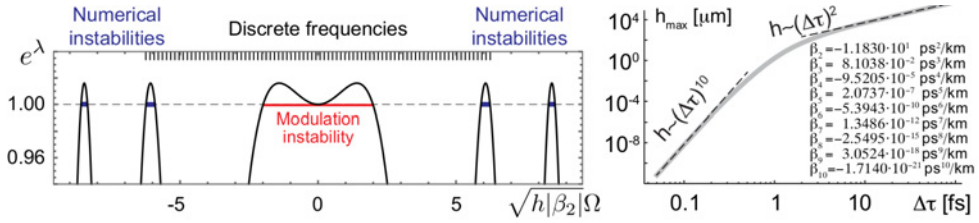


Fig. 5: *Left: True and spurious instabilities. Right: The valid solution step versus temporal resolution for a practically relevant fiber.*

Temporal cavity soliton interaction in a mode-locked laser. Weak interactions of two well-separated temporal cavity solitons (TCS) in a long cavity semiconductor laser were studied numerically and analytically using the DDE mode-locking model [7]. Asymptotic interaction equations governing the slow evolution of the time separation and phase difference of the TCSs were derived and analyzed in the typical parameter range of semiconductor lasers, where the interaction via gain saturation and recovery dominates over the interaction via absorption and field dynamics. Analytical results were compared to direct numerical simulations of the DDE mode-locking model. It was shown that, in addition to usual pulse repulsion leading to harmonic mode-locking regimes, an attractive TCS interaction is also possible in a laser with nonzero linewidth enhancement factor. This attractive interaction can result either in pulse merging (see Figure 6) or in a formation of an incoherent pulse bound state.

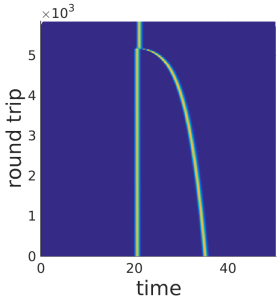


Fig. 6: *Laser intensity map illustrating merging of two mode-locked pulses*

Theory of dynamical systems

The mathematical research on dynamical systems provides the theoretical background for the applied topics in optoelectronics and nonlinear optics of this group. In particular, we further developed the mathematical theory of localized solutions in the large delay limit in delay-differential equations. This enabled us to apply homoclinic bifurcation theory and numerical path-following methods to study a delay-algebraic equation modeling a vertical external-cavity Kerr–Gires–Tournois interferometer in the presence of anti-resonant injection [4]. This system shows the formation of coexisting square-wave patterns and pulse solutions that are organized in a complex structure of snaking branches around a Maxwell point; see Figure 7.

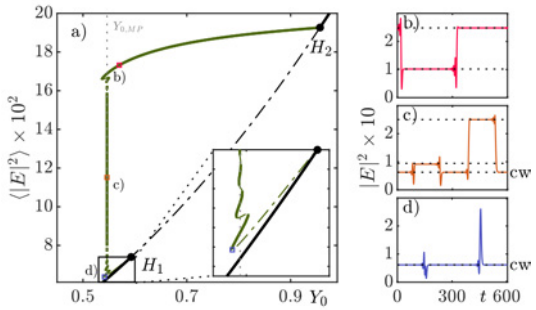


Fig. 7: *Different types of solutions of a delay-algebraic model for the Kerr–Gires–Tournois interferometer. (a): Branch of periodic solutions (green) and continuous wave (CW) states (black). (b): Square wave solutions. (c): Mixed-type solutions around the Maxwell point. (d): Unstable alternating pulse solutions; for details, see [4].*

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

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Deputy Head:	Dr. Jürgen Fuhrmann	
Team:	Priv.-Doz. Dr. Alfonso Caiazzo	Dr. Cristian Cárcamo Sánchez
	Dr. Medine Demir	Priv.-Doz. Dr. Wolfgang Dreyer (long-term guest)
	Dr. Derk Frerichs-Mihov	Dr. Patrick Jaap
	Liam E.J. Johnen (apprentice)	Mihaela Karcheva-Froch (apprentice)
	Sarah Katz	Dr. Christian Merdon
	Dr. Baptiste Moreau	Dr. Ondřej Pártl
	Fedor Romanov (apprentice)	Dr. Franceso Romor
	Daniel Runge	Dr. Holger Stephan
	Timo Streckenbach	Marwa Zainelabdeen
Secretary:	Imke Weitkamp	

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 (PDEs). Many of the research topics have been inspired by problems from applications in fields like computational biomedicine (see the Scientific Highlights article by A. Caiazzo in the WIAS Annual Research Report 2022 on page 15 and under WIAS Research Highlights), numerical methods for charge transport in semiconductors and electrolytes (in cooperation with LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*, RG 1 *Partial Differential Equations*, RG 2 *Laser Dynamics*, and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*), and computational fluid dynamics (CFD).

Numerical analysis for POD-ROMs

Reduced-order models (ROMs) aim to perform very efficient simulations with acceptable accuracy. To this end, one highly resolved simulation (full-order model, FOM) is performed, and main features of the numerical solution are extracted with a proper orthogonal decomposition (POD). The corresponding functions, ideally only very few, are utilized as basis functions for performing simulations for problems with similar data as the FOM.

Numerical analysis of POD-ROMs has been started only quite recently. The state of the art consists in analyzing the POD-ROM problem that has the same data as the FOM. In a series of papers, POD-ROMs for the incompressible Navier–Stokes equations were analyzed. The POD-ROM methods studied in [2] uses as snapshots an approximation of the velocity at the initial time and approximations of the temporal derivative of the velocity at different time instants. Including the latter set is necessary for deriving bounds for the velocity error pointwise in time (maximum at the time instants) and L^2 in space with the currently known technique. The approximation at the initial velocity can be replaced by the mean value of the velocity at the different times so that implementing the ROM to the fluctuations, as done mostly in practice, only requires approximations to the time

derivatives in the set of snapshots. The differences between projecting onto L^2 and H^1 in the POD method are investigated. In both, the FOM and the POD-ROM, a grad-div stabilization term is included. The derived error bounds contain only constants that do not blow up if the viscosity becomes small. Based on simulating POD-ROM velocities in this way, two different procedures to compute approximations to the pressure within the framework of POD-ROMs are analyzed in [3]. Error bounds for the pressure are proved with constants independent of inverse powers of the viscosity. Finally, it is shown in [4] that using second-order accurate and unconditionally stable backward differentiation formulas (BDF2) as time-stepping scheme in POD-ROM methods with snapshots based on difference quotients with respect to time gives both the optimal second-order error bound in time and estimates for the pointwise-in-time and L^2-in-space error. For simplicity, the proof is presented for the heat equation.

Numerical methods for multiscale heterogeneous catalysis

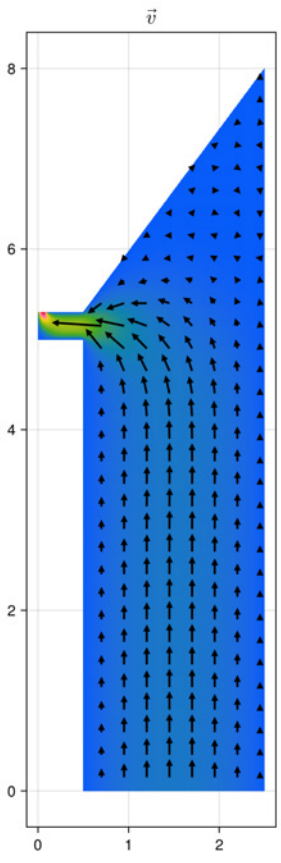

Fig. 1: *Velocity field of flow through an XPS chamber*

Heterogeneous catalysis is a type of catalytic process that usually involves a solid catalyst and gaseous reactants. It primarily involves surface reactions where reactant molecules adsorb onto the surface of the catalyst, undergo chemical transformation, and then desorb as product molecules. Several joint projects with the Fritz Haber Institut (FHI) aim at an efficient and qualitatively and quantitatively accurate modeling and simulation of these processes to help interpreting measurements,e.g., from in-situ surface characterization experiments. The objective of these experiments is to establish a correlation between reactivity, microscopic structure, and reaction conditions at the surface. The reactivity of a catalyst with respect to a specific reaction is described by the so-called *turnover frequency function* that depends on the local reaction concentrations and other reaction conditions like pressure and temperature at the reaction site. This reactivity then acts as a Cauchy boundary condition for the species concentrations and needs to be evaluated during their transport simulation. One challenge consists in modeling this turnover frequency function such that it can be evaluated efficiently and allows high interpretability with respect to the (atomistic) structure of the catalyst. Here, atomistic first-principle kinetic Monte Carlo (kMC) methods have gained popularity in the last years and were extensively studied at the FHI together with a smart way to evaluate the kMC-based reactivities in an efficient way during coupled simulations. The second challenge concerns the efficient simulation of the transport of the reactants and the reaction products and a flow computation through a complex domain, e.g., an X-ray photoelectron spectroscopy (XPS) chamber. However, in the experiments under consideration, the reaction conditions, inlet velocity, and diffusion coefficients of the species are sufficiently well controlled and can be assumed constant, which allows to independently determine the velocity field. For the flow simulation divergence-free finite element methods are employed to ensure physical bounds for the species concentrations, which are computed by finite volume methods.

The DFG project "Atomistic-continuum coupling for heterogeneous catalysis by a reduced basis approach and multilevel on-the-fly sparse grid interpolation" has the aim to speed up the coupling between transport and catalytic response by employing a reduced basis to determine the species concentrations. This is based on the following idea: Given a partition of unity for the species fluxes at the catalytic boundary, the evaluations of any turnover frequency function can be written as a linear combination of this partition. For each element of this partition, one basis function is defined

that solves the corresponding (linear) problem where the nonlinear Cauchy boundary condition is replaced by the element of the partition of unity. It remains to compute the coefficients of these basis functions such that their linear combination solves the nonlinear problem. This is a much smaller problem and, more importantly, the basis functions can be reused if the model for the turnover frequency functions is changed (as long as the involved species and the geometry stay the same). Hence, the approach is well suited for testing a wide range of models, using adaptivity, or performing parameter fitting to help interpreting experimental results. An implementation of this approach is currently developed in Julia, and details on the approach and a first showcase example were published in [5].

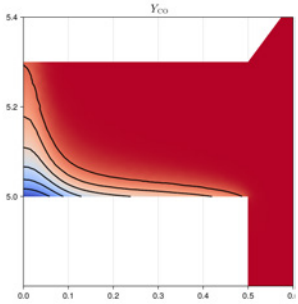

Fig. 2: *Reactant concentration in an XPS chamber in the vicinity of the catalyst surface*

The supervision of the Ph.D. project "Coupled atomistic and nanofluidic simulations for electrocatalysis" funded by the Einstein Center of Catalysis constitutes another cooperation with FHI in this field. This project investigates the coupling of ion transport and electrocatalytic reaction at the nanoscale. KMC-generated reaction data are used to train a neural network that is used as a surface reaction boundary condition to a generalized Nernst–Planck–Poisson system describing ion transport in an electrolyte.

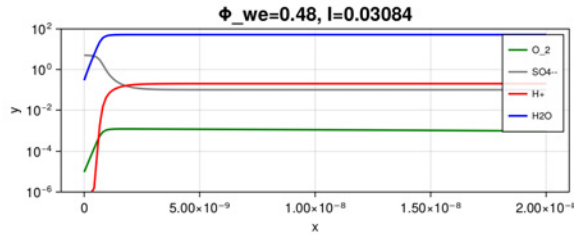

Fig. 3: *Ion concentration near an electrode during an oxygen reduction reaction*

Multiscale modeling and simulation of vascularized tissues

Mathematical and computational modeling of biological tissues can strongly support the potential of non-invasive diagnostic based on medical imaging, such as magnetic resonance elastography (MRE). Combined with available measurements and with robust data assimilation methods, mathematical models can provide the link between observations and clinical biomarkers, i.e., indicators of anomalous conditions or pathologies. In the context of vascularized tissues, fully resolved fluid-structure interaction models require the handling of multiple physics—the solid matrix and the fluid vasculature—and often come with an intrinsic geometrical complexity, which makes them computationally extremely expensive and often numerically intractable.

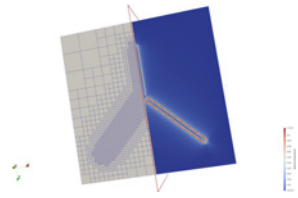

Fig. 4: *Example of multiscale 3D-1D model of vascular tissue showing the mesh around the one-dimensional structure and the displacement field*

The goal of this research is to develop, analyze, and validate suitable reduced-order and multiscale models to simulate the dynamics of a vascular tissue at the *effective* scale, i.e., with the purpose of recovering how the microscale influences the mechanical parameters at the macroscale. Concrete examples of applications concern the sensitivity of parameters to intrinsic poroelastic properties and vascular architecture in biological tissues, such as liver (cardiovascular system) and brain (cerebrospinal fluid).

The considered model describes the system as an elastic matrix (three-dimensional) coupled to a set of thin fluid vessels. Boundary conditions on the tissue-vessel interface can be based on

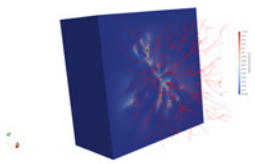

Fig. 5: *Geometry of a complex network*

imposing the deformation of the vessel boundary, or the transfer of the pressure between fluid and tissue. Considering the limit of small vessel radius, each segment of the vasculature is modeled as a one-dimensional manifold, described, e.g., by its centerline. The boundary conditions are imposed using a non-matching immersed method, i.e., introducing singular terms into the elasticity equation for the tissue. These terms can be defined as integral over the vessel boundary or over the centerlines. The main advantage of this approach is that these integrals can be numerically computed using a discretization independent of the tissue dynamics. This property is particularly important to efficiently handle complex geometrical structures without the need of discretizing the vessel details within the computational mesh. In the model proposed in [1], these immersed coupling terms are handled via a Lagrange multiplier on the tissue-vessel interface. Moreover, further computational efficiency can be achieved considering a reduced-order Lagrange space only on the centerline.

This research is partially pursued in collaboration with the Universität Augsburg, the Charité Universitätsmedizin Berlin, the International School for Advanced Studies (SISSA), and the University of Trento (Italy). In this context, the DFG project "Computational multiscale methods for inverse estimation of effective properties of poroelastic tissues," aims at constructing efficient multiscale models of 3D–1D coupled elasticity based on numerical homogenization. Current work focuses on using the results of [1] to build consistent maps between the space of effective (coarse) tissue parameters and the fine vascular scales, and on the usage of neural networks to efficiently compute these maps in the context of inverse problems.

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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:	Vitalii Aksenov Dr. Ingo Bremer Priv.-Doz. Dr. Martin Eigel Hanyue Gu (WIAS Female Master Students Program) Dr. Holger Heitsch Nina Kliche Dr. Robert Lasarzik Charles Miranda Sophie Luisa Plato Dr. Andreas Rathsfeld Janina Schütte David Sommer Okunowa Toluwani (WIAS Female Master Students Program)
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. Our work is related to the main application areas *Energy: Technology, Markets, Networks, Flow and Transport, Nano- and Optoelectronics*, and *Optimization and Control in Technology and Economy*.

We cooperate with RG 1 *Partial Differential Equations* on stochastic homogenization and the analysis of nonlinear evolution equations using maximally dissipative as well as energy-variational solution concepts with a special focus on electrochemical fluids. With RG 3 *Numerical Mathematics and Scientific Computing*, we work together in the numerical approximation of electro-rheological fluids and adaptive stochastic Galerkin finite element methods (FEM). We collaborate with RG 6 *Stochastic Algorithms and Nonparametric Statistics* on the simulation of stochastic processes and stochastic control problems, with RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* on battery-ageing dynamics, and with RG 8 *Nonsmooth Variational Problems and Operator Equations* on machine learning and risk-averse optimization in gas networks.

A special highlight of this year's work has been the organization of the WIAS workshop "Frontiers of Stochastic Optimization and its Applications in Industry," May 10–12, jointly with RG 8. In September, the RG was a driving force in organizing ESGI 175 – The Berlin Study Group with Industry, September 18–22, jointly with RG 7 and Torsten Köhler, with additional funding from the Berlin Mathematics Research Center MATH+.

In the following, selected scientific achievements of the research group's work in 2023 are detailed.

Stochastic and nonsmooth optimization

The research on stochastic and nonsmooth optimization is associated with projects in the programs DFG Transregio (TRR) 154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks*, the Berlin Mathematics Research Center MATH+, and the Gaspard Monge Program for Optimization (PGMO) funded by Fondation Mathématique Jacques Hadamard. Work in TRR 154 was within the third and last funding period. The funding of the running PGMO project (Optimal control problems with probabilistic constraints, with Hasnaa Zidani, Rouen, and Wim van Ackooij, Paris) could be renewed for another year. Within MATH+, one project (weakly coupled mini-grids) is running and another one (SARS-CoV-2 risk assessment and vaccine design, with Max von Kleist and Claudia Schillings, Berlin) starting in January 2024.

The work in TRR 154 focused on the completion of intensive research on time-dependent probabilistic capacity maximization in gas networks. Here, a problem earlier posed by a gas network owner in a purely static setting was dealt with in the context of dynamic gas flow under uncertain load of stochastic and non-stochastic nature (Figure 1, left). A second axis of research was devoted to optimality conditions and to the numerical solution of (static) control problems with uniform state constraints in probabilistic and almost-sure form. This topic initiated an intensive cooperation between RG 4 and RG 8 within TRR 154. It is closely related with the PGMO project which, in contrast, considers time-dependent control problems with a single end-point constraint. A major part of work in the MATH+ project turned around finishing work on battery-aging models including probabilistic constraints and embedding it into the general framework of unit commitment in a mini-grid. The latter question is closely connected with an external cooperation (Tatiana González Grandón, Flensburg, and Nesrine Ouanes, Berlin) on mini-grid management under uncertainty. In this framework, RG 4 participates in a proposal for a HORIZON project Green Rural Industrialization through Decentralized Open-Source Agri-Mini-grids for Africa. Furthermore, the research on stochastic and nonsmooth optimization was applied to a problem proposed by Electricité de France as part of the "ESGI 175 – The Berlin Study Group with Industry" held at WIAS.

Completed external cooperation with colleagues from Erlangen, Dijon, and Detroit led to joint publications in optimal control ([4], [5]). A new cooperation on linear complementarity problems subject to probabilistic constraints was initiated with Martin Schmidt (Trier).

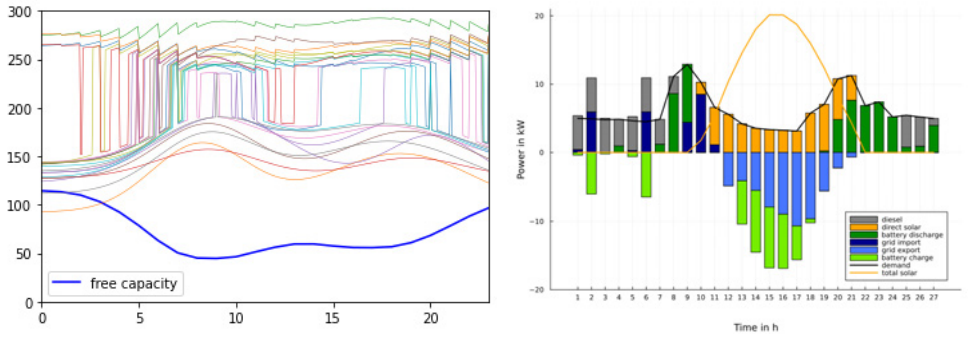


Fig. 1: *Left: Probabilistic free capacity in a gas pipe along with twenty worst-case load scenarios. Right: Optimal dispatch of a mini-grid for high probability of islanding capacity under randomness (solar, demand, disruptions from main grid)*

Optimal control of multifield and multiscale problems

Expanding on the focus of our research in recent years, the concept of energy-variational solutions was proposed in [1] for a general class of evolutionary partial differential equations (PDEs) in a damped Hamiltonian framework with a convex energy defined on a reflexive Banach space. Our main motivation in this paper was to apply the abstract result to different viscoelastic fluid models.

Viscoelastic materials are ubiquitous in the modeling of materials. For instance, human tissues as well as the earth's lithosphere exhibit viscoelastic properties. In contrast to their importance, many viscoelastic fluid models are not very well understood mathematically. In order to handle the inherent nonsmoothness of solutions to these models, often a smoothing term, so-called *stress diffusion*, is added to the equation for the additional stress tensor, which allows to use standard compactness arguments for the analysis. But this regularizing stress diffusion term breaks the kinematic relationship between the variables and often breaks the dissipative structure of the system, or changes the observed phenomena. Therefore, a novel framework for general damped Hamiltonian systems is provided, which especially also allows to prove existence and weak-strong uniqueness results for multiple viscoelastic fluid models without this regularizing stress diffusion. But the abstract framework has the potential to provide novel insights for multiple other evolutionary PDE models, which we will investigate further in the future.

In this direction, a third-party-funded project on "Analysis of energy-variational solutions for hyperbolic conservation laws" could be acquired together with Thomas Eiter from RG 1 within *DFG SPP 2410 Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness*. The associated Ph.D. position could just be filled with a former student of the WIAS Female Master Student Program.

Good progress was made in the third-party-funded project on "Nonlinear electrokinetics in anisotropic microfluids – Analysis, simulation, and optimal control" within the DFG Excellence Cluster MATH+. The numerical simulations of the evolution of the velocity field in an anisotropic electrolyte shows good agreement with experiments. Via an oscillating current on the boundary, an oscillating electric field is built that can be used to mix the contained fluid as can be seen in Figure 2.

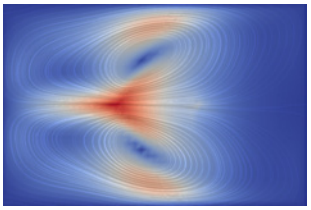
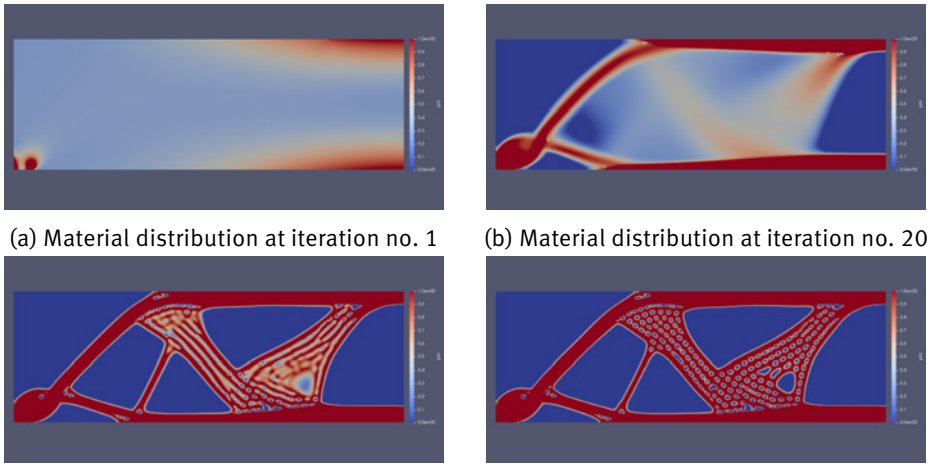


Fig. 2: *Induced velocity field in an anisotropic electrolyte by an oscillating electric field*

Another focus of last year's work was topology optimization for additive manufacturing. There, the creation of porous infill structures is desirable in order to increase the surface-to-volume ratio of the structure, which leads to better thermal or acoustic insulation and can improve the stability with respect to buckling. Recently, a novel approach was introduced that relies on a global minimization problem with global and local volume constraint, where the local volume constraint depends on the stress of the associated mechanical problem. The associated numerical optimization algorithm introduces via a pseudo-time stepping a gradient flow for a nonsmooth, nonlocal energy; see Figure 3. In the recently published article [2], we proved existence of generalized solutions to this problem, where the Allen–Cahn-like equations are fulfilled as a differential inclusion due to the nonsmoothness of the energy.



(a) Material distribution at iteration no. 1 (b) Material distribution at iteration no. 20

(c) Material distribution at iteration no. 40 (d) Material distribution at iteration no. 100

Fig. 3: *Result of a pseudo-time stepping scheme for two-scale topology optimization for a Messerschmitt–Bolkow–Blohm (MBB) beam*

High-dimensional parametrized inverse problems

Weighted sparsity and hierarchical tensors for parametric PDEs. The sparsity of functions plays a fundamental role, in particular, in high-dimensional problems, where the exploitation of this property is often crucial to render numerical methods successful. To evaluate if certain problems can be treated practically, an analysis of the sparsity that can be expected is required. It is well known that solutions of common parametric PDEs can be analyzed in this framework. The data of these PDEs is assumed to depend on a countable (possibly infinite-dimensional) set of parameters, describing variances of data or uncertainties. An important question is to determine how sparsity of data transfers to sparsity of solutions, which leads to the question of what appropriate representations look like. A central tool for the analysis is the Stechkin lemma, leading to best n-term convergence rates as a result of the summability of data and (consequently) solution. In its standard form, this lemma does not exploit the refined notion of weighted sparsity. The weighted Stechkin lemma derived in [7] verifies known results for holomorphic functions, but also allows to obtain optimal convergence rates in cases that were not covered before, in particular, resulting in exponential rates if appropriate summability can be assumed. To make use of this weighted sparsity, a new low-rank tensor format was devised, which consists of sparse component tensors. It was shown that sparsity translates to low-rank approximability under certain assumptions. Moreover, efficient training algorithms based on a modified alternating linear scheme were developed for the sparse format. These have only polynomial complexity scaling in the dimensions and the sparsity, hence enabling efficient simulations of parametric PDEs.

Multilevel neural networks for parametric PDEs. Neural network (NN) expressivity results for approximating functions from common model classes were ubiquitous in the theoretical analysis of Deep Learning in recent years. They hinted at a huge potential to represent even very complicated functions that could not be handled by classical approaches. This has lead to a growing interest in solving differential equations with NNs, which is frequently considered a defining part of

so-called *scientific machine learning*. However, the practical experience with NN approximations, e.g., for PDEs distinctly falls short of the high expectations yet. An obvious reason for this is the extremely challenging optimization process of the nonconvex nonlinear representation. To alleviate this, a multilevel strategy was developed in [6], which encompasses a NN architecture based on convolutional NNs (CNN) and U-nets (depicted in Figure 4) as well as a data decomposition that mimicks the multigrid structure known from finite element simulations. The training of the multilevel architecture is based on coarse-grid data and fine-grid corrections, which in practical experiments show a significantly improved performance in accuracy of PDE solutions when compared to other common NN-based methods such as the popular PINNs (physics-informed neural networks). Moreover, motivated by classical multigrid theory, the training complexity can be reduced by using fewer samples on finer spaces. For this architecture, a complete convergence analysis was carried out, leading to complexity bounds in dependence of the desired approximation accuracy. The results provide a strong motivation to extend the methods to adaptively refined multilevel data and an a posteriori error monitoring, which is a topic of current research.

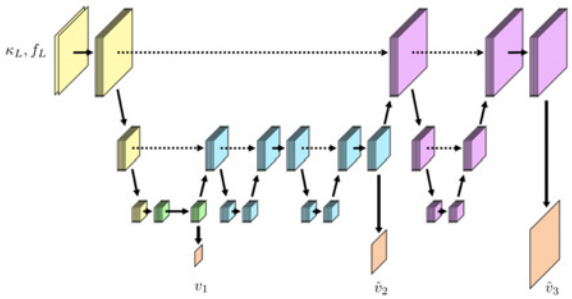


Fig. 4: *Multilevel NN architecture with discretization of data as input. The action of the NN consists of several U-net cycles that are equivalent to classical multigrid iterations. The color-marked layers represent these iterations with different refinement levels (smaller components indicate coarser grids). The output is determined by the sum of a coarse-grid approximation v_1 and subsequent fine-grid corrections $\hat{v}_2, \hat{v}_3$.*

Interacting particle dynamics and gradient flows for inverse problems. Ensemble methods have become ubiquitous for the solution of Bayesian inference problems where state-of-the-art Langevin samplers such as the ensemble Kalman sampler or affine invariant Langevin dynamics (ALDI) use weighted covariance estimates relying on successive evaluations of the forward model or its gradient. A main drawback that these methods have is the required large number of forward calls as well as the possible lack of convergence in the case of more involved posterior measures. The developed method addresses these issues using two ideas. First, several adaptive ensemble enrichment strategies that enlarge the number of particles in the underlying Langevin dynamics were devised. These lead to a significant reduction of the total number of forward model calls. Second, to address more involved target distributions, the method proposes adapted Langevin dynamics based on a homotopy formalism for which convergence is proved; see Figure 5. Additionally, a complexity and convergence analysis for a NN approximation of Langevin dynamics was carried out, which is based on an Euler–Maruyama discretization translated to network layers.

The ALDI method generates gradient flows, transporting measures from a prior to a posterior. The research was extended to the numerical analysis of more general gradient flows for Bayesian inverse problems based on the well-known Jordan–Kinderlehrer–Otto (JKO) scheme and a Lagrangian ansatz, compressed by hierarchical tensor methods to become practical.

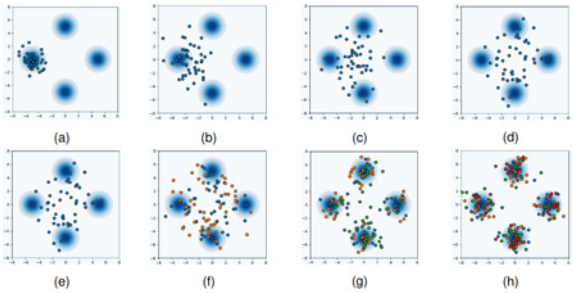


Fig. 5: *Transport of interacting particles from initial distribution to a multimodal target distribution (Gaussian mixture with 4 modes). The proposed method first carries out a homotopy-assisted Langevin dynamics for existing particles (a-d), then performs an enrichment of the existing particles by new ones (red color) based on empirical densities (f-h), leading to an improved accuracy of the target approximation in (h).*

Periodic scattering. For the simulation and for inverse problems of the scattering of acoustic or electro-magnetic waves by periodic surface structures, models for the radiation condition are essential. A general approach for the plane-wave scattering by perturbed planes is to require such a condition over a half-space included in the domain over the perturbed plane. For this it was shown that the differentiated upward propagating radiation condition (UPRC) guarantees a unique solution of the scattering of bounded waves by planar boundaries.

In cooperation with Guanghui Hu (Tianjin), a radiation condition was derived for the case of special inhomogeneous substrate materials, where the refractive index depends periodically on either the vertical (distance to the unperturbed surface plane) or on the horizontal direction (new for transverse-magnetic (TM) polarization).

The popular scattering matrix algorithm called *rigorous coupled-wave analysis* (RCWA) for the simulation of scattering by periodic surfaces is based on the solution operators over slices with inhomogeneous super- and substrates. The existence and boundedness of these operators were proved, and the convergence of the RCWA was analyzed for surfaces with binary slices. The results will be published in a forthcoming preprint.

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4.5 Research Group 5 "Interacting Random Systems"

Head:	Prof. Dr. Wolfgang König
Deputy Head:	Dr. Robert Patterson
Team:	Dr. Tejas Iyer Julian Kern Heide Langhammer Dr. Elena Magnanini Alexandra Quitmann Helia Shafigh César Zarco-Romero Dr. Alexander Zass Dr. Willem van Zuijlen
Secretary:	Christina van de Sand

The focus of the RG 5 *Interacting Random Systems* is populations of spatially distributed objects that experience random changes, most often due to mutual interactions. The group is particularly interested in problems where the number of entities becomes large and finds ways to make reliable predictions about the collective behavior that arises on large scales. Such large scale behavior can include alterations in physical properties and the appearance of regular patterns. The applications and motivations for the research can generally be found in topics arising in the natural sciences, and we are increasingly focusing on problems where spatial and geometric aspects of interactions are crucial for the large-scale behavior.

The post-doctoral composition of the group was stable during 2023 as intensive work took place on projects funded with the German Science Foundation Priority Program *Random Geometric Systems (SPP 2265)* and the German Science Foundation Collaborative Research Center *Scaling Cascades in Complex Systems (CRC 1114)*. During the year, an application for a second phase of funding for our project on spatially distributed coagulating particles was approved as part of the German Science Foundation Priority Program *Random Geometric Systems (SPP 2265)*.

The group is proud to report that Alexandra Quitmann, after having achieved the first ever proof of macroscopically long loops in the interacting Bose gas, successfully defended her Ph.D. thesis during the year and wishes her all the best as she moves on. Doctoral training is a major activity in the group, and Alexandra Quitmann was one of five doctoral students who were members of the group during the year.

The RG 5 *Interacting Random Systems* was involved in the organization of two conferences during 2023:

- Phase Transitions in Spatial Particle Systems, July 31 – August 2, 2023,
- SPP 2265 Summer School: Probability and Geometry on Configuration Spaces, July 17 – 21, 2023.

The head of RG 5, supported by group members, supervised many bachelor's and master's theses at Technische Universität Berlin during the year. These theses dealt with a wide range of topics, some of which arose out of the research in the group, while one helped formulate a doctoral project

that is now in progress. A small number of theses were supervised independently by experienced post-doctoral members of the group. In addition to the regular teaching responsibilities of the group leader at Technische Universität Berlin, one group member lectured at Freie Universität Berlin in order to maintain current teaching experience.

In its efforts to understand real-world systems and effects, the group uses both static and dynamic models for interacting random systems, and in many cases some kind of geometric graph structure is present. The ongoing work on spatially distributed coagulating particles is very interesting, because it touches on all these topics. Our research on this topic was reported at greater length last year, but, because of its significance within the group, we highlight the most important points.

In recent years, we were able to exploit an equivalence between connected component sizes in certain random graphs and the sizes of particles coagulating according to a simple rule [5]. We are now generalizing the techniques for coagulation that we learned while studying the graphical representation. In doing so, we are exploiting a move to a much richer space as a way to express a coagulation process, which is naturally a dynamical model, as a "static" point process with a Gibbsian interaction that is very common in statistical physics. We are particularly interested in the formation of gels (large particles containing a positive fraction of the available mass), which we are able to identify using point process and other methods [4].

Random graphs are a topic of interest to us in their own right, especially when their nodes can be viewed as spatially distributed. This is a topic where we share many interests with the LG DYCOMNET. Much more information is available in the Scientific Highlights article on this topic on page 17.

The following three sections give some sense of the breadth and applicability of further research undertaken in the group:

Diffusion dynamics for colloids and the packing problem

In this work, we investigate a dynamical version of the AO model introduced in 1954 by S. Asakura and F. Oosawa in Chemical Physics. It is given by a size-asymmetric binary mixture in $\mathbb{R}^3$ that describes colloids (large spheres) in a bath (or emulsion) of ideal polymers (small particles). Our results can be found in [1].

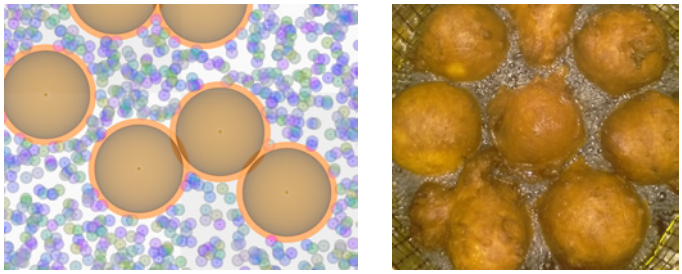

Fig. 1: *Identical hard spheres in a bath of identical small particles. An ideal mathematical representation (left) and a culinary realization (right, jelly doughnuts in particles of frying oil).*
Left: The orange depletion shells around the brown spheres overlap.

We briefly present the model in words: n spheres of equal radius R evolve in a bath of much

smaller ones with radius $r \ll R$. The larger spheres are hard in the sense that they cannot overlap; the smaller spheres (particles), which compose the random medium, are also not allowed to overlap with the large ones. This naturally leads to the presence of a virtual spherical shell around each large sphere, corresponding to the zone in which the centres of the particles are not allowed. This zone, called *depletion* shell, will play a fundamental role in what follows. Finally, the radius r of the particles is taken so small that one can simplify the situation by considering them as an ideal gas: The particles can overlap each other.

We first construct an infinite-dimensional random diffusion dynamics that describes the evolution of this two-type system: The hard spheres and the particles move according to independent Brownian motions, and the only interaction is given by the no-overlap constraint described above. We find that the stationary measure for the system is the uniform distribution of particles and spheres conditioned to satisfy the no-overlap constraint of the AO model.

The marginal of this two-type equilibrium measure for the subsystem of hard spheres presents a new attractive interaction, called *depletion* interaction, due to the fact that the (now hidden) particles form a forbidden region for the hard spheres, thus forcing them closer together. This interaction is proportional to the volume of the depletion shells around the hard spheres (in orange in Figure 1), and is purely 2-body if $r/R \leq \frac{2}{3}\sqrt{3} - 1$. We propose a new gradient random dynamics for the hard spheres that has this marginal as its stationary measure. This dynamics allows us to provide a dynamic solution to the difficult problem of *optimal sphere packing* for any number of spheres and in any dimension: In the asymptotic regime corresponding to a bath with a very high density of particles, the depletion interaction dominates the system, and the optimal configurations tend to maximize their contact number. A companion GitLab page is available with simulations of the two-type and gradient dynamics.

Evolutionary models with fluctuating population size

Models in population genetics try to explain and facilitate the analysis of changes in the genetic composition of a population on evolutionary time scales. To reduce the complexity, many models assume the population size to be constant in time and space. A notable example is the Λ-Fleming–Viot process that models reproduction through a series of so-called *reproduction events* in which a proportion of the population is killed and replaced by offspring.

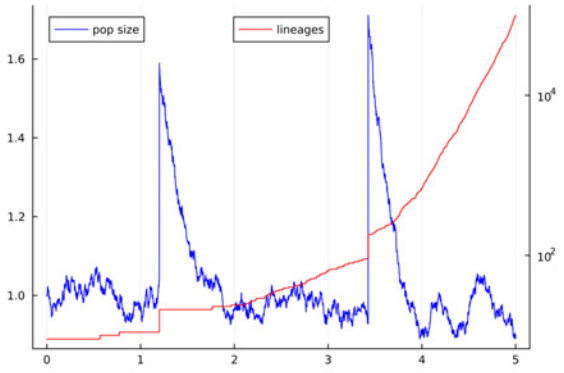

Fig. 2: *Simulation of a (γ, Π)-Fleming–Viot process. In blue: the normalized population size process, scale on the left-hand side. In red: the number of ancestral lineages in the genealogical tree backwards in time, scale on the right-hand side. The code is available through the Julia package GammaPiModel.jl.*

In collaboration with Alison Etheridge (Oxford) and Bastian Wiederhold (Oxford), we are investigating how the behavior of Λ-Fleming–Viot-type models is altered by allowing for variations in the population size. To this end, we developed in [2] the (γ, Π)-*Fleming–Viot process* as a toy model that incorporates reproduction events in which the population size is conserved only on average. Interestingly, the fluctuations in the population size induce a scaling that is fundamentally different from the parabolic scaling in classical models. We showed, however, that the (γ, Π)-Fleming–Viot paradigm can still recover all Λ-Fleming–Viot models, at least through a scaling limit, justifying its use as an extension of the latter.

The genealogy of the population is usually tracked backwards in time through its ancestral tree (which can also be viewed as a coagulation process) in which coalescence of ancestral lineages corresponds to birth events in the population model. To overcome the fact that the genealogical structure becomes intractable when viewed backwards in time, we developed a forward-in-time approach through a so-called *lookdown construction*. In this forward-in-time approach, individual population members have a type, which they inherit from their parent, and which therefore allows genealogies to be reconstructed. Starting from this model, we are able to show that at large times the descendants of one individual will come to dominate the population, forming an ever increasing percentage of the total population, but without ever converging to 100%.

An additional achievement of the work is a new variant of the duality method to prove uniqueness of particular measure-valued processes. This will be particularly valuable for spatial models such as those described in [3, Section 4], for which uniqueness is still partially open.

Lattice models for water droplets

In an ongoing project involving colleagues from RG 1 *Partial Differential Equations* and the Freie Universität Berlin, members of the group are working to extend existing knowledge in the group concerning dynamical large deviations principles and related gradient structures to models for small water droplets suspended in the air within a room. Such *aerosols* are generated, for example, by people as they speak or sneeze and may therefore spread infections. Ultimately, the project aims at a spatially resolved population balance model for aerosols throughout a room; however, it is clear that the loss of water from aerosol particles due to evaporation plays a critical role in determining how they settle out of the air or are entrained by convection currents.

Fig. 3: *Aerosol cloud produced by a sneeze*

In preparation for such a population balance, the RG 5 is working on a stochastic molecular model for individual water droplets. This will give a detailed understanding of how the evaporation rate changes with aerosol radius. Crucially, it will also be capable of extension in a further project to include the effects of solid material in the droplets, which may form a crust as they shrink. In this simplified molecular model, water molecules jump between the sites of fine grid. The jump rate is reduced when another water molecule occupies a neighboring site, reflecting the attractive forces between water molecules while no more than one molecule is allowed to occupy a single site, which approximately captures the very strong short-range mutual repulsion of molecules.

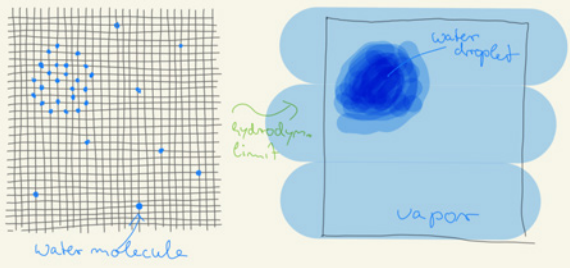

Fig. 4: *Water molecules on a grid approximate a continuous distribution in space*

By proving a large deviations principle for this model in the limit of vanishing grid spacing, we expect to identify the form of the thermodynamical free energy and, more importantly, understand how the transport of molecules is hindered in regions of high concentrations as molecules obstruct each other. Mathematically, this turns out to be very closely related to the *Kawasaki dynamics* for the *Ising model*, which is a classical topic in statistical physics and for which the large deviations principle has not been proved in the low temperature regime of interest in our application.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

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Secretary:	Christine Schneider
Nonresident Member:	Prof. Dr. Peter Friz

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

Members of the research group participated in the DFG Collaborative Research Center SFB 1294 *Data Assimilation*, the *Berlin Center for Machine Learning*, the DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, the DFG International Research Training Group IRTG 2544 *Stochastic Analysis in Interaction*, 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. *Statistical inference* helps to address an important question of reliability of the statistical decision, and it is nowadays an unavoidable element of any statistical analysis. The research includes, e. g., frequentist and Bayesian methods for dimension reduction and manifold learning, change-point detection, regularization and estimation in inverse problems, model selection, feature identification, inference for random

networks and complex statistical objects using optimal transport and Wasserstein barycenter. Research within this subarea covered both theoretical and applied statistical problems.

Highlights 2023:

- The paper "High-probability bounds for stochastic optimization and variational inequalities: The case of unbounded variance" by Abdurakhmon Sadiev, Marina Danilova, Eduard Gorbunov, Samuel Horváth, Gauthier Gidel, Pavel Dvurechensky (RG 6), Alexander Gasnikov, and Peter Richtárik was presented at the International Conference on Machine Learning (ICML) 2023.
- The new application for a joint proposal in the Leibniz Competition under the leadership of ZAS (Leibniz-Zentrum Allgemeine Sprachwissenschaft) was approved. The PIs at WIAS are Vladimir Spokoiny and Karsten Tabelow.
- After the successful defense of Habilitation by Pavel Dvurechensky at the Humboldt-Universität zu Berlin, the Habilitation Committee submitted their positive recommendation to the Faculty Board.
- Jörg Polzehl and Karsten Tabelow published the second revised edition of their monograph "Magnetic Resonance Brain Imaging: Modeling and Data Analysis Using R" with Springer adding very recent new scientific results.

In 2023, the members of the group made some significant contributions to statistical literature.

The paper [5] aimed at revisiting the classical results on Laplace approximation in a modern nonasymptotic and dimension-free form. Such an extension was motivated by applications to high-dimensional statistical and optimization problems. The established results provided explicit nonasymptotic bounds on the quality of a Gaussian approximation of the posterior distribution in total variation distance in terms of the so-called *effective dimension*. This value was defined as the interplay between the information contained in the data and in the prior distribution. In contrast to prominent Bernstein–von Mises results, the impact of the prior is not negligible, and it allows one to keep the effective dimension small or moderate even if the true parameter dimension is huge. We also addressed the issue of using a Gaussian approximation with inexact parameters, with the focus on replacing the maximum a posteriori (MAP) value by the posterior mean and designing the algorithm of Bayesian optimization based on Laplace iterations. The results were specified to the case of nonlinear regression.

We continued the research started by Klochkov, Kroshnin, Zhivotovskiy (Ann. Statist. 2021). We proposed and studied statistical properties of two variants of robust k-means clustering in general metric spaces: one based on the median-of-means approach, and another one based on (adaptive) trimming. It was shown that, under the assumption of finite second moment of a distribution, given a lower bound p on the mass of a cluster, these methods achieve nearly minimax rate in terms of p, k, and sample size n, with sub-Gaussian tail bound. Moreover, trimmed k-means allows us to replace the second moment with the minimal k-means distortion that can be much smaller for well-clustered distributions. The preprints are under preparation.

Within the MATH$^+$ project EF3-8 "Analysis of brain signals by Bayesian optimal transport" (jointly with Technische Universität Berlin), we considered the population Wasserstein barycenter problem from the perspective of the Bayesian approach. Based on the formulation of the Wasserstein barycenter problem as an optimization problem, we constructed a quasi-log likelihood and use it

to construct a Laplace approximation for the corresponding posterior distribution. The latter was used to propose concentration results that depend on the effective dimension of the problem. Preliminary numerical results illustrate the effectiveness of a two-sample test procedure based on these theoretical results. In the broader sense, this approach is planned to be applied to general optimization problems, mimicking gradient- and Hessian-free second-order optimization procedures.

Approximating Wasserstein barycenter is a computationally intensive optimization problem, which motivates the development of efficient numerical algorithms for its solution. In Alexander Rogozin, Alexander Beznosikov, Darina Dvinskikh, Pavel Dvurechenky et al.: *Decentralized saddle point problems via non-Euclidean mirror prox* (accepted to Optim. Methods Soft.), we built on previous research that had proposed an equivalent saddle-point reformulation of the Wasserstein barycenter problem. To scale up the computations, we proposed a decentralized distributed version of the mirror-prox algorithm. Specifically, we focused on smooth convex-concave saddle-point problems in a decentralized distributed setting, where a finite-sum objective is distributed among the nodes of a computational network, and local objectives depend on groups of local and global variables. We estimated the oracle and communication complexities of the algorithm showing that they are optimal by proving the corresponding lower bounds. We demonstrated the effectiveness of our proposed algorithm by applying it to the problem of computing Wasserstein barycenters. Besides the above work, in 2023, we also studied other questions related to the computation of optimal transport distances: first-order algorithms for the Euclidean-regularized optimal transport problems, higher-order, and (distributed) first-order algorithms applied to classical entropy-regularized optimal transport problems. An important feature of the latter is that the communication network may change with time while the algorithm works.

An important part of the research in the group is dedicated to optimization under inexactness, including stochastic optimization motivated by machine learning applications. A highlight of 2023 in this direction is the research on algorithms for stochastic optimization with heavy-tailed noise. For optimization problems, and, more generally, variational inequalities, a series of clipped stochastic algorithms was proposed. The main idea is to clip stochastic gradients when they are too large in the norm due to the heavy tails of the noise distribution. Carefully treating the emerging bias-variance trade-off, complexity guarantees for these algorithms were proved in terms of the high probability of a solution to the problem at hand. Such guarantees are more reliable compared to the standard in-expectation guarantees. The obtained results were published in the proceedings of the International Conference on Machine Learning (ICML) 2023 [4] and were submitted to the International Conference on Learning Representations (ICLR) 2024. Further, together with J.-J. Zhu (WG DOC), motivated by robust machine learning, we proposed and studied the infinite-dimensional Mixed Functional Nash Equilibrium problem, which is a joint optimization problem over the space of measures and a space of functions. We motivated this problem with a number of applications such as the Wasserstein barycenter problem, training of implicit generative models, and distributionally robust optimization. For the setting when the function space is a reproducing kernel Hilbert space, we propose and theoretically analyze an infinite-dimensional mirror-prox algorithm. The results are available in WIAS Preprint no. 3032 and submitted to the Artificial Intelligence and Statistics Conference (AISTATS) 2024.

The research group contributes to the WIAS main application area Quantitative Biomedicine, espe-

cially for (quantitative) imaging problems and in neuroscientific applications. One major achievement in 2023 was the publication of the second revised edition of the Springer monograph "Magnetic Resonance Brain Imaging: Modeling and Data Analysis Using R" by Jörg Polzehl and Karsten Tabelow that includes a complete new chapter on the analysis of inversion recovery magnetic resonance imaging (MRI) data that was, among others, the subject of the MATH$^+$ project EF3-11 "Quantitative tissue pressure imaging via PDE-informed assimilation of MR data" with RG 3 *Numerical Mathematics and Scientific Computing*. Furthermore, the second edition monograph is contributing to the goal of full reproducibility of research result by providing all code and data for download and processing. Within EF3-11, we showed that the new methods for inversion recovery MRI data presented in the monograph can be used to improve the results of the displacement field estimation for magnetic resonance elastography (MRE). This research is complemented by new results on the validity of the axisymmetric diffusion kurtosis imaging model and an analysis of the assumptions of the analytical comparison; see also the Scientific Highlights article "Data-driven Regularization and Quantitative Imaging" on page 40.

The research group is actively contributing to the Mathematical Research Data Initiative (MaRDI) (http://www.mardi4nfdi.de/ Within its task area "Cooperations with other disciplines" and in cooperation with RG 1 *Partial Differential Equations*, we developed a common ontology for mathematical algorithms and mathematical models to be used in the MaRDI knowledge graph and the respective databases. These enable researchers to find, e.g., mathematical models for real-world problems together with the algorithms to solve the mathematical tasks therein and the respective software and publications in an easy and machine-readable manner. This will help researchers to browse the state-of-the-art in the respective field, avoid re-invention of the wheel, and ease the research progress based on existing knowledge. Within the task area "Statistics and machine learning," we started working on the description of statistical methodology and its relation to statistical software also based on an ontology. As R is the lingua franca of statitical software, focus is on the thousands of R packages that are hosted on CRAN and are referenced from the MaRDI portal (http://portal.mardi4nfdi.de/). The research group also contributes to the management of MaRDI and the strategic development of the consortium.

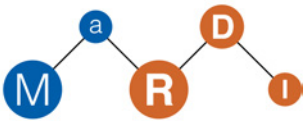

Fig. 1: *The Mathematical Research Data Initiative will contribute to build the National Research Data Infrastructure (NFDI) for mathematics*

Stochastic modeling, optimization, and algorithms

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

Highlights 2023:

- The Focus Platform *Quantitative Analysis of Rough and Stochastic Systems* has successfully completed its work, and will be transformed to a *Research Focus* of RG 6.
- The research monograph "Rough Volatility", edited by Christian Bayer, Peter K. Friz, Masaaki Fukasawa, Jim Gatheral, Antoine Jacquier, and Mathieu Rosenbaum, will be published by SIAM.
- The article "A reproducing kernel Hilbert space approach to singular local stochastic volatility McKean–Vlasov models" by Christian Bayer, Denis Belomestny, Oleg Butkovsky, and John G.M. Schoenmakers was accepted for publication in Finance Stoch.
- The article "Robust multiple stopping – A duality approach" by Roger Laeven, John G.M. Schoenmakers, Mitja Stadje, and Nikolaus Schweizer was accepted for publication in Math. Oper. Res.
- The article "Primal-dual regression approach for Markov decision processes with general state and action space" by Denis Belomestny and John G.M. Schoenmakers was accepted for publication in SIAM J. Control Optim.
- The article "From optimal martingales to randomized dual optimal stopping" by Denis Belomestny and John G.M. Schoenmakers was accepted and published in Quant. Finance (June 2023).

The research on nonlinear Markov or McKean–Vlasov (MV) 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. The study of singular McKean–Vlasov equations, developed in WIAS Preprint no. 2921, that turn up in the smile calibration problem for plain vanilla options for instance, was substantially revised in the year under report, and finally accepted in Finance Stoch.

In the area of optimal control, a regression-based primal-dual martingale approach for solving finite time-horizon *Markov decision processes* with general state and action space, developed in WIAS Preprint no. 2957 was substantially revised in the year under report, and finally accepted in SIAM J. Control Optim.

In a joint project with the University of Amsterdam, a new method for solving general optimal stopping problems with randomly arriving opportunities to stop was developed and published in WIAS Preprint no. 3056. Such problems occur naturally in applications with market frictions. Pivotal to this approach is that the method operates on random rather than deterministic time scales. Along this way, the original problem was converted into an equivalent discrete-time optimal stopping problem with natural number-valued stopping times and infinite time horizon. In this setting, existing methods for finite horizon problems were revisited from a theoretical and a numerical point of view.

The work on numerical quadrature methods for solutions of stochastic differential equations based on numerical smoothing of discontinuous target functionals was continued. These methods exhibit considerably faster convergence speeds to the true expectation especially for financial options (with nonsmooth payoffs) or calculations of probabilities of events or even densities. Additionally, optimal damping regimes for Fourier pricing of European options in multidimensional markets were developed. Damping is required in order to enforce integrability of the Fourier transforms of payoff

functions, a necessary requirement for fast Fourier pricing methods. However, while admissible ranges of damping parameters are widely reported in the literature, optimal choices within these ranges are essentially neglected. Numerical experiments supported by theory presented in WIAS Preprint no. 2968 show that the choice of damping parameters has a significant impact on the accuracy of the pricing routine. In addition, well-performing yet simple rules for the choice of damping parameters are given.

Focus Platform *Quantitative Analysis of Rough and Stochastic Systems*

The investigation of rough volatility models continued. In [7], we studied local volatility under rough volatility. Basket options were studied in related work. We also pioneered a new connection between stochastic and rough analysis.

The development of efficient Markovian approximations to rough volatility models was continued. Efficient numerical simulation methods for the rough Heston model are developed based on new Markovian approximations constructed by optimizing the L^1 distance between the true and the approximating kernel; see WIAS Preprint no. 3044. The rough Heston model is very popular, but accurate simulations remain a difficult open problem due to the highly singular nature of the model. Markovian approximations result in standard, but highly stiff stochastic differential equations, which can be accurately simulated by a combination of splitting and moment-matching methods; see WIAS Preprint no. 3045.

The work on the log-ordinary differential equation (ODE) method for solving controlled differential equations driven by (deterministic) rough paths was continued. An algorithm allowing adaptive control of the time steps as well as the local degree of the method was developed and tested in numerous numerical examples, including examples from machine learning; see WIAS Preprint no. 3013.

New pricing methods for local stochastic volatility models were developed based on deriving pathwise representations of the conditional expectation of the payoff given the stochastic volatility process; see WIAS Preprint no. 3034. Indeed, such conditional expectations can be described as solutions of rough partial differential equations, thereby isolating the "quasi-Markovian" structure induced by the price dynamics. From a numerical point of view, this approach can be seen as a smoothing technique.

The research on signature methods for optimal stopping and pricing of American options continued. In WIAS Preprint no. 3068, signature-based variants of the Longstaff–Schwartz and the dual martingale methods were developed and theoretically analyzed for a very general class of (non-Markovian) processes. As verified by numerical examples, the range of applicability of the methods is thereby pushed considerably beyond the standard (Markovian) domain. Research on signature methods for optimal stopping problems and other classes of stochastic optimal control problems continues.

Research focused on the application of signature methods to Machine Learning. In an ongoing project with Christian Bayer, Simon Breneis, and Peter K. Friz, we show stability bounds for residual neural networks in the average regime with respect to the weight distribution. Work in progress with Joscha Diehl and Leonard Schmitz (both Greifswald) shows how these methods apply to polynomial

feature extraction for image recognition.

At the theoretical level, together with Carlo Bellingeri (Technische Universität Berlin) and Emilio Ferrucci (Oxford), we show that an Itô formula holds for branched rough paths of arbitrary regularity and with no restrictions on the type of lift. In particular, we include all semimartingales and Lévy processes with and without jumps. We are also able to generalize the stochastic exponential to arbitrary branched rough paths, thus providing a version of Kailath–Segall polynomials for non-semimartingale processes. Joint work Ilya Chevyrev (Edinburgh), Joscha Diehl, and Kurusch Ebrahimi-Fard (Trondheim) reveals the algebraic structure of a two-parameter extension of the iterated-integrals signature to be the free 2-groupoid supported on the shuffle algebra.

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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. André H. Erhardt Christine Keller Dr. Manuel Landstorfer Dr. Leonie Schmeller Alireza Selahi
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, for singularly perturbed problems, rigorous analysis of the derived models, and analysis of hysteresis properties. Application areas focus on fundamental processes that drive micro- and nano-structuring of multiphase materials and their interfaces, electrochemical processes as well as electro-magneto-mechanical components. For these application areas the research group develops material models for liquid polymers, hydrogels, active gels, polyelectrolyte gels, and models for biological ion channels, used to understand problems in cell biology and tissue engineering. This is combined with models for lithium-ion batteries and for electro-catalytic applications, as well as models for magnetorestrictive materials. For the corresponding, typically, free boundary problems of multiphase and multiscale systems of partial differential equations (PDEs) the research group also develops mathematical theory and numerical algorithms.

RG 7 was invited to organize as editors two special issues that appeared in 2023 on mathematical methods in the application fields of renewable energies in Wagner and Timme (2023) and biomedical applications in Erhardt et al. (2023).

Multiphase flow problems in soft and living materials

In 2023, research studies of the RG 7 were published for a range of multiphase problems in soft matter and biological systems, where we developed material models, mathematical theory, and numerical algorithms often in close collaboration with experimentalists in the applied fields. The research was mostly funded by the 1st and 2nd funding period within the DFG Priority Program SPP 2171 *Dynamic Wetting of Flexible, Adaptive and Switchable Surfaces* and within the Berlin Mathematics Research Center MATH+ (subproject AA1-12). These papers address liquid-liquid phase separation of the protein FUS (FUsed in Sarcoma), which is considered to play a role in a number of neurodegenerative diseases. The work develops a microscopically informed mean-field theory and compares experimental results conducted at the Max-Planck-Institut für Molekulare Zellbiologie und Genetik (Dresden) [1]. They also address the mechanical properties of articular cartilage, where we develop hydrogel-type models and experiments for fiber-reinforced hydrated

networks (Moore et al. (2023)) in collaboration with colleagues at Imperial College London and further collaborators.

Together with colleagues at the Julius Wolff Institute (Charité), we combine agent-based models (ABM) with strain-stiffening hydrogels to predict the evolution of patterns of cell populations on an extracellular matrix [2]. In collaboration with WG BIP *Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes* (Dirk Peschka), the mathematical theory and numerical algorithms for hydrogels and their free boundary problems with liquid droplets and films were developed in Schmeller and Peschka (2023a), Schmeller and Peschka (2023b), as well as for liquid-liquid interfaces in Shiri et al. (2023) and form a part of the Dissertation by Leonie Schmeller on "Multiphase dynamic systems at finite-strain elasticity," defended on Sept. 26, 2023, at the Institute of Mathematics of the Technische Universität Berlin (with distinction: *summa cum laude*). A considerable part of the publications concerned the analysis of thermodynamically consistant models for electrochemical systems consisting of a polyelectrolyte gel in an ionic liquid bath, conducted together with colleagues at the University of Oxford, University of Bristol, and University College London. The analysis of phase field models showed new oscillatory phase-separated states that were investigated using singular perturbation techniques at the bath-gel double layer [3]. Similar asymptotic techniques were used for the development of a sharp-interface approximation of the Ohta–Kawasaki model for symmetric diblock copolymers in Barua et al. (2023). We will describe two of these studies in more detail.

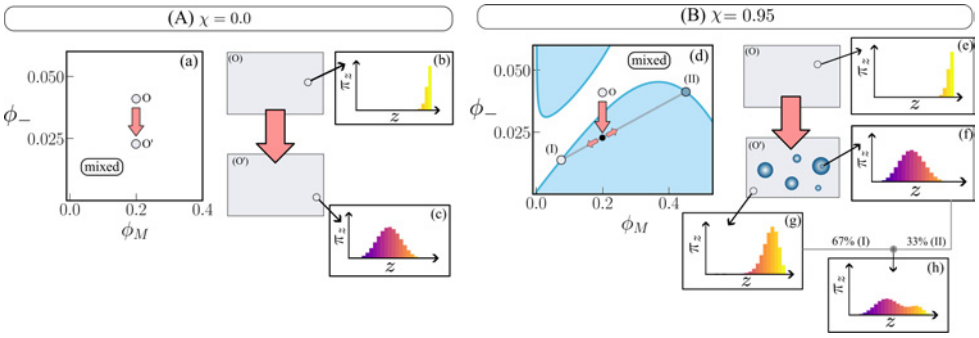

Fig. 1: *Phase separation as a charge regulation mechanism. (A) Solution with non-hydrophobic polymers ($\chi = 0$); (B) Solution of hydrophobic polymers that phase separate upon quenching ($\chi = 0.95$).*

Charge regulation of liquid-liquid phase separation in polyelectrolyte solutions. Charge regulation is an inert, yet often neglected property of systems of polyelectrolyte solutions. Jointly with collaborators from the Université de Lille, University College London, and University of Oxford, we demonstrate in [4] the impact of charge regulation on liquid-liquid phase separation of polyelectrolyte solutions. We explicitly account for variability in the charge states of the polyelectrolyte chains. We investigated the process for a single polyelectrolyte species whose charge states arise from protonation-deprotonation processes in the presence of a dissolved acid, whose anions serve as screening counterions. We derive analytical solutions for the total concentration of polymers, the concentration of counterions, and the charge distributions of polymers to characterize how parameter values and solution acidity influence equilibrium charge distributions. Our analysis of the interplay between charge regulation, solution acidity, and phase separation shows that charge regulation has a significant impact on polymer solubility and allows for nonlinear responses to

the solution acidity. In particular, re-entrant phase behavior is possible in response to increasing solution acidity. Moreover, we show that phase separation can, in turn, yield to the coexistence of local environments characterized by different charge distributions.

Cellular self-organization on strain-stiffening hydrogels. In [2], we focus on the mechanical interactions of a population of cells migrating on hydrogel sheets. The work is meant to accompany *in vitro* experimental work in order to gain a fundamental understanding of the intricate mechanical interplay between cells and the extracellular matrix (ECM) in tissue formation. For this we developed a model framework that couples the derivation of a continuum two-phase model of a viscoelastic hydrogel with an agent-based model (ABM) that governs the migration decisions of each cell as it interacts with the hydrogel and other cells of the population. While the elasticity of hydrogels can, in general, be understood on the basis of the classical theory of rubber elasticity such as for synthetic polymers for the network phase, the elastic modulus of biopolymer networks in natural hydrogels, such as actin, fibrin, or collagen, typically exhibits strain-stiffening properties.

For the analysis of the coupled hydrogel-ABM model our focus was on the geometrical set-up of a fixed hydrogel sheet for which we investigated the stress-strain state by applying specific loads at the fixed boundaries of a rectangular sheet, leaving the other two boundaries free. We compare scenarios that also allow for possible exchange of the solvent phase through the free boundaries. In addition, we compared our results with those using a neo-Hooke model for the nonlinear elastic network to contrast the effects of strain-stiffening on pattern formation of the cell population.

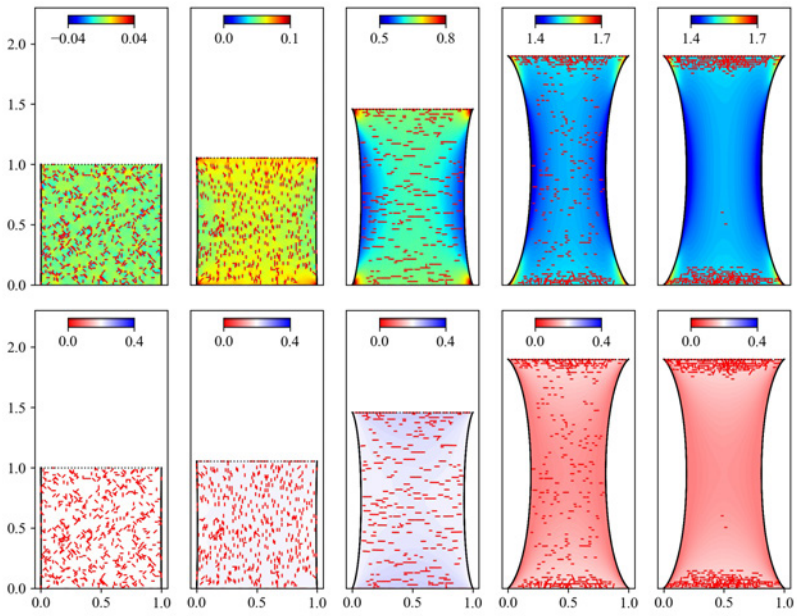

Fig. 2: *Gent-type hydrogel with non-conserved solvent concentration and increasing strain from left to right. The upper panel shows strains, and the lower panel shows concentrations.*

One of the surprising results concerning cell orientation and migration on hydrogels is that at small strain applied on the hydrogel sheet, cells orient vertically, towards the direction of stretch, until a critical value of the applied strain is reached, where the orientation of the cells rapidly flip to the

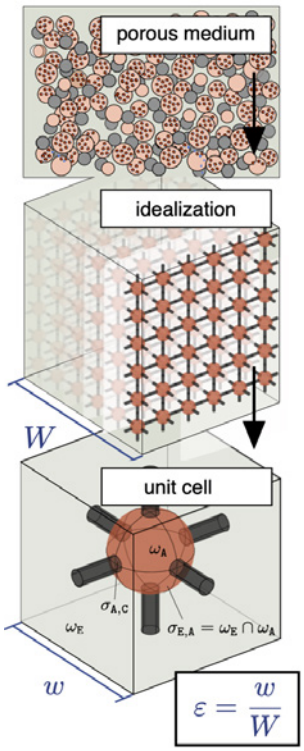

Fig. 3: *Sketch of the spatial periodic homogenization technique.*

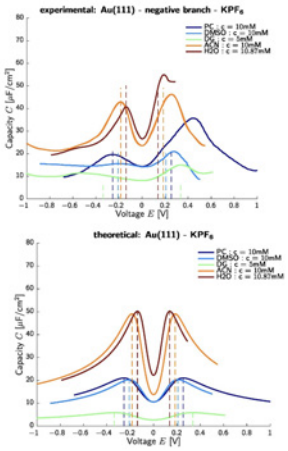

Fig. 4: *Comparison of the experimental data (top) for Au(111)|10 mM KPF6 (5 mM for DG) and theoretical data (bottom) (Fig. 7 from Shatla–Landstorfer–Baltruschat (2021))*

horizontal direction. The value of this critical strain is dependent on the strength of the traction force of the cells. For higher strain applied via stretching the hydrogel sheet, we observe a dramatic morphological change for the Gent-type hydrogel as compared to the only slightly perturbed shape for the neo-Hooke hydrogel model. This has, in turn, a significant effect on the migration of cells being pushed much more quickly towards the clamped boundaries and suppressing chain formation of the cells.

Mathematical models and theory of electrochemical processes

Within RG 7, the whole spectrum of modern mathematical modeling and simulation for electrochemical systems is carried out. Based on non-equilibrium thermodynamics and its coupling to electrodynamics in Müller and Landstorfer (2023), we develop fundamental models for electrolytes, (intercalation) electrodes, and electrochemical reactions that are employed in project-based applications such as electrocatalysis, bio-electrochemical systems, or various batteries. The development of models for lithium-ion batteries [5, 6] is a core competence of RG 7 that is continuously expanded by internal and external cooperations, third-party project funding, and guided by new material developments. A further key feature of RG 7 is the numerical computation of the derived, in general, PDE-based mathematical model to carry out validation studies as well as simulations for the various applications. Mathematical techniques, such as asymptotic expansions, (periodic) homogenization theory (see Figure 3), and modern numerical methods are important tools for RG 7 and continuously further developed in cooperation with RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, and RG 4 *Nonlinear Optimization and Inverse Problems*.

In 2023, three MATH+ subprojects (AA4-8, AA4-9, AA1-14) were running, and one new MATH+ subproject (PaA-2 "Modeling battery electrodes with mechanical interactions and multiple phase transitions upon ion insertion," PIs: Manuel Landstorfer, Matthias Liero) was granted.

Fundamental models for electrochemical systems. In 2023, we continued the research work on electrolyte models, especially on the solvation effect of various solvent molecules. This is important for a variety of applications where water as a solvent cannot be used. Surprisingly, systematic experimental investigations of equal salts, e.g., KPF_6, in a sequence of solvents, e.g., ACN (acetonitrile), DMC (dimethyl carbonate), and others are rare. By the initiative of RG 7, experimental measurements on this aspect were carried out, see Shatla–Landstorfer–Baltruschat (2021), and led to the first, detailed insights on the behavior of the different solvents in an electrochemical environment. This was investigated by differential capacity measurements, which can be computed by the mathematical models of RG 7 and were measured by the group of Helmut Baltruschat from Universität Bonn (see Figure 4). The research in 2023 focused on the aspect of solvent adsorption on the electrode surface and the question if this entails a jump of the electrostatic potential across the (singular) electrode surface. While this *perception* is widespread in theoretical electrochemistry, it has some major drawbacks concerning thermodynamic consistency. However, the experimental impact of solvent adsorption on electrode surfaces is eminent. It shows itself in a shift of the *potential of zero charge* as well as in compressing and widening of the differential capacity (for various solvents, see Figure 4). We developed a (surface) thermodynamic model that accounts for an electrode-solvent free energy interaction on the surface and that naturally predicts these effects,

without assuming a discontinuity of the electrostatic potential. This model is currently investigated in detail and validated on experimental data, which shows already great potential to answer some long-standing questions on solvent-electrode interactions.

The MATH+ subproject AA4-8 "Recovery of battery ageing dynamics with multiple timescales is headed by Martin Eigel (RG 4), Martin Heida (RG 1), and Manuel Landstorfer (RG 7), with Alireza Selahi (RG 7) working as a Ph.D. student on the project. The project aims at developing a data-driven methodology to recover the dynamics of battery aging based on a parametrized mathematical model and experimental data. We succeeded in determining the evolution of certain parameters of the model as a function of the cycling number. These parameters satisfy an evolution equation, where the right-hand side was determined by leveraging methods of Bayesian inverse problems, given numerically generated data of the charge-discharge cycle of a lithium-ion battery (LIB).

In 2023, we considered two different time scales for the spatially homogenized model framework [5]. The small time scale reflects one charge-discharge cycle, while the large time scale captures the battery lifetime over thousands of cycles. The goal was to apply the methods of homogenization theory to gain insights into possible scale separations. Two different approaches were investigated: One is the classical theory of homogenization, and the other one is the theory of multiple time scale dynamics. After a short evaluation of both methods, we decided on the asymptotic expansion method. For a reduced and simplified model, it was possible to show the scale separation between a single charge-discharge cycle and the long time scale that counts the actual number of cycles. This is, from a mathematical point of view, the justification that within a single cycle, the parameters may be assumed to be constant while varying over the number of cycles in the manner described above. However, we were already able to show in a different scaling a more realistic feedback loop between a single cycle and its impact on the parameter variation, which is currently being investigated in more detail.

The MATH+ subproject AA1-14 "Development of an ion-channel model-framework for in-vitro assisted Interpretation of current voltage relations with Jürgen Fuhrmann (RG 3), Manuel Landstorfer (RG 7), and Barbara Wagner (RG 7) as PIs and Christine Keller (RG 7) as a Ph.D. student, aims to develop a PDE-based model framework to predict current-voltage relations of calcium ion channels in biological applications. A key feature of this modeling procedure is the ability to vary salt concentrations, applied voltages, and channel elasticity to support the interpretation of measured results.

A fundamental aspect of ion channels is their high selectivity for certain ions, which is controlled by the selectivity filter region within the pore. We placed particular emphasis on consistent modeling of this selectivity filter. Our approach is to treat this region as an additional embedded domain with surface charges. It is thought to behave like a solid or polymer electrolyte, where ions passing through the channel interact with immobile species that form the selectivity filter. An illustration is given in Figure 5. In addition, de- and re-solvation effects are considered within the free energy density of the system and by chemical reactions at interfaces that are included as Neumann interface conditions.

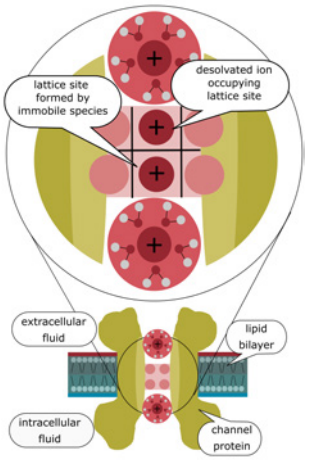

Fig. 5: *Sketch of the extracellular and intracellular fluid connected by a channel that is a selectivity filter*

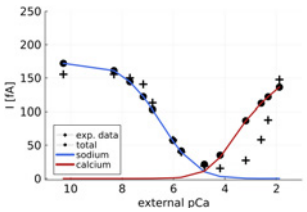

Fig. 6: *Model simulation (circles), experimental data (crosses), sodium (blue), and calcium current (red)*

The system is solved numerically in Julia using the Voronoi finite volume method. In a first validation study, the model was compared to experimental data, where a calcium selective ion channel was studied by measuring the total ionic current for different extracellular calcium concentrations. It was found that for low calcium concentrations a sodium current was measured. However, for higher calcium concentrations the sodium current decreases, and the calcium current is dominant. The model shows a good agreement with the experimental data and is able to depict this behavior, as shown in Figure 6. A first parameter study indicates that both mobility and electrostatic forces (surface charges) do have an influence on the ion current flowing through the channel.

Hysteresis, electromagnetic-mechanical components, and uncertainty quantification

The investigations on uncertainty quantification for models involving hysteresis operators were continued. Using experimental data for Terfenol-D, provided by Carmine S. Clemente and Daniele Davino (Benevento, Italy), appropriate values for the parameters in a model following Sec. 5.1 of Davino–Krejčí–Visone (2013) were computed. Information on the uncertainty of these parameters was determined by using the software package UQLab (Marelli–Sudret (2014), https://www.uqlab.com/); see [8].

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

Head: Prof. Dr. Michael Hintermüller

Deputy Head: Dr. Caroline Geiersbach

Team:
Dr. Amal Alphonse
Dr. Marcelo Bongarti
Prof. Dr. Martin Brokate (long-term guest)
Sarah Essadi
Dr. Moritz Flaschel
Maximilian Fröhlich
Sophie Gehricke (WIAS Female Master Students Program)
Dr. Patrick Jaap (later RG 3)
Stefan Kater
Dr. Denis Korolev
Dr. Ioannis Papadopoulos
Clemens Sirotenko
Luise Teigeler (WIAS Female Master Students Program)
Mike Theiß
Qi Wang

Secretary: Pia Pfau

The research group RG 8 *Nonsmooth Variational Problems and Operator Equations* continued its work in the area of optimization and equilibrium problems involving nonsmooth structures. The group focuses on the mathematical modeling, analysis of the underlying variational problems and operator equations, and development and implementation of numerical solution methods. Research is informed by physics-based applications, often involving partial differential equations (PDEs), and as a rule containing nonsmooth constituents. This contributes to the institute's main application areas *Energy: Technology, Markets, Networks*, *Quantitative Biomedicine*, *Optimization and Control in Technology and Economy*, *Flow and Transport*, as well as aspects of *Materials Modeling*. In view of these applications, the group's work includes generalized Nash equilibrium problems and mean field games, quasi-variational inequalities, physics and model-based image processing, optimal control of PDEs, and optimization problems involving fluid flows. The group continues to strengthen its presence in the fields of data-driven or neural network-based optimization as well as nonsmooth problems under uncertainty.

Michael Hintermüller is currently spokesperson of the Berlin Mathematics Research Center MATH+. He is additionally serving as a scientist-in-charge of the MATH+ Emerging Field 3 (EF3) Model-Based Imaging. The group gained several new postdoctoral researchers and Ph.D. students thanks to the initiation of several projects. Within MATH+, work began in project EF1-15: "Robust multilevel training for artificial neural networks," EF3-12: "Integrated learning and variational methods for quantitative dynamic imaging," and AA4-13: "Equilibria for distributed multi-modal energy systems under uncertainty." Dr. Ioannis Papadopoulus joined the group from Imperial College London as a MATH+ Dirichlet postdoctoral fellow; his work is focused on numerical analysis and scientific

computing. Steven-Marian Stengl successfully defended his dissertation entitled "Existence Theorems, Stationarity Conditions and Adaptive Numerical Methods for Generalized Nash Equilibrium Problems Constrained by Partial Differential Equations."

RG 8 has two ongoing projects within the third and final phase of the Collaborative Research Center CRC/TRR 154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks* and supported the organization of the semi-annual meeting in 2023. The SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* is winding down at the end of a second phase of funding. A special issue book collecting the research achievements of the second phase is being compiled for publication under Birkhäuser and is currently at the reviewing stage. The SPP also partly funded the European Conference on Computational Optimization 2023, held in Heidelberg, as well as the workshop "Frontiers of Stochastic Optimization and its Applications in Industry;" members of the group participated in and contributed to the organization of both events.

Denis Korolev and Michael Hintermüller are actively involved in the collaborative project ML4SIM "Machine Learning for Simulation Intelligence in Composite Process Design" together with the Leibniz-Institut für Verbundwerkstoffe, Deutsches Forschungszentrum für Künstliche Intelligenz (German Research Center for Artificial Intelligence), Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), and the Fraunhofer-Institut für Techno- und Wirtschaftsmathematik. Consortium meetings were held in May at IPF Dresden and at the Weierstrass Institute in November. These meetings not only serve to discuss individual research results, but also aim to establish a common scientific language across diverse research groups and foster interdisciplinary experiences. The partners also discussed the potential opportunities to continue the research cooperation on the intersection of mathematics, computer science, and composite materials.

Additionally, the research group was co-organizer and supporter of the Mathematics and Image Analysis Conference (MIA) in Berlin, together with Humboldt-Universität zu Berlin and Technische Universität Berlin. The conference took place in February.

Optimization with applications in physics-based systems

Optimal control of a nonsmooth Cahn–Hilliard/Navier–Stokes system. In [1], a strong stationarity system for the optimal control of a semi-discrete in time Cahn–Hilliard/Navier–Stokes system was derived. The nonsmoothness stems from a double obstacle potential in the Ginzburg–Landau free energy associated with the Cahn–Hilliard component of the above system and gives rise to a variational inequality problem in the state system. Such a setting is relevant in mathematical models of physical systems of demixing with deep temperature quenches or, e.g., in polymer membrane formation under rapid wall hardening. Mathematically, the nonsmoothness gives rise to a degenerate constraint system in the associated optimization problem, thus preventing the application of the well-established Karush–Kuhn–Tucker theory in Banach spaces. For the derivation of strong stationarity of an optimal solution, in [1] the Hadamard directional differentiability of the control-to-state map was shown, and it was then used directly to characterize strong stationarity. In contrast to other forms of stationarity conditions such as weak, C-, or M-stationarity, strong stationarity is the most desirable among the primal-dual stationarity conditions as it represents

the strongest available filter to avoid spurious stationary points. This newly derived stationarity characterization is planned to be exploited in the design of numerical solvers such as the bundle-free technique introduced earlier by Michael Hintermüller and Thomas M. Surowiec (Simula Research Laboratory) for the optimal control of the obstacle problem.

Optimization under uncertainty. In 2023, work began on two projects with applications in energy. The first is project B02 "Multicriteria optimization using the example of gas markets" within the third phase of Collaborative Research Center CRC/TRR 154 and headed by the co-PIs Michael Hintermüller and Caroline Geiersbach. The second project is MATH+ AA4-13: "Equilibria for distributed multi-modal energy systems under uncertainty" headed by Michael Hintermüller, Caroline Geiersbach, Pavel Dvurechensky (RG 6), and Aswin Kannan (Humboldt-Universität zu Berlin). Both projects involve, among other aspects, incorporating uncertainty into physics-based generalized Nash equilibrium problems.

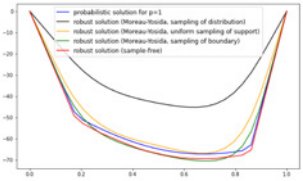

Fig. 1: *Comparison of optimal controls obtained using probability function, regularization, or exact formula*

In view of this application, work began on characterizing optimality for the single-player model, where uncertainty enters in the form of a random PDE. First steps were made in characterizing optimality for stochastic optimization problems over Banach spaces with random state constraints in [2], which was a joint project with RG 4 *Nonlinear Optimization and Inverse Problems*. Several constraint models were compared, namely in probabilistic, almost sure, and robust forms. For an optimization problem with an elliptic PDE with a random right-hand side, necessary (and if possible, sufficient) conditions were given for optimality. This work informed further numerical studies for the same system in [3]. Different numerical approaches were compared for the solution to the problem with almost sure state constraints. Experiments demonstrated that the obtained formula for the subdifferential of the probability function can be used as an approximation of the almost sure model. This was compared to an approach involving Moreau–Yosida regularization of the state constraints with various sampling strategies. An example of this comparison is shown in Figure 1.

Mean field games

The group continued its research in constrained mean field games. In this project, the analysis of a noncooperative differential N-player game was studied. The modeling of the game, at an individual level, is as follows:

$$\begin{aligned} &\text{minimize} && J^i(\alpha^i, x^i; \mu^{i,N}) \text{ over } A^i_{ad} \times X^i_{ad} \times \mathcal{AC}(0,T;\mathcal{P}(\mathbb{R}^d)) \\ &\text{subject to} && \dot{x}^i = Ax^i + B\mathbb{E}_{\mu^{i,N}}[id] + \alpha^i, \quad x^i(0) = x^i_0 \in \mathbb{R}^d, \end{aligned}$$

where A^i_{ad} are box constraints for the control, X^i_{ad} are conic constraints for the state, and $\mathcal{AC}(0,T;\mathcal{P}(\mathbb{R}^d))$ is the space of all absolutely continuous flows of probability measures. The objective function involves nonsmoothness (ℓ^1 norm) in the tracking terms of the state functions and a standard quadratic control cost. A generalized Nash equilibrium of this constrained game exists, and a limiting model leads to a representative agent's optimal control problem.

A special case of the latter model is given by the following PDE formulation:

$$\begin{cases} -\partial_t u(t,x) + H(x, Du(t,x); m(t,x)) = 0\,, \\ \partial_t m(t,x) + \nabla \cdot \big(D_p H(x, Du(t,x); m(t,x)) m(t,x)\big) = 0\,, \end{cases}$$

where m is the density of a probability measure, and u is the value function. The mean field PDE system is understood as a coupled backward-forward system of PDEs. The first is the Hamilton–Jacobi equation, and its study requires, in our case, the notion of lower semicontinuous viscosity solutions. The latter is the continuity equation, and it results from the dynamics and the mean field term and is to be understood in the distributional sense.

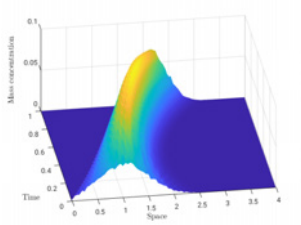

Fig. 2: *$\overline{\mu}$ with no active constraints*

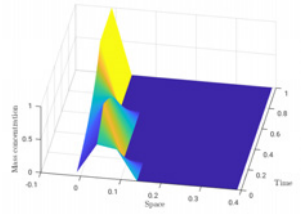

Fig. 3: *$\overline{\mu}$ with active state constraints*

Further, a numerical algorithm was developed to solve the mean field game with a quadratic objective function. The algorithm can be seen as a fixed-point algorithm in the mean field $\overline{\mu}$. For each new solution $\overline{\mu}$ of the continuity equation, one can solve the representative agent problem by an augmented Lagrangian algorithm to update the flux pertaining to the continuity equation. Figure 2 and Figure 3 show examples in one dimension of a density of $\overline{\mu}$ with no active constraints and with active state constraints, respectively. A subsequent study will involve stochastic dynamics without common noise, as well as explore constrained multi-player systems governed by a centralized control.

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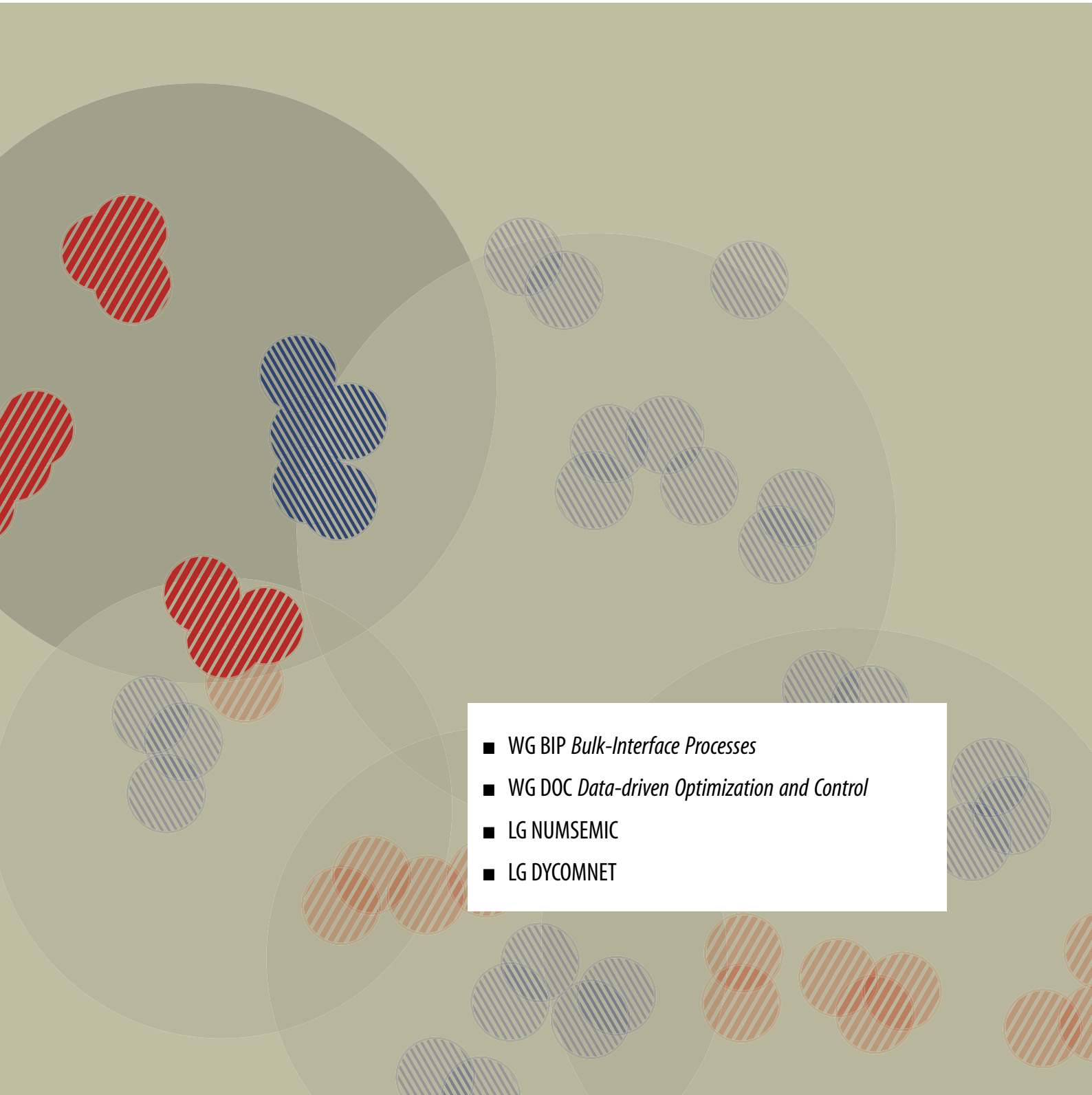
5 Flexible Research Platform



- WG BIP *Bulk-Interface Processes*
- WG DOC *Data-driven Optimization and Control*
- LG NUMSEMIC
- LG DYCOMNET

5.1 Weierstrass Group BIP "Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes"

Head: Prof. Dr. Marita Thomas
Team: Dr. Dirk Peschka
Secretary: Andrea Eismann

WG BIP was established as an element of the Flexible Research Platform at WIAS in April 2017, partially funded by WIAS budget resources. After a first successful period of three years, the group was positively evaluated in spring 2020, and a second three-year funding period was granted. In accordance with the WIAS strategy, the group terminated in June 2023 after six years of successful research.

The research goal of WG BIP consisted in developing mathematical methods for systems with bulk-interface processes. This concerned 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 provided the basis for the development of numerical algorithms supporting simulations for applications with bulk-interface interaction. During the first funding period, WG BIP contributed with its research projects to the three WIAS main application areas *Nano- and Optoelectronics*, *Materials Modeling*, and *Flow and Transport*. Since the projects on mechanically strained optoelectronic devices were considered successfully closed by the start of the second funding period, from July 2020 on, the group continued and intensified its research on applications within the areas *Materials Modeling* and *Flow and Transport*, in particular, on:

(1) Dissipative processes in elastic solids with bulk-interface interaction, such as, e.g., damage, fracture, plastification, and

(2) Multiphase flows with free boundaries.

The group also pursued the long-term goal of further directing the research within (1) and (2) towards applications in biology.

WG BIP contributed to organizing the WIAS seminar on Materials Modeling and to the Langenbach Seminar on Nonlinear Partial Differential Equations. In the winter term 2020–2021, the WG BIP co-organized a Thematic Einstein Semester on "Energy-Based Mathematical Methods for Reactive Multiphase Flows". The ZAMM special issue "Energy-Based Mathematical Methods for Reactive Multiphase Flows" related to this event appeared in July 2023, and it features 10 articles dedicated to recent results in the thermodynamically consistent modeling and in the development of mathematical tools suited to solve complex problems in materials science.

In 2023, group members also contributed to the organization of the conference "Variational and Geometric Structures for Evolution" that took place on October 9–13, 2023, in Levico Terme (Italy), funded by CIRM Centro Internazionale per la Ricerca Matematica, the DFG-CRC 1114 *Scaling Cascades in Complex Systems*, the DFG-SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*, and by the grant PRIN 2017 "Gradient flows, optimal

transport and metric measure structures" (U Bocconi, Milano). The workshop was dedicated to analytical methods for the exploration and identification of variational and geometric structures for evolutionary problems with a focus on applications to dissipative models and systems governed by reaction-diffusion mechanisms. It featured 28 invited talks and a special session to mark the 65th birthday of Alexander Mielke, whose work has set a cornerstone in this field.

In 2023, following a restructuring process that was started already in 2022 in view of the group's planned termination in June 2023, the group saw further changes in its staff. By now, all former group members have obtained new positions at universities or in other WIAS research groups, and it is a pleasure to report here on these successes: Dirk Peschka held a guest professorship at Freie Universität (FU) Berlin in summer term 2023, where he gave lectures on Linear Algebra I and a course on numerical methods in fluid dynamics. Moreover, his application for a project within the DFG-funded Priority Program SPP 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates* was successfully granted in 2022. With funding for his own position in the project "Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows," Dirk Peschka joined RG 1 *Partial Differential Equations* in October 2023 to continue his research on structure-preserving numerical methods for complex fluid flows with free boundaries. Also Marita Thomas, who has held the W2 Professorship for Applied Analysis at Freie Universität Berlin since August 2022, has joined the research team of RG 1 for two more years to continue her research on ongoing projects with the group members. In the course of her call to FU Berlin, it was possible to offer positions to the former WG BIP members Sven Tornquist and Andrea Zafferi at FU Berlin, where they will submit their Ph.D. theses and may subsequently continue their work on postdoc positions. Furthermore, also the former group members M. Hassan Farshbaf Shaker and Xin Liu have obtained professorships elsewhere. M. Hassan Farshbaf Shaker started his new position as a W2 Professor at the Hochschule für Technik und Wirtschaft Berlin (HTW Berlin) in April 2022, and Xin Liu was awarded an assistant professorship at the Department of Mathematics at Texas A & M University.

The WG BIP now happily looks back on six years of successful research in the fruitful and cooperative research atmosphere at the WIAS. Some of the research results of the WG BIP are described in more detail in the Scientific Highlights article on page 10.

5.2 Weierstrass Group DOC "Data-driven Optimization and Control"

Head: Dr. Jia-Jie Zhu
Team: Ling Liang
René Saitenmacher
Secretary: Christine Schneider

WG DOC was established as a unit of the Flexible Research Platform at WIAS in June 2021, funded by WIAS budget resources. The group has successfully undergone the first interim review and will be prolonged to May, 2027. In 2023, a postdoctoral scholar, Ling Liang, funded by the Berlin Mathemacics Research Center MATH+, has done a research stay with the group, before continuing his career in the US. In addition, a new Ph.D. student, René Saitenmacher, has joined the group. The WG has successfully acquired the MATH+ subproject AA5-10 (jointly with partner institutions) on "Robust data-driven reduced-order models for cardiovascular imaging of turbulent flows," in collaboration with Alfonso Caiazzo (RG 3 *Numerical Mathematics and Scientific Computing*) and the Charité, Berlin. This will fund one postdoc position—in the intersection of numerical partial differential equations (PDEs) and machine learning—to be filled in early 2024. In 2023, WG DOC leader Jia-Jie Zhu gave nine invited talks, which greatly boosted the visibility of the group in the international research community. Notably, his invited talk at an International Conference on Machine Learning (ICML) workshop, in Hawaii, USA, has generated significant interest towards our research in the machine learning community.

Another milestone for WG DOC in 2023 was the successful proposal for funding from the DFG (German Research Foundation) for an international collaboration. The project, titled "Workshop on Optimal Transport from Theory to Applications – Interfacing Dynamical Systems, Optimization, and Machine Learning," has been granted (Project Number 536048694), co-organized by Jia-Jie Zhu in collaboration with Matthias Liero (RG 1 *Partial Differential Equations*), Pavel Dvurechensky (RG 6 *Stochastic Algorithms and Nonparametric Statistics*), and Gabriele Steidl (Technische Universität Berlin). This endeavor reflects our commitment to interdisciplinary research and highlights our role at the forefront of integrating dynamical systems, optimization, and machine learning in the realm of optimal transport.

WG DOC's overarching goal is to study mathematical foundations and applications of machine learning and computational optimization algorithms. One of WG DOC's focal topics is the theory and application of robust machine learning algorithms and statistical inference. We are heavily invested in optimal transport theory and kernel methods for machine learning, such as applications to generative modeling. On the other hand, we have acquired significant expertise in optimization and learning with probability measures. This also fits into the research landscape of WIAS, such as in transport, gradient flows, mechanics, PDE and dynamical systems research.

Building upon our previous works in distributionally robust optimization and kernel methods using the kernel maximum mean discrepancy (MMD), e.g., [2, 1], we further expand our expertise in

achieving robust learning and estimation under stronger forms of structured distribution shift—those caused by causal confounding and heterogeneity within the data sets. In [4], together with collaborators at the Max-Planck-Institut für Intelligente Systeme, Tübingen, we invented a new estimation algorithm that beats state-of-the-art performance in conditional moment restriction for estimation. In our ICML 2023 paper [3], following our previous work [4], we apply our kernel geometry to construct the first (generalized) moment method (GMM) (and empirical likelihood (EL)) estimation method that allows us to consider all distributions including continuous distributions. Existing MM or EL methods use the f-divergence; hence, the probability distributions considered there must be absolutely continuous with respect to empirical (atomic) distributions. In addition to achieving optimal statistical efficiency, using the kernelized geometry-based computational algorithms, we also achieve practical performance exceeding state-of-the-art estimation methods in small to moderate sample-size regimes, as well as matching performance in large-data regimes. This is the first work that introduces a new geometric perspective in EL and GMM, which also sets the state-of-the-art performance benchmark.

We also deepened our investigation of the measure optimization problem, e.g., with application in distributionally robust optimization and optimal transport, in collaboration with Pavel Dvurechensky (RG 6). In that direction, we have currently a preprint under review, entitled "Analysis of kernel mirror prox for measure optimization." In that work, we provided algorithmic analysis for a new type of mirror descent algorithm for measure optimization, which can be applied to general machine learning and measure optimization with convergence guarantees. To fully attack the problems in machine learning that involve measure optimization, such as generative modeling, we are in the process of establishing cooperations with other experts at WIAS. For example, we are exploring novel applications of principled Wasserstein gradient flow theory, PDE, and optimal transport, via interactions with experts such as Alexander Mielke (RG 1).

Last but not least, another focus of WG DOC is in data-driven modeling and control of dynamical systems. This research direction draws from the foundational works in kernel discrepancy measures and data-driven modeling schemes principled in statistical learning theory. For example, we recently completed a few preprints, e.g., on data-driven modeling of dynamical systems using kernel conditions mean embeddings [5], a framework that is the adjoint of the Koopman operator perspective, and on Wasserstein nonlinear distributionally robust control [6].

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5.3 Leibniz Group NUMSEMIC "Numerical Methods for Innovative Semiconductor Devices"

Head: Priv.-Doz. Dr. Patricio Farrell

Team: Dr. Yiannis Hadjimichael
Dr. Daniel Fritsch
Dilara Abdel
Zeina Amer

Secretary: Imke Weitkamp

Fig. 1: *Leibniz Group NUMSEMIC (left to right): Patricio Farrell, Dilara Abdel, Yiannis Hadjimichael, Daniel Fritsch, and Zeina Amer. Not in picture: Imke Weitkamp.*

The Leibniz Group NUMSEMIC was established on the WIAS Flexible Research Plattform in January 2020 after successfully winning a grant within the Leibniz competition. For six years, it is funded by the Leibniz Association and covers three of WIAS's main application areas: *Materials Modeling*, *Energy: Technology, Markets, Networks*, and *Nano- and Optoelectronics*. The aim of this group is to develop partial differential equation (PDE) models as well as physics-preserving numerical techniques for new semiconductor materials and technologies. During 2023, Dilara Abdel submitted her Ph.D. thesis. The group successfully acquired a MATH+ project, supported a short-term scientific mission within the Leibniz Research Alliance "Health Technologies" that was supervised by Costanza Manganelli (IHP) and participated in the 175th European Study Group with Industry hosted at WIAS.

Furthermore, Patricio Farrell completed his habilitation at Freie Universität Berlin, became a *Brain City Ambassador* for the Senate of Berlin, and was voted among the *Top 40 under 40* by the business magazine "Capital." Futhermore, he gave an invited talk at the conference on "Device Physics Characterization and Interpretation in Perovskite and Organic Materials" and was invited to work as a guest professor at the University of Florence.

The following topics drive our research:

- **Electro-mechanical models and simulations**, e.g., to understand transport in bent nanowires,
- **Two-dimensional memristive devices**,
- Models and simulations of charge transport in **perovskite solar cells**,
- Opto-electronic **laser models and simulations**,
- Inclusion of **atomistic effects** in drift-diffusion models.

We present these applications in more detail.

Fig. 2: A bent nanowire

Electro-mechanical models and simulations. Together with Christian Merdon (RG 3 *Numerical Mathematics and Scientific Computing*), Yiannis Hadjimichael and Patricio Farrell develop numerical techniques to simulate charge transport in bent nanowires. The difficulty here is to combine the nonlinear van Roosbroeck system, which models charge transport in semiconductors, with an appropriate model from continuum mechanics to take into account the deformations. A model that describes the bending of nanowires due to a lattice number mismatch as well as piezoelectric effects was proposed and numerically solved using the finite element method. Our numerical simulations show that the curvature of bent nanowires agrees well with analytical derivations. The relevant code is included in the `StrainedBandstructures.jl` package.

The interaction between strain and piezoelectricity in bent nanowires has a significant impact on the band structures and, consequently, the charge transport properties. We study the effects of strain on various crystal nanostructures and utilize the `S/PHI/nX package` (partially developed at WIAS) to gain insights into the optoelectronic properties of heterostructures. This work is a collaboration with the Paul-Drude-Institut für Festkörperelektronik (PDI).

In general, it is important to understand how band-edge energies are impacted by general strain profiles. Daniel Fritsch investigated how to find the eigenvalues from a Bir–Pikus Hamiltonian and identify them with heavy hole, light hole, and split-off band edge energies. This work is in collaboration with the Leibniz Institute for High Performance Microelectronics (IHP).

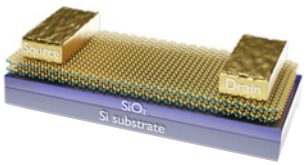

Fig. 3: Two-dimensional memristor from [1]

Two-dimensional memristive devices. The von Neumann architecture is far from ideal for AI applications due to its unacceptably high energy consumption. Memristors help to emulate the extremely efficient computing power of human brains. Dilara Abdel and Patricio Farrell develop together with researchers from TU Ilmenau complex charge transport models that incorporate mobile point defects and Schottky barrier lowering to theoretically understand the shape and asymmetries of the hysteresis curves observed in experiments [1].

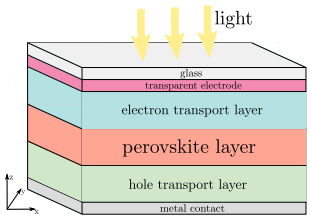

Fig. 4: Perovskite solar cell

Perovskite solar cells. In recent years, perovskite solar cells (PSCs) have become one of the fastest growing technologies within photovoltaics. Two advantages of PSCs stand out: On the one hand, certain architectures have significantly lower production costs than conventional solar cells. On the other hand, in 2020 silicon-perovskite tandem cells have become more efficient than classical single junction silicon solar cells. A record efficiency of 32.5% has been demonstrated. Further efficiency gains are likely. However, the commercialization of PSCs is still in its early stages.

With Nicola Courtier (University of Oxford), alternative current density descriptions for the inclusion of volume exclusion effects are numerically compared [2]. The simulations are performed with `ChargeTransport.jl`, a software package developed in cooperation with Jürgen Fuhrmann (RG 3) for the simulation of charge transport in semiconductors. Apart from numerical simulations, also the numerical analysis, including entropy dissipation relationships, of the model was analyzed with colleagues from the University of Lille/INRIA Lille [3].

Laser models and simulations. Together with Hans Wenzel (Ferdinand-Braun-Institut, FBH), Eduard Kuhn, and Markus Kantner (both RG 2 *Laser Dynamics*), Zeina Amer and Patricio Farrell develop optoelectronic models and simulations within `ChargeTransport.jl`, coupling charge transport to a Helmholtz problem.

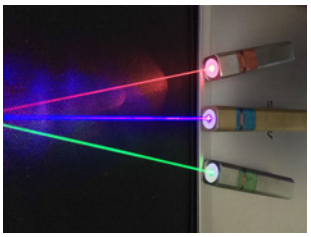

Fig. 5: *Lasers. Source: Pang Kakit CC BY-SA 3.0.*

Coupling with atomistic effects. LG NUMSEMIC investigates together with researchers from Tyndall National Institute, INRIA Lille, and Thomas Koprucki (RG 1 *Partial Differential Equations*) how to combine random atomic fluctuations in band edges with macroscale drift diffusion processes. To this end, spatially randomly varying band edges were implemented in `ddfermi` [4, 5].

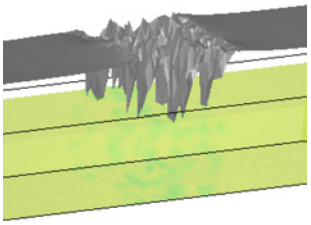

Fig. 6: *Random fluctuations in the band edge energy on atomic scale*

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[4] R. Finn, M. O'Donovan, P. Farrell, J. Moatti, T. Streckenbach, T. Koprucki, S. Schulz, *Theoretical study of the impact of alloy disorder on carrier transport and recombination processes in deep UV (Al, Ga)N light emitters*, Appl. Phys. Lett., **122** (2023), pp. 241104/1–241104/7.

[5] P. Farrell, J. Moatti, M. O'Donovan, S. Schulz, T. Koprucki, *Importance of satisfying thermodynamic consistency in optoelectronic device simulations for high carrier densities*, Opt. Quantum Electron., **55** (2023), pp. 978/1–978/12.

5.4 Leibniz Group DYCOMNET "Probabilistic Methods for Dynamic Communication Networks"

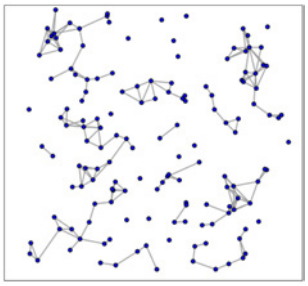

Fig. 1: *Realization of a soft-Boolean model with local interference. Poisson points are connected by an edge based on their mutual distance, individual random weights, and sufficiently small local interference.*

Head: Prof. Dr. Benedikt Jahnel

Team: Dr. Sanjoy Kumar Jhawar
Jonas Köppl
Dr. Lukas Lüchtrath
Anh Duc Vu

Secretary: Christina van de Sand

The Leibniz junior research group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks* is cofunded by the Weierstrass Institute and the Leibniz Association through the *Leibniz Competition 2020*. 2023 is the third year within the anticipated five-year total runtime of the group. Broadly speaking, LG DYCOMNET's goal is to perform state-of-the-art research in the domain of complex spatially distributed communication networks using methods from stochastic geometry and statistical mechanics. A prototypical example is the modeling and analysis of dynamic peer-to-peer networks via the theory of random point processes, interacting particle systems and large deviations theory. LG DYCOMNET thrives to exhibit rigorous results, for example, for connectivity properties of such networks, manifesting themselves, e.g., via percolation phase transitions.

In 2023, our postdoc Sanjoy Kumar Jhawar left the group (starting a new position at INRIA Paris, France) but, due to a successful application at the cluster of excellence MATH+, LG DYCOMNET will grow again with a new postdoc position (to be filled in early 2024) working in the field of *data transmission in dynamical random networks*.

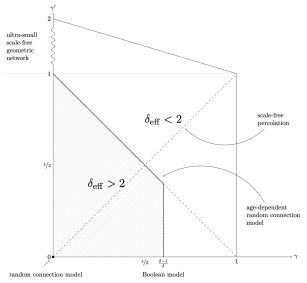

Fig. 2: *Phase diagram for the presence and absence of a subcritical phase in a multi-parameter longe-range percolation model*

The LG DYCOMNET has produced seven preprints in 2023 and has seen a number of its previous preprints being published in A* journals in probability theory and applied mathematics, such as, for example, the *Electronic Journal of Probability* or *IEEE Transactions on Information Theory*. In the context of percolation theory, the preprints [3] and [5] feature a variety of random graphs, both as random sublattices of $\mathbb{Z}^d$ and in the continuum, both as directed and undirected networks, and both with and without long-range correlations. Using a divers set of methods such as martingale approximations, multi-scale analysis, and coupling techniques, members of the group have successfully established criteria for the existence and absence of infinite connected components, which serve as a key performance indicator for the connectivity in such networks. In [2], the modeling and analysis goes substantially beyond the static settings mentioned above and analyzes the evolution of an infection on a non-mixing random environment, thereby exhibiting parameter regimes for survival and extinction of the infection. The preprint [6] takes a slightly different perspective and analyzes the limiting spatial distribution of vertices with a fixed given degree in a high-density network in which nodes are connected via the so-called *preferential attachment kernel*. The vertices additionally carry individual weights that also control the likelihood of being connected, and the central result in the paper features precise criteria, in terms of the small weight quantiles, for the limiting object to be a Poisson point process. As a second line of research, the works [1], [4] are dedicated to the analysis of models from statistical mechanics, both with and without dynamical aspects. In [4], long-standing questions about the attractor of low-dimensional not necessarily

translation-invariant reversible interacting particle systems are addressed. In this situation, members of the group were able to derive general criteria for the dynamic ergodicity of the system. On the other hand, in [1] the classical static Widom–Rowlinson model is considered in a random environment of percolation type. Using the Papangelou intensity approach, it is shown that, both on the lattice and in the continuum, even in a subcritical percolation environment, the quenched system features non-removable discontinuities reminiscent of the so-called *Griffiths singularities* in disordered systems.

Finally, the success of LG DYCOMNET in 2023 is underlined by the invitation of Jonas Köppl to the *10th Heidelberg Laureate Forum*, which is a competitively awarded opportunity for excellent young scientists to meet elite international researchers in their respective field. Members of the team have given about 25 presentations at national and international conferences and research institutions including some outreach talks.

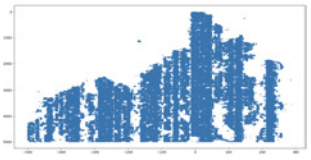

Fig. 3: *Realization of the dissipation of an infection (top to bottom) in a randomly stretched lattice*

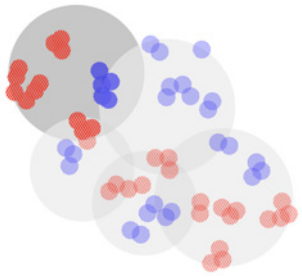

Fig. 4: *Realization of the Widom–Rowlinson model on a cluster of the Poisson–Boolean model. Red and blue Widom–Rowlinson points can not overlap when a marked Boolean ball is added (solid colors).*

References

[1] B. Jahnel, Ch. Külske, A. Zass, *Locality properties for discrete and continuum Widom–Rowlinson models in random environments*, WIAS Preprint no. 3054, 2023.

[2] B. Jahnel, A.D. Vu, *A long-range contact process in a random environment*, WIAS Preprint no. 3047, 2023.

[3] B. Jahnel, J. Köppl, B. Lodewijks, A. Tóbiás, *Percolation in lattice k-neighbor graphs*, WIAS Preprint no. 3028, 2023.

[4] B. Jahnel, J. Köppl, *On the long-time behaviour of reversible interacting particle systems in one and two dimensions*, WIAS Preprint no. 3004, 2023.

[5] B. Jahnel, L. Lüchtrath, *Existence of subcritical percolation phases for generalised weight-dependent random connection models*, WIAS Preprint no. 2993, 2023.

[6] Ch. Hirsch, B. Jahnel, S. Jhawar, P. Juhász, *Poisson approximation of fixed-degree nodes in weighted random connection models*, WIAS Preprint no. 3057, 2023.

A Facts and Figures

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

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

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

A.1.1 Awards and Distinctions

1. P. Farrell, *Online portrait as Brain City Berlin Ambassador (https://braincity.berlin/en/brains-of-berlin/brains-of-berlin-n/dr-patricio-farrell)*, September 20.
2. ———, *Capital – "Top 40 unter 40" for extraordinary talents from science and society*, November 18, 2023.
3. P. Friz, *MATH+ Distinguished Fellowship*.
4. M. Hintermüller, *Board Member of Berlin's non-university research institutions initiative BR50 (Berlin Research 50)*.
5. ———, *Chair of the Berlin Mathematics Research Center MATH+*.
6. ———, *Spokesperson of MaRDI – The Mathematical Research Data Initiative within the National Research Data Infrastructure*.
7. D. Hömberg, *Chair of the European Consortium for Mathematics in Industry (ECMI)'s Research and Innovation Committee*.
8. ———, *Head of the Secretariat of the International Mathematical Union (IMU)*.
9. ———, *Treasurer of IMU*.
10. J. Köppl, *chosen to participate in the Heidelberg Laureate Forum in September 2023*.
11. A. Mielke, *Chair of the Council of the Berlin Mathematics Research Center MATH+*.
12. ———, *MATH+ Distinguished Fellowship*.
13. ———, *Member of Prize Committee for the Enrico Magenes Prize 2023 of the Unione Matematica Italiana*.
14. M. Radziunas, *Honorary Associate Professor of Macquarie University 2021–2023, Sydney, Australia*.

A.1.2 Habilitations

1. P. Dvurechensky, *Large-scale numerical optimization: Inexact oracle, primal-dual analysis, ill-conditioned problems*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, November 20.
2. P. Farrell, *Quantum computing*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, January 25.

A.1.3 Defenses of Ph.D. Theses

1. F. Besold, *Adaptive weights clustering and community detection*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, February 2.
2. J. Holley, *Stress-constrained topology optimization with application to the design of electrical machines*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, May 3.
3. A. Quitmann, *Phase transitions in random loop models*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 17.
4. St.-M. Stengl, *Existence theorems, stationarity conditions and adaptive numerical methods for generalized Nash equilibrium problems constrained by partial differential equations*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, January 25.

5. D. Frerichs-Mihov, *On slope limiting techniques and deep learning techniques for the numerical solution of convection-dominated convection-diffusion problems*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, November 2.
6. P. Jaap, *Efficient and globally convergent minimization algorithms for small- and finite-strain plasticity problems*, Technische Universität Dresden, Bereich Mathematik und Naturwissenschaften, supervisor: Prof. Dr. O. Sander, August 21.
7. M. O'Donovan, *Theory of carrier transport in III-nitride based heterostructures*, Tyndall National Institute, Photonics, supervisors: Dr. St. Schulz, Prof. E. O'Reilly, March 23.
8. L. Schmeller, *Multi-phase dynamic systems at finite-strain elasticity mathematical modeling, existence theory and numerical solutions*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. B. Wagner, Dr. D. Peschka, September 26.
9. J.P. Thiele, *Error-controlled space-time finite elements, algorithms and implementations for nonstationary problems*, Leibniz Universität Hannover, Fakultät für Mathematik und Physik, supervisor: Prof. Dr. Th. Wick, November 1.

A.1.4 Supervision of Undergraduate Theses

1. N. Anderson, *Explizite s-stufige Peer-Methoden zur numerischen Lösung von Anfangswertproblemen* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, June 26.
2. T. Berg, *Exploring the Riesz isomorphism* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. M. Hammer, Prof. Dr. W. König, August 23.
3. Y. Bokredenghel, *Homogenization of elliptic long-range operators on random point processes* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 27.
4. P. Duschl, *Ein interagierendes Bose-Gas im hydrodynamischen Grenzwert* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, August 8.
5. K. Fischer, *Development of a FEM solver for 1D and 2D linear elliptic PDEs and applications in machine learning* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: A. Selahi, April 3.
6. M. Hennicke, *Konzentrationsungleichungen mit der Entropie-Methode und dem Satz von Sanov* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, October 6.
7. L. Hinz, *Ein Markov'sches Modell für zufälligen Zugang zum Kommunikationsmedium* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, July 28.
8. D. Houben, *Empirical Markowitz portfolio optimization with constraints* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, February 5.
9. L.H. Huber, *Support vector machines – Concepts and related optimization problems* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, January 30.
10. A. Jayaprakash, *A comparison of deep learning methods for time series forecasting with limited data* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, February 8.

11. H. Karanbash, *Finite element methods for the Stokes equations with non-constant viscosity* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, November 15.
12. M.R. Khrais, *ENO and WENO for convection-dominated convection-diffusion-reaction equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, May 16.
13. A. Klepoch, *Optimale Steuerung eines Räuber-Beute Modells für die biologische Schädlingsbekämpfung* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, April 13.
14. G. Konopka, *Das Simplexverfahren der linearen Optimierung* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, September 22.
15. Th.C. Le, *The throughput in an ALOHA model with several channels* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 10.
16. X. Lu, *Grad-div stabilization for incompressible Stokes equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, May 30.
17. K.L. McLain, *Finite element methods for the shallow water equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, May 3.
18. H. Mückler, *Große Abweichungen in Erdös-Rényi-Graphen und Graphon* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, January 2.
19. C. Savelsberg, *Gibbs partition* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, February 9.
20. L. Schnee, *Various representations of different rate functions for selected large deviation principles* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. W. van Zuijlen, June 10.
21. M. Seyferth, *On the staggered grid discretization of the total variation in a bilevel optimization problem for image denoising* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Prof. Dr. M. Hintermüller, Dr. K. Papafitsoros, September 8.
22. M.A. Śliwińska, *Analysis of a biomechanical model for growth* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. M. Liero, July 26.
23. F. Sun, *Grenzwertsätze für die Inkremente des Brown'schen Blatts und der Brown'schen Bewegung* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 15.
24. N.H. Ta, *Abgeänderte Pascoletti–Serafini Skalarisierung für multikriterielle Optimierung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, January 30.
25. H.A. Vu, *Grundlagen der Extremwerttheorie und Zwischenskalenordnungsstatistik* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 5.
26. F. Weber, *Verfahren zur Berechnung und Approximation von Konditionszahlen einer Matrix* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, January 9.
27. R. Wolfgramm, *Die höchsten Peaks eines Gauß'schen Feldes in einer großen Box* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, October 30.

28. Ch. Wysocki, *Konvergenzanalyse für Gauss–Newton–Verfahren* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, February 6.
29. D. Xing, *k-Nachbarn Perkolation* (bachelor's thesis), Technische Universität Braunschweig, supervisor: Prof. Dr. B. Jahnel, July 17.
30. M. Zainelabdeen Sedahmed Abdelhameed, *Pressure- and convection-robust finite element discretizations for flow problems* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. Ch. Merdon, April 11.
31. A.-A. Zepernick, *A survey on interpolation and projection operators* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, April 25.
32. T. Zhang, *Spatial preferential attachment networks: Power laws* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, September 21.
33. H. Zhou, *Direct solvers for large sparse linear systems of equations* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, June 26.
34. D. Zorawski, *Nichtlineare Optimierung mit Sparsity-Nebenbedingungen – Theorie und Algorithmen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 16.

A.2 Grants[1]

European Union, Brussels

- **European Metrology Programme for Innovation and Research (EMPIR)**
  Invertible Neural Networks for applications in metrology (as a part of the ATMOC Project "Traceable metrology of soft X-ray to IR optical constants and nanofilms for advanced manufacturing")

  In close collaboration with the Physikalisch-Technische Bundesanstalt (PTB), the project of RG 4 is concerned with the development of efficient neural network architectures for the reliable evaluation of Bayesian inverse problems. For this, invertible neural networks representing normalizing flows is examined. Moreover, a continuous differential equation perspective on neural networks is analyzed, which should allow for an efficient optimization procedure. The project is motivated by application requirements in the ATMOC project, where in particular geometry parameters as a part of the quality management in semiconductor manufacturing have to be inferred from scattering data.

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 has been 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 2023, WIAS again dedicated considerable financial and personal resources to the Center: Its director, Prof. M. Hintermüller (RG 8) was elected spokesperson of MATH+ in November 2022. He, Prof. A. Mielke (RG 1), Prof. W. König (RG 5), Dr. U. Bandelow (RG 2), Prof. P. Friz (RG 6), Prof. V. Spokoiny (RG 6), Prof. M. Thomas (WG BIP), Dr. Chr. Bayer (RG 6), and Dr. R. Henrion (RG 4) were members of the MATH+ Council; Dr. U. Bandelow (RG 2), Scientist in Charge of the Application Area AA2 "Nano and Quantum Technologies," Prof. P. Friz (RG 6) and Dr. R. Henrion (RG 4), Scientists in Charge of the Application Area AA4 "Energy Transition," Prof. M. Hintermüller (RG 8), Scientist in Charge of the Application Area AA5 "Variational Problems in Data-Driven Applications," Prof. M. Hintermüller (RG 8) and Prof. V. Spokoiny (RG 6), Scientists in Charge of the Emerging Field EF3 "Model-based Imaging," and Dr. Chr. Bayer (RG 6) and Prof. W. König (RG 5), Scientists in Charge of the Emerging Field EF45 "Multi-Agent Social Systems;" and WIAS members participated in the successful running of the following subprojects:

AA1-14 "Development of an ion-channel model-framework for in-vitro assisted interpretation of current voltage relations" (in RG 3 and RG 7)

AA2-12 "Nonlinear electrokinetics in anisotropic microfluids – Analysis, simulation, and optimal control" (in RG 4)

AA2-13 "Data-driven stochastic modeling of semiconductor lasers" (in RG 2)

AA2-17 "Coherent transport of semiconductor spin-qubits: Modeling, simulation and optimal control" (in RG 2)

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

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

AA4-7 “Decision-making for energy network dynamics” (in RG 8)

AA4-8 “Recovery of battery ageing dynamics with multiple timescales” (in RG 1, RG 4, and RG 7)

AA4-9 “Volatile electricity markets and battery storage: A model-based approach for optimal control” (in RG 6 and RG 7)

AA4-10 “Modeling and optimization of weakly coupled minigrids under uncertainty” (in RG 4)

AA4-13 “Equilibria for distributed multi-modal energy systems under uncertainty” (in RG 6 and RG 8)

AA5-2 “Robust multilevel training of artificial neural networks” (in RG 8)

AA5-4 “Bayesian optimization and inference for deep networks” (in RG 6)

AA5-5 “Wasserstein gradient flows for generalized transport in Bayesian inversion” (in RG 4)

AA5-7 “Integrated learning and variational methods for quantitative dynamic imaging” (in RG 8)

EF1-17 “Data-driven robust model predictive control under distribution shift” (in RG 8 and WG DOC)

EF3-11 “Quantitative tissue pressure imaging via PDE-informed assimilation of MR data” (in RG 3 and RG 6)

EF4-10 “Coherent movements in co-evolving agent-message systems” (in RG 5)

IN-11 “Identifying and efficiently computing band-edge energies for charge transport simulations in strained materials” (in RG 3 and LG NUMSEMIC)

Approved subprojects, starting in 2024:

AA2-21 “Strain engineering for functional heterostructures: Aspects of elasticity” (in RG 1)

AA5-10 “Robust data-driven reduced-order models for cardiovascular imaging of turbulent flows” (in RG 3 and WG DOC)

EF45-3 “Data transmission in dynamical random networks” (in LG DYCOMNET)

EF6-1 “Heterogeneous data integration to infer SARS-COV-2 variant specific immunity for risk assessment and vaccine design” (in RG 4)

PaA-1 “Electronics of nanotextured perovskite devices” (in LG NUMSEMIC)

PaA-2 “Modeling battery electrodes with mechanical interactions and multiple phase transitions upon ion insertion” (in RG 1 and RG 7)

PaA-5 “AI based simulation of transient physical systems – From benchmarks to hybrid solutions” (in RG 4)

- **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

  The second funding period of this transregio research center, funded by the DFG since October 2014, has ended in June 2022. The application for a third (and last) funding period until June 2026 has been successful. The Weierstrass Institute participates in the subprojects “Chance constraints with feedback and integrality” (in RG 4), “Multicriteria optimization subject to equilibrium constraints using the example of gas markets,” and “Stochastic gradient methods for almost sure state constraints for optimal control of gas flow under uncertainty” (both in RG 8). The common focus of these subprojects is on the consideration of uncertainty and equilibrium problems in risk averse optimal control of transient gas flow through a network.

- **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, and changed from the second into the third funding period in the middle of 2022, which will last until June 30, 2026. WIAS members participate in the subprojects

B09 “Materials with discontinuities on many scales” (in RG 1 and WG BIP with FU Berlin) and C02 “Interface dynamics: Bridging stochastic and hydrodynamic descriptions” (in RG 5 and WG BIP, with FU Berlin).

- **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 and was initially funded for the duration of four years. In 2021, the second funding was granted for another four years until June 2025. 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 (in RG 6), on prior selection for semi- and non-parametric statistics applied to SDEs, and the Universität Potsdam, on sequential Monte Carlo methods for high-dimensional inference problems arising from SDEs.

- **Priority Program SPP 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. Michael 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 started in 2020 and was extended cost neutrally until December 2024.

  WIAS participates in the second funding period with the coordination funds and the subprojects “A non-smooth phase-field approach to shape optimization with instationary fluid flow,” “Constrained mean field games: Analysis and algorithms,” and “A unified approach to optimal uncertainty quantification and risk-averse optimization with quasi-variational inequality constraints” (all three in RG 8).

- **Priority Program SPP 2171: “Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates,”** 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 three-dimensional 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 “Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows” (in WG BIP; duration Sep. 2019 – Dec. 2025) and the tandem project “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 – March 2025).

- **Priority Program SPP 2256: “Variationelle Methoden zur Vorhersage komplexer Phänomene in Strukturen und Materialien der Ingenieurwissenschaften” (Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials)**, Universität Regensburg

  The aim of this priority program, whose first funding period started in July 2020, is the development of analytical and numerical tools for the solution of problems in the continuum mechanics of solids. The research in the priority program is grouped in three major research directions: multiscale and multiphysics problems, coupling of dimensions, and evolution of microstructure. Within this general scope, mathematical

tools from the field of variational analysis are of great interest. They include the theories of homogenization, relaxation, Γ-convergence, and variational time evolution. WIAS contributes to the priority program with three subprojects: "Fractal and stochastic homogenization using variational methods," "Analysis for thermo-mechanical models with internal variables" (both in RG 1), and "Nonlinear fracture dynamics: Modelling, analysis, approximation and applications" (WG BIP with Universität Siegen and Karlsruhe Institute of Technology).

- **Priority Program SPP 2265: "Zufällige geometrische Systeme" (Random Geometric Systems)**, WIAS

  The head of RG 5, Prof. Wolfgang König, is the coordinator of this priority program, which aims at solving various problems that originate from a counterplay between randomness and space. There are many motivations from rich applications in the Sciences, but also intrinsic interest from researchers in probability. The first funding period officially started in October 2020. The second period was granted for 2024–2026.

  WIAS participates with the subprojects "Spatial coagulation and gelation" and "The statistical mechanics of the interlacement point processes" (in RG 5 and LG DYCOMNET).
  For more information see https://spp2265.wias-berlin.de/.

- **Priority Program SPP 2298: "Theoretical Foundations of Deep Learning,"** Ludwig-Maximilians-Universität München

  As a part of this priority program, the subproject "Adaptive neural tensor networks for parametric PDEs" is a cooperation project of RG 4 with Lars Grasedyck (RWTH Aachen). It is concerned with the development of a posteriori error estimators and adaptive methods for neural networks. The objective is to reliably approximate solutions of high-dimensional partial differential equations as well as the related inverse problems. It is a central goal to unveil the connections between tensor network and neural network representations and to exploit the combination of beneficial mathematical and algorithmic properties.

- **Priority Program SPP 2410 "Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness (CoScaRa),"** Universität Stuttgart

  Nonlinear hyperbolic balance laws are ubiquitous in the modeling of fluid mechanical processes. They enable the development of powerful numerical simulation methods that back decision-making for critical applications such as in-silico aircraft design or climate change research. However, fundamental questions about distinctive hyperbolic features remain open including the multi-scale interference of shock and shear waves, or the interplay of hyperbolic transport and random environments. The largely unsolved well-posedness problem for multi-dimensional inviscid flow equations is deeply connected to the laws of turbulent fluid motion in the high Reynolds number limit. Further progress requires a concerted effort of both fluid mechanics and the mathematical fields of analysis, numerics, and stochastics.

  WIAS participates in this first funding period with the subproject "Analysis of energy-variational solutions for hyperbolic conservation laws." The project is a joint effort of RG 1 and RG 4, duration: December 2023 – November 2026.

- **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 until February 2023. One of the two spokespersons was Prof. Peter Friz (RG 6). The unit worked 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 "Numerical analysis of rough PDEs" (in RG 6) were 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.

- **ANR-DFG Funding Programme for the Humanities and Social Sciences**
  "COFNET: Compositional functions networks – Adaptive learning for high-dimensional approximation and uncertainty quantification"

  This cooperation project of RG 4 with Anthony Nouy (Centrale Nantes) examines compositions of functions as a new regularity class that in principle can be represented in neural and tensor networks. Main goals are the analysis of backward stochastic differential equation (BSDE) solutions and transport maps in terms of such compositions, the development of new tensor formats that are tailored to represent functions compositions, and the development of active and passive learning algorithms via optimal sampling techniques in a new COFNET format.

- **RFBR-DFG Cooperation: Joint German-Russian Research Projects**
  "Collective dynamics of heterogeneous networks of active elements" (in RG 2)

  The project was established jointly with the Institute of Applied Physics of the Russian Academy of Sciences (Nishny Novgorod) and is devoted to the investigation of the dynamics of large networks of active elements. After the Russian invasion to Ukraine, all collaborations with Russian partners have been suspended. The funds of the project were used for other scientific cooperation, in particular, for the workshop "Dynamics in Coupled Network Systems 2023 (DCNS23)."

- **Normalverfahren (Individual Grants)**

  "Hybrid chip-scale frequency combs combining III-V quantum-dash mode-locked lasers and high-Q silicon-nitride microresonator" (HybridCombs; in RG 2)

  "Underlying nonlinear science of hybrid SOA-fiber laser systems with feedback" (SOA-FibLas; in RG 2)

  "Recursive and sparse approximation in reinforcement learning with application" (in RG 6)

  "Atomistic-continuum coupling for heterogeneous catalysis by a reduced basis approach and multilevel on-the-fly sparse grid interpolation" (in RG 3)

- **Eigene Stelle (Temporary Positions for Principal Investigators)**

  "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; see SPP 2171, Dr. D. Peschka)

  "Fraktale und stochastische Homogenisierung mithilfe variationeller Methoden" (Fractal and stochastic homogenization using variational methods; see SPP 2256, Dr. M. Heida)

Leibniz-Gemeinschaft (Leibniz Association), Berlin

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

  "Leibniz-MMS: Mathematische Modellierung und Simulation" (Leibniz MMS: Mathematical Modeling and Simulation; January 2021 – June 2024, in Director's office)

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

  "Numerical Methods for Innovative Semiconductor Devices" (January 2020 – December 2024, in LG NUMSEMIC)

  "Probabilistic Methods for Dynamic Communication Networks" (January 2021 – December 2025, in LG DYCOMNET)

  "UVSimTec: UV Lasers: From Modeling and Simulation to Technology" (January 2022 – December 2026, in RG 1, RG 2, and RG 3 in a consortium with Friedrich-Alexander-Universität Erlangen-Nürnberg, Leibniz-Institut für Kristallzüchtung, Ferdinand-Braun-Institut – Leibniz-Institut für Höchstfrequenztechnik, and Technische Universität Berlin)

"ML4Sim: Machine Learning for Simulation Intelligence in Composite Process Design," contribution of WIAS (RG 8) to a project coordinated by the Leibniz-Institut für Verbundwerkstoffe GmbH (IVW) Kaiserslautern. Further partners: Fraunhofer ITWM, DFKI Kaiserslautern, and Leibniz IPF Dresden (January 2022 – December 2024)

"Excellence in Photonic Crystal Surface Emitting Lasers," contribution of RGs 2, 3 and LG NUMSEMIC to a Leibniz Association's Cooperative Excellence project led by the Ferdinand Braun Institute (FBH). Further partner: Center of Excellence for Photonic-Crystal Surface-Emitting Lasers at Kyoto University (April 2023 – April 2026)

Approved project, starting in 2024:

"Linguistic Meaning and Bayesian Modelling," joint project with RG 6, coordinated by the Leibniz-Centre General Linguistics (ZAS) in the program "Leibniz Collaborative Excellence"

Einstein Stiftung Berlin (Einstein Foundation Berlin)

- Einstein Research Unit (ERU-QD) "Perspectives of a Quantum Digital Transformation: Near-term Quantum Computational Devices and Quantum Processors"

  "Approximating combinatorial optimization problems" and "Classical-quantum time-sharing and variational manifolds" (both in RG 8)

National Research Data Infrastructure

- MaRDI (see page 49)

  "Library of statistical methods und software and integration into the MaRDI platform" (October 1, 2021 – September 30, 2026; in RG 6)

  "Interdisciplinary workflows, standardization of mathematical descriptions in the natural sciences and integration into the MaRDI platform" (October 1, 2021 – September 30, 2026; in RG 1)

  "Mathematical methods and workflows for imaging problems and integration into the MaRDI platform" (October 1, 2021 – September 30, 2026; in RG 6)

  Consortium Management (October 1, 2021 – September 30, 2026; in RG 1, RG 6, and RG 8)

International projects

- Fondation Mathématique Jacques Hadamard (FMJH): "Optimal control problems with probabilistic constraints" and "Bi-level probabilistic sizing and dispatch of mini-grids" (both in RG 4)

Mission-oriented research (example)

- Ferdinand Braun Institute, Berlin: "Simulation of the spatio-temporal dynamics of high-power semiconductor lasers" (in RG 2)

A.3 Membership in Editorial Boards[2]

1. J. Sprekels, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
2. ———, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
3. ———, Editorial Board, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
4. Ch. Bayer, Associate Editor, Quantitative Finance, Taylor & Francis Online, London, UK.
5. A.H. Erhardt, Editorial Board, Frontiers in Applied Mathematics & Statistics, Section Mathematical and Statistical Physics, Frontiers Media S.A., Lausanne, Switzerland.
6. ———, Editorial Board, Frontiers in Physics, Section Mathematical and Statistical Physics, Frontiers Media S.A., Lausanne, Switzerland.
7. P. Friz, Associate Editor, Electronic Communications in Probability, Institute of Mathematical Statistics, Bethesda, USA.
8. ———, Associate Editor, Electronic Journal of Probability, Institute of Mathematical Statistics, Bethesda, USA.
9. C. Geiersbach, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Heidelberg.
10. ———, Editorial Board, Computational Optimization and Applications, Springer-Verlag, Heidelberg.
11. R. Henrion, Associate Editor, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
12. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
13. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
14. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
15. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
16. M. Hintermüller, Associate Editor, ESAIM: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
17. ———, Associate Editor, Advances in Continuous and Discrete Models: Theory and Modern Applications, Springer Nature, New York, USA.
18. ———, Associate Editor, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, USA.
19. ———, Editorial Board, Interfaces and Free Boundaries, European Mathematical Society Publishing House, Zurich, Switzerland.
20. ———, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
21. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
22. ———, Editorial Board, Optimization Methods and Software, Taylor & Francis, Oxford, UK.

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

23. ———, Editorial Board, Foundations of Data Science, American Institute of Mathematical Sciences, Springfield, USA.
24. ———, Series Editor, International Series of Numerical Mathematics, Springer-Verlag, Basel, Switzerland.
25. ———, Series Editor, Handbook of Numerical Analysis, Elsevier, Amsterdam, Netherlands.
26. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
27. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
28. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
29. ———, Editorial Board, Bernoulli Journal, International Statistical Institute/Bernoulli Society for Mathematical Statistics and Probability, The Hague, Netherlands.
30. ———, Series Editor, Pathways in Mathematics, Birkhäuser, Basel, Switzerland.
31. A. Mielke, Associate Editor, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
32. ———, Associate Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
33. ———, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
34. M. Radziunas, Editorial Board, Mathematical Modelling and Analysis, Vilnius Gediminas Technical University, Vilnius, Lithuania.
35. J.G.M. Schoenmakers, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
36. M. Thomas, Associate Editor, Discrete & Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences, Springfield, USA.
37. B. Wagner, Editorial Board, SIAM Journal on Applied Mathematics, Society for Industrial and Applied Mathematics, Philadelphia, USA.

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

MIA 2023 – Mathematics and Image Analysis
Berlin, February 1–3
Organized by: WIAS (RG 8), HU Berlin, TU Berlin
Supported by: Réseau Thématique CNRS 2286 Mathématiques de l'Imagerie et de ses Applications(RT MIA), HU Berlin, TU Berlin, WIAS

The MIA conference series was initiated in Paris in 2000 by the French Mathematics of Imaging group, RT CNRS 2286 Mathématiques de l'Imagerie et de ses Applications (http://gdr-mia.math.cnrs.fr). It has been subsequently held every two years at the Institute Henri Poincaré in Paris. Since 2014, German scientists have been involved in the organization of the conference, and it was decided to organize it alternately in Paris and Berlin. The focus of the conference series is on applications in imaging and image processing. Topics included: inverse problems, mathematics of visualization, motion analysis, video processing, statistical and data science, partial differential equations and variational methods, and deep learning methods. The conference in 2023 featured 18 invited speakers and a poster session; a total of 93 researchers attended. A French-German Mathematics in Imaging Ph.D. Prize was also awarded.

Leibniz MMS Days 2023
Potsdam, April 17–19
Organized by: ATB Potsdam, WIAS
Supported by: MMS

The Leibniz MMS Days are the central annual workshop of the Leibniz Research Network "Mathematical Modeling and Simulation (MMS)." In 2023, this workshop took place from April 17 to 19 at the Leibniz Institute for Agricultural Engineering and Bioeconomy (ATB) in Potsdam. The meeting represented another important step in the further development of the network's activities. It was attended by 61 scientists from 21 institutions. Two key-note talks were given by Melina Freitag (Universität Potsdam) "From models to data and back – An introduction to data assimilation algorithms" and Nicolas Gauger (Rheinland-Pfälzische Technische Universität Kaiserlautern) on "Grey-box data-driven turbulence modeling." Furthermore, ATB Director Barbara Sturm gave an impulse lecture on "Digital Twins – Unravelling the black box that is food processing." There were general plenary contributions and discussions on MMS-related topics at large, and in particular on research software, research data, reproducibility, Open Science, Data Science, and other topics.

17th Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis
Berlin, April 27–29
Organized by: WIAS (RG 6), TU Berlin, University of Oxford
Supported by: DFG FOR 2402, DFG IRTG 2544, University of Oxford, TU Berlin, DataSig, WIAS

Around 50 participants attended the 17th Berlin-Oxford Workshop in April of this year. As in previous years, participants were predominantly from the UK and Germany, but we also had several participants from France and Austria. The workshop continued the tradition of previous meetings, with a focus on Applied Stochastic Analysis, including, but not restricted to, the resolution of ill-posed stochastic partial differential equations (SPDEs) to new ways of handling high-dimensional data. More specifically, talks were divided into sections on "Rough Paths and Regularity," "Signatures and Data Science," "Numerical Analysis/Mathematical Finance," "SPDEs," and "Further Topics in Stochastic Analysis." The 16th meeting took place in Oxford in December 2022, a 18th meeting is again scheduled for Oxford.

Frontiers of Stochastic Optimization and its Applications in Industry
Berlin, May 10–12
Organized by: WIAS (RG 4 and RG 8), EDF Palaiseau, Simula Research Laboratory, Oslo
Supported by: Fondation Mathématique Jacques Hadamard, DFG SPP 1962, WIAS

The workshop was initiated against the background that stochastic optimization has been a driving factor for new mathematics for a long time. This is especially the case for methods and theory of nonsmooth optimization, new tools from variational analysis, and randomized solution algorithms for large-scale optimization problems. There are many instances arising from important industrial applications such as energy systems and markets, gas networks, and structural engineering. Due to advances in computing capacity and increasingly larger data sets, recent times have seen a surge of interest in robust optimal control, stochastic optimization of partial differential equations, and data-driven optimization. Presented topics of leading international scientists have demonstrated the interplay of stochastic optimization with other branches of mathematics and its applications in industry. The workshop was attended by 28 participants from 8 countries.

Nonlinear Dynamics in Semiconductor Lasers 2023
Berlin, July 3–5
Organized by: WIAS (RG 2) and Ferdinand Braun Institute
Supported by: MATH+, WIAS

There were several focal points covering a variety of the aspects of nonlinear dynamics and complex phenomena in photonic and optoelectronic devices. Special attention was paid to the theoretical description of noise in narrow-linewidth semiconductor lasers as well as the characterization of phase noise by statistical methods, which was covered in several presentations. The scientific program included 30 invited talks, 8 contributed talks, and 7 posters, which were presented in an evening poster session. In total, 61 participants from 17 countries actively participated in the workshop.

SPP 2265 Summer School: Probability and Geometry on Configuration Spaces
Berlin, July 17–21
Organized by: WIAS (RG 5)
Supported by: DFG SPP 2265

The summer school was one of the activities of the Priority Program SPP 2265 *Random Geometric Systems*. It was devoted to configuration spaces, seen through the different lenses of analysis, geometry, and probability. The aim of the school was to bring together different communities in the theory of point processes, configuration-space analysis, and particle systems. This was accomplished thanks to four minicourses, by Ronan Herry (Centre Henri Lebesgue, Rennes) on "Probabilistic and geometric aspects of Poisson point processes," by Benedikt Jahnel (LG DYCOMNET) on "Continuum percolation in random environments," by Alessia Nota (University of L'Aquila) on "Lorentz gas dynamics: Particle systems and scaling limits with some perspectives on the role of long-range interactions," and by Elena Pulvirenti (TU Delft) on "The Widom–Rowlinson model: From phase transition to metastability." Building on these, the central topics of the school were further developed by the invited talks, given by six young scientists who presented their recent results, leading to interesting discussions among the participants.

The summer school, which took place in the wonderful location of the Harnack Haus in Berlin-Dahlem, was attended by about 40 participants, among them several junior scientists (bachelor's and master's students). The organizers were Lorenzo Dello Schiavo (Institute of Science and Technology Austria (ISTA)) and Alexander Zass (RG 5).

Phase Transitions in Spatial Particle Systems
Berlin, July 31 – August 2
Organized by: WIAS (RG 5)
Supported by: DFG SPP 2265

The workshop was another of the activities of the Priority Program SPP 2265 *Random Geometric Systems*. It was devoted to various types of phase transitions in various kinds of interacting spatial particle systems. Examples include condensation in randomly growing structures, percolation in randomly connecting models, and gelation in random coagulation models, and also hard-sphere dynamics. There were two minicourses by Lorenzo Bertini (Università degli Studi di Roma "La Sapienza") on large deviations for Kac-like walks and by Stefan Großkinsky (Universität Augsburg) on condensation phenomena in interacting particle systems. Eight more talks on various kinds of phase transitions in spatial particle systems lead to fruitful discussions and exchange. All talks were given in presence in the wonderful location of the Harnack-Haus in Berlin-Dahlem. The workshop hosted about 30–35 participants. The organizers were Markus Heydenreich (LMU Munich) and Wolfgang König (RG 5).

BioPhysMed – Biophysics-based Modeling and Data Assimilation in Medical Imaging
Berlin, August 30 – September 1
Organized by: WIAS (RG 3: A. Caiazzo, RG 6: K. Tabelow), D. Peterseim (U Augsburg), I. Sack (Charité Berlin)
Supported by: MATH+

The workshop was held at WIAS on August 30 to September 1. The event featured 10 interdisciplinary keynote talks from international experts in mathematical modeling, scientific computing, inverse problems, biomechanics, and medical imaging. The program was completed by 13 contributed talks in three thematics sessions (Multiscale Biomechanics, AI & Data Assimilation, MRE & Cardiovascular Imaging), and by a session dedicated to research data management (one talk presenting the Mathematical Research Data Initiative MaRDI and a group discussion). All talks were followed by intense and stimulating discussions, highlighting the importance of exchanging scientific results and challenges across different communities. There have been 47 onsite participants, 42 percent from abroad.

Colloquium on the Occasion of Alexander Mielke's 65th Birthday
September 6
Organized by: WIAS (RG 1), TU Vienna
Supported by: DFG

On September 6, 2023, Alexander Mielke's 65th birthday was celebrated with a scientific colloquium. The event started with welcome addresses by the institute's director and close colleagues. The scientific part of the event featured presentations by renowned speakers such as Rupert Klein (FU Berlin), Felix Otto (MPI Leipzig), and Riccarda Rossi (U Brescia).

Energetic Methods for Multi-Component Reactive Mixtures: Modelling, Stability, and Asymptotic Analysis
Berlin, September 13–15
Organized by: WIAS (RG 1: K. Hopf, M. Kniely)
Supported by: DFG

The workshop was devoted to various aspects in the modeling and analysis of reaction-diffusion systems and fluid models, including viscoelastic fluids and multiphase flows. Special emphasis was put on energy and entropy methods, which are known as a versatile tool in the context of complex systems subject to temperature effects, electrostatic forces, and compressibility. The scientific program consisted of 10 invited lectures, 12 contributed talks, and three poster presentations. Bringing together 42 scientists from 8 European countries, the workshop also enabled fruitful discussions among the participants on their ongoing research and possible future collaborations.

ESGI 175 – The Berlin Study Group with Industry
Berlin, September 18–22
Organized by: WIAS
Supported by: ECMI, MATH+, WIAS

The Berlin Study Group with Industry was a practical workshop where four companies submitted altogether five mathematical problems beforehand to be solved by the participants; mostly in the form of a modeling or an optimization problem. It brought together European experts, many of them with a large experience in this type of events. The altogether 59 participants from eight countries worked in suitably arranged groups around each problem and discussed their results with company representatives at the end of the week. The outcome was summarized in reports for the participating companies and presented to them. The results were very well received. The in this way special and outstanding workshop was also a starting point for further industrial cooperation with at least one of the participating companies.

First NFDI-Berlin-Brandenburg meeting
Berlin, October 12
Organized by: WIAS, MaRDI
Supported by: MaRDI

The MaRDI (Mathematical Research Data Initiative) team at WIAS organized this first regional networking event, where all NFDI (National Research Data Infrastructure) consortia within the Berlin-Brandenburg area were invited to. The main goal was to establish contact between the members of the various consortia and to identify common fields of interest with the aim to develop collaborative projects. The one-day event saw 25 out of the 27 NFDI consortia represented among the 65 participants who came from more than 120 regional research institutes and universities. The group had collectively identified five topics that both addressed the wide interests of and relevance to the consortia present. These included the acceptance of stakeholders of the FAIR principles and research data management (RDM), longevity of services developed in the NFDI, RDM in curriculum, collaborations with industry and international partners and ontologies in knowledge graphs. The meeting came to a positive conclusion with plans of moving forward on areas in smaller groups such as developing a general RDM curriculum and ontologies. Overall, it was a success with high engagement and lively discussions.

International Workshop: Dynamics in Coupled Network Systems
Berlin, November 20–22
Organized by: WIAS (RG 2: M. Wolfrum), T. Pereira (University of São Carlos), S. Yanchuk (University College Cork/ PIK Potsdam)
Supported by: DFG

The workshop brought together mathematicians and experts from various fields of applications (neuronal systems, power grids, chemical oscillations) to discuss recent developments and further perspectives of network dynamical systems from an interdisciplinary perspective. A specific focus was on adaptive networks, structured networks, emergent collective dynamics, heterogeneous networks, and networks with multiple time scale dynamics. The workshop included 28 scientific talks, six posters and two contributed talks and was attended by 46 participants from seven countries.

MaRDI Annual Workshop 2023
Berlin, November 28–30
Organized by: WIAS, MaRDI
Supported by: MaRDI

From November 28 to 30, 2023, the Mathematical Research Data Initiative MaRDI held its 3rd Annual Meeting in Berlin at WIAS. The focus this year was on consolidating MaRDI services in preparation of the progress report and the future development of MaRDI. Three speakers from the National Research Data Initiatives NFDI4DataScience, KonsortSWD, and NFDI4Biodiversity were invited to give impulse talks on the possibility of engagement with consortia outside of the natural and mathematical sciences sphere. The talks were followed by an open plenary

discussion on how mathematics and services developed within MaRDI could be adapted and extended in a way that would be mutually beneficial. Demo sessions on the current services that are in development and active were presented to the group with BarCamp discussions on how integration of services to our MaRDI Portal, central entry point, would be done. Where the first two years were focused on starting and building on the work done, the meeting in 2023 gave us a sense of our success, areas to focus until the end of our first phase and how to develop beyond that.

A.4.2 Oberwolfach Workshops co-organized by WIAS

Variational Methods for Evolution
Mathematisches Forschungsinstitut Oberwolfach, December 3–8
Organized by: Franca Hoffmann (Pasadena), Alexander Mielke (RG 1), Mark Peletier (Eindhoven), Dejan Slepcev (Pittsburgh)

The workshop was the fifth edition of a series started in 2011. About 45 mathematicians from classical continuum mechanics, mathematical physics, stochastic and applied analysis interacted with researchers from geometry, data science, and machine learning. About 25 talks covered a wide range of topics on discrete and continuous evolutionary systems, where the variational approaches such as gradient structures, minimizing-movement schemes, or optimal transport. Multiscale problems and discrete-to-continuum limits were studied using EDP convergence, which means convergence of gradient systems in the sense of the energy-dissipation principle. The WIAS was represented by four participants.

A.5 Membership in Organizing Committees of non-WIAS Meetings[3]

1. A. Mielke, co-organizer, *Workshop "Variational Methods for Evolution"*, Mathematisches Forschungsinstitut Oberwolfach, December 3–8.
2. M. Eigel, organizer of the Minisymposium MS135 "Randomized Solvers in Large-Scale Scientific Computing II", *SIAM Conference on Computational Science and Engineering (CSE23)*, Amsterdam, Netherlands, February 26 – March 3.
3. ———, co-organizer of the Minisymposium MS9 "UQ and Data Assimilation with Sparse, Low-rank Tensor, and Machine Learning Methods", *5th International Conference on Uncertainty Quantification in Computational Science and Engineering (UNCECOMP 2023)*, Athens, Greece, June 12–14.
4. ———, co-organizer of the Minisymposium MS24 "Tensor Networks and Compositional Functions for High-Dimensional Approximation", *International Conference on Spectral and High Order Methods (ICOSAHOM 2023)*, Yonsei University, Seoul, Korea (Republic of), August 14–18.
5. Th. Eiter, co-organizer of the Minisymposium 00608 "Limit Behavior and Asymptotic Properties in Fluid Mechanics", *10th International Congress on Industrial and Applied Mathematics (ICIAM 2023)*, Waseda University, Tokyo, Japan, August 20–25.
6. P. Farrell, co-organizer of the Minisymposium MS230 "Modern Directions in Electronic Devices: Neuromorphic Devices, Memristors and Quantum Technologies", *SIAM Conference on Computational Science and Engineering (CSE23)*, Amsterdam, Netherlands, February 26 – March 3.
7. P.K. Friz, co-organizer, *Stochastics, Statistics, Machine Learning and their Applications to Sustainable Finance and Energy Markets*, Wolfgang Pauli Institute (WPI), Vienna, Austria, September 12–14.
8. C. Geiersbach, organizer of the Session S19 "Optimization of Differential Equations", *93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2023)*, Technische Universität Dresden, May 30 – June 2.
9. ———, organizer of the Focus Session "Optimization under Uncertainty", *European Conference on Computational Optimization (EUCCO)*, Universität Heidelberg, September 25–27.
10. R. Henrion, member of the Scientific Committee, *Nonsmooth And Variational Analysis (NAVAL) Conference*, Université de Bourgogne, Dijon, France, June 26–28.
11. M. Hintermüller, organizer of the Session PP 1962 "Non-Smooth and Complementarity-Based Distributed Parameter Systems: Simulation and Hierarchical Optimization", *93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2023)*, Technische Universität Dresden, May 30 – June 2.
12. ———, co-organizer of the Minisymposium MS 35 "PDE-Constrained Optimization with Nonsmooth Structures or under Uncertainty", *SIAM Conference on Optimization (OP23)*, Seattle, USA, May 31 – June 3.
13. ———, co-organizer of the Minisymposium 00687 "Recent Advances in Deep Learning-Based Inverse and Imaging Problems", *10th International Congress on Industrial and Applied Mathematics (ICIAM 2023)*, Waseda University, Tokyo, Japan, August 20–25.
14. D. Hömberg, co-organizer of the Minisymposium MS17 "ECMI SIG: Mathematics for the Digital Factory", *22nd European Conference on Mathematics for Industry (ECMI2023)*, Wrocław University of Science and Technology Congress Centre, Poland, June 26–30.

[3] Membership in organizing committees of non-WIAS meetings by nonresident members have been listed in front of those by the WIAS staff members.

15. ———, co-organizer, *preparatory winter school within the project "Ethiopian Norwegian Network in Computational Mathematics" (ENNCoMat)*, Addis Ababa University, Ethiopia, November 27 – December 1.
16. ———, co-organizer, *First Ethiopian Study Group with Industry*, Addis Ababa University, Ethiopia, December 4–8.
17. Th. Koprucki, K. Tabelow, co-organizers of Minisymposium MS 05 "Towards a Digital Infrastructure for Mathematical Research", *DMV Annual Meeting 2023*, Technische Universität Ilmenau, September 25–28.
18. M. Landstorfer, co-organizer of the Minisymposium 01140 "Modelling and Simulation of Electro-Chemomechanical Processes in Batteries and Fuel Cells", *10th International Congress on Industrial and Applied Mathematics (ICIAM 2023)*, Waseda University, Tokyo, Japan, August 20–25.
19. M. Liero, A. Stephan, co-organizers of the Minisymposium 01181 "Variational Methods for Multi-scale Dynamics", *10th International Congress on Industrial and Applied Mathematics (ICIAM 2023)*, Waseda University, Tokyo, Japan, August 20–25.
20. D. Peschka, B. Wagner, co-organizers, *SPP 2171 Workshop "Wetting of Flexible, Adaptive, and Switchable Substrates" 2023*, Technische Universität Berlin, December 4–7.
21. J. Schütte, co-organizer, *Mini-Workshop "Nonlinear Approximation of High-dimensional Functions in Scientific Computing"*, Mathematisches Forschungsinstitut Oberwolfach, October 15–20.
22. L. Schütz, co-organizer, *PhD Workshop 2023 of CRC 1114* Scaling Cascades in Complex Systems, Freie Universität Berlin, Brandenburg an der Havel, September 25–28.
23. K. Tabelow, co-organizer of the Minisymposium: MS 5 "Towards a Digital Infrastructure for Mathematical Research", *DMV Annual Meeting 2023*, Technische Universität Ilmenau, September 25–28.
24. M. Thomas, co-organizer of the Section 14 "Applied Analysis", *93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2023)*, Technische Universität Dresden, May 30 – June 2.
25. ———, co-organizer, *Variational and Geometric Structures for Evolution*, Centro Internazionale per la Ricerca Matematica (CIRM), Levico Terme, Italy, October 9–13.

A.6 Publications

A.6.1 Monographs

[1] M. Brokate, J. Zimmer, F. Lindemann, *Analysis 1 – Ein zuverlässiger und verständlicher Begleiter für Studium und Prüfung*, Springer Spektrum, Berlin, Heidelberg, 2023, XII, 298 pages. doi:10.1007/978-3-662-67776-6.

[2] Ch. Bayer, P.K. Friz, M. Fukasawa, J. Gatheral, A. Jacquier, M. Rosenbaum, eds., *Rough Volatility*, Society for Industrial and Applied Mathematics, Philadelphia, 2023, xxviii + 263 pages. doi:10.1137/1.9781611977783.

[3] J. Polzehl, K. Tabelow, *Magnetic Resonance Brain Imaging: Modeling and Data Analysis using R, 2nd Revised Edition*, Series: Use R!, Springer International Publishing, Cham, 2023, 258 pages. doi:10.1007/978-3-031-38949-8.

A.6.2 Editorship of Proceedings and Collected Editions

[1] A.H. Erhardt, K. Tsaneva-Atanasova, G.T. Lines, E.A. Martens, eds., *Dynamical Systems, PDEs and Networks for Biomedical Applications: Mathematical Modeling, Analysis and Simulations*, Special Edition, articles published in Frontiers of Physics, Frontiers in Applied Mathematics and Statistics, and Frontiers in Physiology, Frontiers Media SA, Lausanne, Switzerland, 2023, 207 pages. doi:10.3389/978-2-8325-1458-0.

[2] E. Franck, J. Fuhrmann, V. Michel-Dansac, L. Navoret, eds., *Finite Volumes for Complex Applications X – Volume 1, Elliptic and Parabolic Problems: FVCA10, Strasbourg, France, October 30, 2023 – November 03, 2023, Invited Contributions*, vol. 432 of Springer Proceedings in Mathematics & Statistics, Springer International Publishing, Cham, 2023, 396 pages. doi:10.1007/978-3-031-40864-9.

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[4] M. Liero, M. Thomas, D. Peschka, eds., *Special Issue on Energy-based Mathematical Methods for Reactive Multiphase Flows*, vol. 103 of Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), no. 7, Wiley-VCH Verlag, Weinheim, 2023. doi:10.1002/zamm.202302012.

[5] B. Wagner, M. Timme, eds., *Special Issue "The Mathematics in Renewable Energy"*, vol. 34 of European Journal of Applied Mathematics, no. 3, Springer Nature, Heidelberg et al., 2023, 190 pages. doi:10.1017/S0956792523000013.

A.6.3 Outstanding Contributions to Monographs

[1] N. Tupitsa, P. Dvurechensky, D. Dvinskikh, A. Gasnikov, *Section: Computational Optimal Transport*, P.M. Pardalos, O.A. Prokopyev, eds., Encyclopedia of Optimization, Springer International Publishing, Cham, published online on 11.07.2023. doi:10.1007/978-3-030-54621-2_861-1.

Contributions to Monographs (to appear)

[1] A. Gasnikov, D. Dvinskikh, P. Dvurechensky, E. Gorbunov, A. Beznosikov, A. Lobanov, *Randomized gradient-free methods in convex optimization*, Encyclopedia of Optimization, Springer International Publishing.

[2] D. Kamzolov, A. Gasnikov, P. Dvurechensky, A. Agafonov, M. Takac, *Exploiting higher-order derivates in convex optimization methods*, Encyclopedia of Optimization, Springer International Publishing.

A.6.4 Articles in Refereed Journals[4]

[1] M. Brokate, C. Christof, *Strong stationarity conditions for optimal control problems governed by a rate-independent evolution variational inequality*, SIAM J. Control Optim., 61 (2023), pp. 2222–2250. doi:10.1137/22M1494403.

[2] P. Colli, G. Gilardi, A. Signori, J. Sprekels, *Cahn–Hilliard–Brinkman model for tumor growth with possibly singular potentials*, Nonlinearity, 36 (2023), pp. 4470–4500. doi:https://doi.org/10.1088/1361-6544/ace2a7.

[3] ———, *Optimal control of a nonconserved phase field model of Caginalp type with thermal memory and double obstacle potential*, Discrete Contin. Dyn. Syst. Ser. S, 16 (2023), pp. 2305–2325. doi:10.3934/dcdss.2022210.

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[5] ———, *Optimal temperature distribution for a nonisothermal Cahn–Hilliard system with source term*, Appl. Math. Optim., 88 (2023), pp. 68/1–68/31. doi:10.1007/s00245-023-10039-9.

[6] ———, *On a Cahn–Hilliard system with source term and thermal memory*, Nonlinear Analysis, 240 (2024), pp. 113461/1–113461/16 (published online on 14.12.2023). doi:10.1016/j.na.2023.113461.

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[11] N.N. Nefedov, A.O. Orlov, L. Recke, K.R. Schneider, *Nonsmooth regular perturbations of singularly perturbed problems*, J. Dynam. Differential Equations, 375 (2023), pp. 206–236. doi:10.1016/j.jde.2023.08.006.

[12] J. Sprekels, F. Tröltzsch, *Second-order sufficient conditions for sparse optimal control of singular Allen–Cahn systems with dynamic boundary conditions*, Discrete Contin. Dyn. Syst. Ser. S, 16 (2023), pp. 3784–3812. doi:10.3934/dcdss.2023163.

[13] D. Abdel, C. Chainais-Hillairet, P. Farrell, M. Herda, *Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells*, IMA J. Numer. Anal., published online on 10.6.2023. doi:10.1093/imanum/drad034.

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Contributions to Collected Editions (to appear)

[1] B. Schembera, F. Wübbeling, H. Kleikamp, Ch. Biedinger, J. Fiedler, M. Reidelbach, A. Shehu, B. Schmidt, Th. Koprucki, D. Iglezakis, D. Göddeke, *Ontologies for models and algorithms in applied mathematics and related disciplines*, in: 17th International Conference on Metadata and Semantics Research, E. Garoufallou, A. Vlachidis, eds., Communications in Computer and Information Science, Springer, Cham.

A.7 Preprints, Reports

A.7.1 WIAS Preprints Series[5]

[1] P. Colli, G. Gilardi, A. Signori, J. Sprekels, *Optimal temperature distribution for a nonisothermal Cahn–Hilliard system in two dimensions with source term and double obstacle potential*, Preprint no. 3003, WIAS, Berlin, 2023.

[2] ———, *Optimal temperature distribution for a nonisothermal Cahn–Hilliard system with source term*, Preprint no. 2997, WIAS, Berlin, 2023.

[3] K.M. Gambaryan, O. Ernst, T. Boeck, O. Marquardt, *Energy level alignment of confined hole states in $InAs_{1-x-y}Sb_xP_y$ double quantum dots*, Preprint no. 3040, WIAS, Berlin, 2023.

[4] J. Sprekels, F. Tröltzsch, *Second-order sufficient conditions for sparse optimal control of singular Allen–Cahn systems with dynamic boundary conditions*, Preprint no. 3005, WIAS, Berlin, 2023.

[5] ———, *Second-order sufficient conditions in the sparse optimal control of a phase field tumor growth model with logarithmic potential*, Preprint no. 3020, WIAS, Berlin, 2023.

[6] D. Abdel, A. Glitzky, M. Liero, *Analysis of a drift-diffusion model for perovskite solar cells*, Preprint no. 3073, WIAS, Berlin, 2023.

[7] A. Alphonse, D. Caetano, A. Djurdjevac, Ch.M. Elliott, *Function spaces, time derivatives and compactness for evolving families of Banach spaces with applications to PDEs*, Preprint no. 2994, WIAS, Berlin, 2023.

[8] S. Amiranashvili, R. Čiegis, *Stability of the higher-order splitting methods for the generalized nonlinear Schrödinger equation*, Preprint no. 3070, WIAS, Berlin, 2023.

[9] Ch. Bayer, S. Breneis, *Efficient option pricing in the rough Heston model using weak simulation schemes*, Preprint no. 3045, WIAS, Berlin, 2023.

[10] ———, *Weak Markovian approximations of rough Heston*, Preprint no. 3044, WIAS, Berlin, 2023.

[11] Ch. Bayer, S. Breneis, T. Lyons, *An adaptive algorithm for rough differential equations*, Preprint no. 3013, WIAS, Berlin, 2023.

[12] P. Bank, Ch. Bayer, P. Friz, L. Pelizzari, *Rough PDEs for local stochastic volatility models*, Preprint no. 3034, WIAS, Berlin, 2023.

[13] Ch. Bayer, L. Pelizzari, J.G.M. Schoenmakers, *Primal and dual optimal stopping with signatures*, Preprint no. 3068, WIAS, Berlin, 2023.

[14] M. Bongarti, M. Hintermüller, *Optimal boundary control of the isothermal semilinear Euler equation for gas dynamics on a network*, Preprint no. 3016, WIAS, Berlin, 2023.

[15] M. Demir, V. John, *Pressure-robust approximation of the incompressible Navier–Stokes equations in a rotating frame of reference*, Preprint no. 3058, WIAS, Berlin, 2023.

[16] P. Dvurechensky, J.-J. Zhu, *Kernel mirror prox and RKHS gradient flow for mixed functional Nash equilibrium*, Preprint no. 3032, WIAS, Berlin, 2023.

[17] M. Eigel, N. Hegemann, *Guaranteed quasi-error reduction of adaptive Galerkin FEM for parametric PDEs with lognormal coefficients*, Preprint no. 3036, WIAS, Berlin, 2023.

[18] P. Trunschke, M. Eigel, A. Nouy, *Weighted sparsity and sparse tensor networks for least squares approximation*, Preprint no. 3049, WIAS, Berlin, 2023.

[19] C. Heiss, I. Gühring, M. Eigel, *Multilevel CNNs for parametric PDEs*, Preprint no. 3035, WIAS, Berlin, 2023.

[5] 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.

[20] M. Eigel, Ch. Miranda, *Functional SDE approximation inspired by a deep operator network architecture*, Preprint no. 3079, WIAS, Berlin, 2023.

[21] M. Eigel, Ch. Miranda, J. Schütte, D. Sommer, *Approximating Langevin Monte Carlo with ResNet-like neural network architectures*, Preprint no. 3077, WIAS, Berlin, 2023.

[22] Th. Eiter, Y. Shibata, *Viscous flow past a translating body with oscillating boundary*, Preprint no. 3000, WIAS, Berlin, 2023.

[23] A. Erhardt, D. Peschka, Ch. Dazzi, L. Schmeller, A. Petersen, S. Checa, A. Münch, B. Wagner, *Modeling cellular self-organization in strain-stiffening hydrogels*, Preprint no. 3076, WIAS, Berlin, 2023.

[24] L. Ermoneit, B. Schmidt, Th. Koprucki, J. Fuhrmann, T. Breiten, A. Sala, N. Ciroth, R. Xue, L.R. Schreiber, M. Kantner, *Optimal control of conveyor-mode spin-qubit shuttling in a Si/SiGe quantum bus in the presence of charged defects*, Preprint no. 3082, WIAS, Berlin, 2023.

[25] D. Frerichs-Mihov, L. Henning, V. John, *On loss functionals for physics-informed neural networks for convection-dominated convection-diffusion problems*, Preprint no. 3063, WIAS, Berlin, 2023.

[26] D. Frerichs-Mihov, M. Zainelabdeen, V. John, *On collocation points for physics-informed neural networks applied to convection-dominated convection-diffusion problems*, Preprint no. 3074, WIAS, Berlin, 2023.

[27] C. Geiersbach, T. Suchan, K. Welker, *Optimization of piecewise smooth shapes under uncertainty using the example of Navier–Stokes flow*, Preprint no. 3037, WIAS, Berlin, 2023.

[28] ———, *Stochastic augmented Lagrangian method in shape spaces*, Preprint no. 3010, WIAS, Berlin, 2023.

[29] C. Geiersbach, R. Henrion, *Optimality conditions in control problems with random state constraints in probabilistic or almost-sure form*, Preprint no. 3021, WIAS, Berlin, 2023.

[30] C. Geiersbach, R. Henrion, P. Pérez-Aroz, *Numerical solution of an optimal control problem with probabilistic and almost sure state constraints*, Preprint no. 3062, WIAS, Berlin, 2023.

[31] A. Glitzky, M. Liero, *A drift-diffusion based electrothermal model for organic thin-film devices including electrical and thermal environment*, Preprint no. 3012, WIAS, Berlin, 2023.

[32] Y. Hadjimichael, Ch. Merdon, M. Liero, P. Farrell, *An energy-based finite-strain model for 3D heterostructured materials and its validation by curvature analysis*, Preprint no. 3064, WIAS, Berlin, 2023.

[33] M. Heida, *Finite volumes for simulation of large molecules*, Preprint no. 3018, WIAS, Berlin, 2023.

[34] ———, *On the computation of high dimensional Voronoi diagrams*, Preprint no. 3041, WIAS, Berlin, 2023.

[35] Y. Bokredenghel, M. Heida, *Quenched homogenization of infinite range random conductance model on stationary point processes*, Preprint no. 3017, WIAS, Berlin, 2023.

[36] H. Heitsch, R. Henrion, C. Tischendorf, *Probabilistic maximization of time-dependent capacities in a gas network*, Preprint no. 3066, WIAS, Berlin, 2023.

[37] N. Ouanes, T. González Grandón, H. Heitsch, R. Henrion, *Optimizing the economic dispatch of weakly-connected mini-grids under uncertainty using joint chance constraints*, Preprint no. 3069, WIAS, Berlin, 2023.

[38] W. van Ackooij, R. Henrion, H. Zidani, *Pontryagin's principle for some probabilistic control problems*, Preprint no. 3050, WIAS, Berlin, 2023.

[39] M. Hintermüller, D. Korolev, *A hybrid physics-informed neural network based multiscale solver as a partial differential equation constrained optimization problem*, Preprint no. 3052, WIAS, Berlin, 2023.

[40] M.J. Arenas, D. Hömberg, R. Lasarzik, *Optimal beam forming for laser materials processing*, Preprint no. 3080, WIAS, Berlin, 2023.

[41] M. Ebeling-Rump, D. Hömberg, R. Lasarzik, *On a two-scale phasefield model for topology optimization*, Preprint no. 3026, WIAS, Berlin, 2023.

[42] K. Hopf, A. Jüngel, *Convergence of a finite volume scheme and dissipative measure-valued–strong stability for a hyperbolic-parabolic cross-diffusion system*, Preprint no. 3006, WIAS, Berlin, 2023.

[43] T. Iyer, B. Lodewijks, *On the structure of genealogical trees associated with explosive Crump–Mode–Jagers branching processes*, Preprint no. 3060, WIAS, Berlin, 2023.

[44] L. Andreis, T. Iyer, E. Magnanini, *Gelation, hydrodynamic limits and uniqueness in cluster coagulation processes*, Preprint no. 3039, WIAS, Berlin, 2023.

[45] Ch. Hirsch, B. Jahnel, S.K. Jhawar, P. Juhász, *Poisson approximation of fixed-degree nodes in weighted random connection models*, Preprint no. 3057, WIAS, Berlin, 2023.

[46] B. Jahnel, J. Köppl, *On the long-time behaviour of reversible interacting particle systems in one and two dimensions*, Preprint no. 3004, WIAS, Berlin, 2023.

[47] ———, *Trajectorial dissipation of Φ-entropies for interacting particle systems*, Preprint no. 3019, WIAS, Berlin, 2023.

[48] B. Jahnel, J. Köppl, B. Lodewijks, A. Tóbiás, *Percolation in lattice k-neighbor graphs*, Preprint no. 3028, WIAS, Berlin, 2023.

[49] B. Jahnel, L. Lüchtrath, *Existence of subcritical percolation phases for generalised weight-dependent random connection models*, Preprint no. 2993, WIAS, Berlin, 2023.

[50] B. Jahnel, A.D. Vu, *A long-range contact process in a random environment*, Preprint no. 3047, WIAS, Berlin, 2023.

[51] B. Jahnel, Ch. Külske, A. Zass, *Locality properties for discrete and continuum Widom–Rowlinson models in random environments*, Preprint no. 3054, WIAS, Berlin, 2023.

[52] V. John, Ch. Merdon, M. Zainelabdeen, *Augmenting the grad-div stabilization for Taylor–Hood finite elements with a vorticity stabilization*, Preprint no. 3055, WIAS, Berlin, 2023.

[53] Ch. Keller, J. Fuhrmann, M. Landstorfer, B. Wagner, *A model framework for ion channels with selectivity filters based on continuum non-equilibrium thermodynamics*, Preprint no. 3072, WIAS, Berlin, 2023.

[54] J. Kern, *Exponential equivalence for misanthrope processes in contact with weak reservoirs and applications to totally asymmetric exclusion processes*, Preprint no. 3051, WIAS, Berlin, 2023.

[55] J. Kern, B. Wiederhold, *A Lambda-Fleming–Viot type model with intrinsically varying population size*, Preprint no. 3053, WIAS, Berlin, 2023.

[56] M. Fradon, J. Kern, S. Rœlly, A. Zass, *Diffusion dynamics for an infinite system of two-type spheres and the associated depletion effect*, Preprint no. 3024, WIAS, Berlin, 2023.

[57] C.S. Clemente, D. Davino, O. Klein, C. Visone, *On forward and inverse uncertainty quantification for a model for a magneto mechanical device involving a hysteresis operator*, Preprint no. 3009, WIAS, Berlin, 2023.

[58] W. König, Ch. Kwofie, *The throughput in multi-channel (slotted) ALOHA: Large deviations and analysis of bad events*, Preprint no. 2991, WIAS, Berlin, 2023.

[59] W. König, N. Pétrélis, R. Soares dos Santos, W. van Zuijlen, *Weakly self-avoiding walk in a Pareto-distributed random potential*, Preprint no. 3023, WIAS, Berlin, 2023.

[60] W. König, Q. Vogel, A. Zass, *Off-diagonal long-range order for the free Bose gas via the Feynman–Kac formula*, Preprint no. 3067, WIAS, Berlin, 2023.

[61] E. Kuhn, *Simulation of the mode dynamics in broad-ridge laser diodes*, Preprint no. 3061, WIAS, Berlin, 2023.

[62] E. Kuhn, A. Tränhardt, *Influence of scattering effects on the interaction between longitudinal modes in laser diodes*, Preprint no. 3038, WIAS, Berlin, 2023.

[63] A. Agosti, R. Lasarzik, E. Rocca, *Energy-variational solutions for viscoelastic fluid models*, Preprint no. 3048, WIAS, Berlin, 2023.

[64] P. Gracar, L. Lüchtrath, Ch. Mönch, *The emergence of a giant component in one-dimensional inhomogeneous networks with long-range effects*, Preprint no. 3011, WIAS, Berlin, 2023.

[65] L. Mertensk̈otter, M. Kantner, *Bayesian estimation of laser linewidth from delayed self-heterodyne measurements*, Preprint no. 3014, WIAS, Berlin, 2023.

[66] ———, *Frequency noise characterization of narrow-linewidth lasers: A Bayesian approach*, Preprint no. 3065, WIAS, Berlin, 2023.

[67] A. Mielke, *An introduction to the analysis of gradients systems*, Preprint no. 3022, WIAS, Berlin, 2023.

[68] ———, *Non-equilibrium steady states as saddle points and EDP-convergence for slow-fast gradient systems*, Preprint no. 2998, WIAS, Berlin, 2023.

[69] A. Mielke, T. Roubíček, U. Stefanelli, *A model of gravitational differentiation of compressible self-gravitating planets*, Preprint no. 3015, WIAS, Berlin, 2023.

[70] A. Mielke, R. Rossi, A. Stephan, *On time-splitting methods for gradient flows with two dissipation mechanisms*, Preprint no. 3033, WIAS, Berlin, 2023.

[71] A. Mielke, St. Schindler, *Convergence to self-similar profiles in reaction-diffusion systems*, Preprint no. 3008, WIAS, Berlin, 2023.

[72] ———, *Existence of similarity profiles for diffusion equations and systems*, Preprint no. 3007, WIAS, Berlin, 2023.

[73] ———, *Self-similar pattern in coupled parabolic systems as non-equilibrium steady states*, Preprint no. 2992, WIAS, Berlin, 2023.

[74] A. Zafferi, K. Huber, D. Peschka, J. Vrijmoed, T. John, M. Thomas, *A porous-media model for reactive fluid-rock interaction in a dehydrating rock*, Preprint no. 2999, WIAS, Berlin, 2023.

[75] A. Quitmann, *A note on the monomer-dimer model*, Preprint no. 3046, WIAS, Berlin, 2023.

[76] N. Forien, M. Quattropani, A. Quitmann, L. Taggi, *Coexistence, enhancements and short loops in random walk loop soups*, Preprint no. 3029, WIAS, Berlin, 2023.

[77] M. Radziunas, E. Kuhn, H. Wenzel, *Solving a spectral problem for large-area photonic crystal surface-emitting lasers*, Preprint no. 3059, WIAS, Berlin, 2023.

[78] M. Radziunas, E. Kuhn, H. Wenzel, B. King, P. Crump, *Optical mode calculation in large-area photonic crystal surface-emitting lasers*, Preprint no. 3075, WIAS, Berlin, 2023.

[79] A. Rathsfeld, *Convergence of the method of rigorous coupled-wave analysis for the diffraction by two-dimensional periodic surface structures*, Preprint no. 3081, WIAS, Berlin, 2023.

[80] L. Schmeller, D. Peschka, *Sharp-interface limits of Cahn–Hilliard models and mechanics with moving contact lines*, Preprint no. 2990, WIAS, Berlin, 2023.

[81] L. Araujo, C. Lasser, B. Schmidt, *FSSH-2: Fewest Switches Surface Hopping with robust switching probability*, Preprint no. 3071, WIAS, Berlin, 2023.

[82] P. Gelss, S. Matera, R. Klein, B. Schmidt, *Quantum dynamics of coupled excitons and phonons in chain-like systems: Tensor train approaches and higher-order propagators*, Preprint no. 2995, WIAS, Berlin, 2023.

[83] J. Riedel, P. Gelss, R. Klein, B. Schmidt, *WaveTrain: A Python package for numerical quantum mechanics of chain-like systems based on tensor trains*, Preprint no. 2996, WIAS, Berlin, 2023.

[84] J.A. Dekker, R.J.A. Laeven, J.G.M. Schoenmakers, M.H. Vellekoop, *Optimal stopping with randomly arriving opportunities to stop*, Preprint no. 3056, WIAS, Berlin, 2023.

[85] D. Sommer, R. Gruhlke, M. Kirstein, M. Eigel, C. Schillings, *Generative modelling with tensor train approximations of Hamilton–Jacobi–Bellman equations*, Preprint no. 3078, WIAS, Berlin, 2023.

[86] A. Stephan, *Trotter-type formula for operator semigroups on product spaces*, Preprint no. 3030, WIAS, Berlin, 2023.

[87] M. Stöhr, E.R. Koch, J. Javaloyes, S.V. Gurevich, M. Wolfrum, *Square waves and Bykov T-points in a delay algebraic model for the Kerr–Gires–Tournois interferometer*, Preprint no. 3043, WIAS, Berlin, 2023.

[88] M. Thomas, S. Tornquist, Ch. Wieners, *Approximating dynamic phase-field fracture in viscoelastic materials with a first-order formulation for velocity and stress*, Preprint no. 3002, WIAS, Berlin, 2023.

[89] W. van Oosterhout, M. Liero, *Finite-strain poro-visco-elasticity with degenerate mobility*, Preprint no. 3027, WIAS, Berlin, 2023.

[90] A.G. Vladimirov, *Temporal cavity soliton interaction in passively mode-locked semiconductor lasers*, Preprint no. 3001, WIAS, Berlin, 2023.

[91] A.G. Vladimirov, D. Dolinina, *Neutral delay differential equation Kerr cavity model*, Preprint no. 3025, WIAS, Berlin, 2023.

[92] G.L. Celora, R. Blossey, A. Münch, B. Wagner, *Counterion-controlled phase equilibria in a charge-regulated polymer solution*, Preprint no. 3031, WIAS, Berlin, 2023.

[93] O. Burylko, M. Wolfrum, S. Yanchuk, J. Kurths, *Time-reversible dynamics in a system of two coupled active rotators*, Preprint no. 3042, WIAS, Berlin, 2023.

A.7.2 Preprints/Reports in other Institutions

[1] B. Spetzler, D. Abdel, F. Schwierz, M. Ziegler, P. Farrell, *The role of mobile point defects in two-dimensional memristive devices*, arXiv:2304.06527, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.06527.

[2] O. Butkovsky, S. Gallay, *Weak existence for SDEs with singular drifts and fractional Brownian or Levy noise beyond the subcritical regime*, arXiv:2311.12013, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2311.12013.

[3] O. Butkovsky, K. Lê, L. Mytnik, *Stochastic equations with singular drift driven by fractional Brownian motion*, arXiv:2302.11937, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2302.11937.

[4] R. Araya, A. Caiazzo, F. Chouly, *Stokes problem with slip boundary conditions using stabilized finite elements combined with Nitsche*, hal-04077986, Hyper Articles en Ligne (HAL), Lyon, France, 2023.

[5] F. Galarce, J. Mura, A. Caiazzo, *Bias and multiscale correction methods for variational state estimation algorithms*, arXiv:2311.14031, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2311.14031.

[6] E. Gorbunov, A. Sadiev, D. Dolinova, S. Horvát, G. Gidel, P. Dvurechensky, A. Gasnikov, P. Richtárik, *High-probability convergence for composite and distributed stochastic minimization and variational inequalities with heavy-tailed noise*, arXiv:2310.01860, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2310.01860.

[7] N. Kornilov, A. Gasnikov, P. Dvurechensky, D. Dvinskikh, *Gradient free methods for non-smooth convex stochastic optimization with heavy-tailed noise on convex compact*, arXiv:2304.02442, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.02442.

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[9] D.A. Pasechnyuk, M. Persiianov, P. Dvurechensky, A. Gasnikov, *Algorithms for Euclidean-regularised optimal transport*, arXiv:2307.00321, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2307.00321.

[10] A. Sadiev, E. Gorbunov, S. Horváth, G. Gidel, P. Dvurechensky, A. Gasnikov, P. Peter, *High-probability bounds for stochastic optimization and variational inequalities: The case of unbounded variance*, arXiv:2302.00999, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2302.00999.

[11] O. Yufereva, M. Persiianov, P. Dvurechensky, A. Gasnikov, D. Kovalev, *Decentralized convex optimization on time-varying networks with application to Wasserstein barycenters*, arXiv:2205.15669, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2205.15669.

[12] E. Gladin, A. Gasnikov, P. Dvurechensky, *Accuracy certificates for convex minimization with inexact Oracle*, arXiv:2310.00523, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2310.00523.

[13] P. Trunschke, A. Nouy, M. Eigel, *Weighted sparsity and sparse tensor networks for least squares approximation*, arXiv:2310.08942, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2310.08942.

[14] P. Farrell, J. Moatti, M. O'Donovan, St. Schulz, Th. Koprucki, *Importance of satisfying thermodynamic consistency in light emitting diode simulations*, hal-04012467, Hyper Articles en Ligne (HAL), Lyon, France, 2023.

[15] J. Boddapati, M. Flaschel, S. Kumar, L. De Lorenzis, Ch. Daralo, *Single-test evaluation of directional elastic properties of anisotropic structured materials*, arXiv:2304.09112, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.09112.

[16] M. Flaschel, H. Yu, N. Reiter, J. Hinrichsen, S. Budday, P. Steinmann, S. Kumar, L. De Lorenzis, *Automated discovery of interpretable hyperelastic material models for human brain tissue with EUCLID*, arXiv:2305.16362, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2305.16362.

[17] B. García-Archilla, V. John, S. Katz, J. Novo, *POD-ROMs for incompressible flows including snapshots of the temporal derivative of the full order solution: Error bounds for the pressure*, arXiv:2304.08313, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.08313.

[18] M. Kantner, L. Mertensk̈otter, *Accurate evaluation of self-heterodyne laser linewidth measurements using Wiener filters*, arXiv:2301.10645, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2301.10645.

[19] L. Liang, D. Sun, K.-Ch. Toh, *A squared smoothing Newton method for semidefinite programming*, arXiv:2303.05825, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2303.05825.

[20] P.L. Lederer, Ch. Merdon, *Gradient-robust hybrid DG discretizations for the compressible Stokes equations*, arXiv.2311.06098, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2311.06098.

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[22] I.P.A. Papadopoulos, T.S. Gutleb, J.A. Carrillo, S. Olver, *A frame approach for equations involving the fractional Laplacian*, arXiv:2311.12451, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2311.12451.

[23] T.S. Gutleb, I.P.A. Papadopoulos, *Explicit fractional Laplacians and Riesz potentials of classical functions*, arXiv:2311.10896, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2311.10896.

[24] D.M. Kane, M. Radziunas, *Chaos spectrum – Semiconductor laser with delayed optical feedback*, arXiv.2312.14353, Cornell University, Ithaca, 2023. doi:10.48550/arXiv.2312.14353.

[25] B. Schembera, F. Wübbeling, H. Kleikamp, Ch. Bledinger, J. Fiedler, M. Reidelbach, A. Shehu, B. Schmidt, Th. Koprucki, D. Iglezakis, D. Göddeke, *Ontologies for models and algorithms in applied mathematics and related disciplines*, arXiv:2310.20443, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2310.20443.

[26] A. Kofler, F. Altekrüger, F.A. Ba, Ch. Kolbitsch, E. Papoutsellis, D. Schote, C. Sirotenko, F.F. Zimmermann, K. Papafitsoros, *Learning regularization parameter-maps for variational image reconstruction*

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[27] ———, *Unrolled three-operator splitting for parameter-map learning in low dose X-ray CT reconstruction*, arXiv:2304.08350, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.08350.

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[29] ———, *Mixed Laplace approximation for marginal posterior and Bayesian inference in error-in-operator model*, arXiv:2305.08193, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2305.09336.

[30] ———, *Nonlinear regression: Finite sample guarantees*, arXiv:2305.08193, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2305.08193.

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[32] J.M. Oeschger, K. Tabelow, S. Mohammadi, *Investigating apparent differences between standard DKI and axisymmetric DKI and its consequences for biophysical parameter estimates*, bioRxiv:2023.06.21.545891, Cold Spring Harbor Laboratory, New York, USA, 2023. doi:10.1101/2023.06.21.545891.

[33] K. Ebrahimi-Fard, F. Patras, N. Tapia, L. Zambotti, *Shifted substitution in non-commutative multivariate power series with a view toward free probability*, arXiv:2204.01445, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2204.01445.

[34] F. Goth, R. Alves, M. Braun, L.J. Castro, G. Chourdakis, S. Christ, J. Cohen, F. Erxleben, J.-N. Grad, M. Hagdorn, T. Hodges, G. Juckeland, D. Kempf, A.-L. Lamprecht, J. Linxweiler, M. Schwarzmeier, H. Seibold, J.P. Thiele, H. von Waldow, S. Wittke, *Foundational competencies and responsibilities of a research software engineer*, arXiv:2311.11457, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2311.11457.

[35] J.-J. Zhu, *Propagating kernel ambiguity sets in nonlinear data-driven dynamics models*, arXiv:2304.14057, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.14057.

[36] Z. Zhong, J.-J. Zhu, *Nonlinear Wasserstein distributionally robust optimal control*, arXiv:2304.07415, Cornell University, Ithaca, USA, 2023. doi:10.48550/arXiv.2304.07415.

A.8 Talks and Posters

A.8.1 Main and Plenary Talks

1. M. Radziunas, *Modeling of photonic crystal surface-emitting lasers*, 26th International Conference on Mathematical Modelling and Analysis, May 30 – June 2, University of Latvia, Jurmala, Latvia, May 30.
2. V. Spokoiny, *Estimation and inference for error-in-operator model*, Mathematics in Armenia: Advances and Perspectives, July 2–8, Yerevan State University and National Academy of Sciences, Institute of Mathematics, Yerevan, Armenia, July 3.

A.8.2 Scientific Talks (Invited)

1. M. Brokate, *Strong stationarity conditions for an optimal control problem involving a rate-independent variational inequality*, International Conference on Optimization: SIGOPT 2023, March 14–16, Brandenburgische Technische Universität Cottbus-Senftenberg, March 15.
2. ———, *Derivatives and optimal control of a scalar sweeping process*, Variational Analysis and Optimization Seminar, University of Michigan, Ann Arbor, USA, March 31.
3. ———, *Derivatives and optimal control of a sweeping process*, 93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2023), Session S19 "Optimization of Differential Equations", May 30 – June 2, Technische Universität Dresden, June 2.
4. J. Rehberg, *Maximal parabolic regularity for the treatment of real world problems*, Oberseminar für Optimale Steuerung und Inverse Probleme, Universität Duisburg-Essen, Fakultät für Mathematik, May 4.
5. J. Sprekels, *Sparse optimal control of singular Allen–Cahn systems with dynamic boundary conditions*, Kolloquium, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, April 18.
6. V. Aksenov, *Simulation of Wasserstein gradient flows with low-rank tensor methods for sampling*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00837 "Particle Methods for Bayesian Inference", August 20–25, Waseda University, Tokyo, Japan, August 24.
7. A. Alphonse, *Analysis of a quasi-variational contact problem arising in thermoelasticity*, European Conference on Computational Optimization (EUCCO), Session "Non-smooth Optimization", September 25–27, Universität Heidelberg, September 25.
8. S. Amiranashvili, *Numerical aspects of modulation instability*, 26th International Conference on Mathematical Modelling and Analysis, May 30 – June 2, University of Latvia, Jurmala, Latvia, June 1.
9. ———, *Numerical aspects of modulation instability*, Extreme Waves 2023, August 28 – September 1, Max-Planck-Institut für Physik komplexer Systeme, Dresden, August 28.
10. U. Bandelow, *Laserdynamik – mathematische Modellierung*, MBI-Technikerschulung 2023, October 16, Max-Born-Institut, Wandlitz.
11. ———, *Modeling and simulation of semiconductor devices: From high-power lasers to quantum technologies*, Winter School on III-Sb Applications: Non-Volatile Memories – A Modelling Perspective, February 27 – March 3, Technische Universität Berlin, February 27.
12. ———, *Ultrashort solitons in the regime of event horizons in nonlinear optical media*, Extreme Waves 2023, August 28 – September 1, Max-Planck-Institut für Physik komplexer Systeme, Dresden, August 29.
13. ———, *Unusual scenarios in the context of the modulation instability*, Dissipative Solitons, Turbulence and Extreme Events in Nonlinear Photonics, September 6–8, International Solvay Institutes, Brussels, Belgium, September 7.

14. ———, *Unusual wave-mixing processes in the context of the modulation instability*, XIX International Workshop on Instabilities and Nonequilibrium Structures – INES 2023, December 4–8, Pontificia Universidad Catolica de Valparaiso, Chile, December 7.
15. Ch. Bayer, *Rough PDEs for local stochastic volatility models*, Rough Volatility Workshop, November 21–22, Sorbonne Université, Institut Henri Poincaré, Paris, France.
16. ———, *Optimal stopping with signatures*, Probabilistic Methods, Signatures, Cubature and Geometry, January 9–11, University of York, Department of Mathematics, UK, January 9.
17. ———, *Optimal stopping with signatures (online talk)*, North British Probability Seminar, University of Edinburgh, UK, March 29.
18. ———, *Optimal stopping with signatures*, Quantitative Finance Conference, April 12–15, University of Cambridge, Centre for Financial Research, UK, April 13.
19. ———, *Markovian approximations to rough volatility models*, Volatility is rough, Isle of Skye Workshop, May 21–25, Sabhal Mòr Ostaig, Sleat, Isle of Skye, UK, May 25.
20. ———, *Non-Markovian models in finance*, Stochastic Numerics and Statistical Learning: Theory and Applications 2023 Workshop, May 26 – June 1, King Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences, Thuwal, Saudi Arabia, May 27.
21. ———, *Signatures and applications*, 3 talks, 4th Workshop on Stochastic Methods in Finance and Physics, July 17–21, Institute of Applied and Computational Mathematics (IACM), Heraklion, Kreta, Greece, July 18–21.
22. ———, *Optimal stopping with signatures*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00322 “Methodological Advancement in Rough Paths and Data Science”, August 20–25, Waseda University, Tokyo, Japan, August 24.
23. ———, *Markovian approximations to rough volatility models*, Stochastics around Finance, August 28–30, Kanazawa University, Natural Science and Technology, Kanazawa, Japan, August 28.
24. ———, *Optimal stopping with signatures*, Workshop on Stochastic Control Theory, October 25–26, KTH Royal Institute of Technology, Department of Mathematics, Stockholm, Sweden, October 26.
25. ———, *Optimal stopping with signatures*, University of Dundee, School of Science and Engineering, UK, November 13.
26. ———, *Markovian approximations to rough volatility models*, Heriot-Watt University, Mathematical Institute, Edinburgh, UK, November 15.
27. M. Bongarti, *Network boundary control of the semilinear isothermal Euler equation modeling gas transport on a network of pipelines*, 93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2023), Session S19 “Optimization of Differential Equations”, May 30 – June 2, Technische Universität Dresden, June 2.
28. S. Breneis, *Weak Markovian approximations of rough Heston*, 17th Oxford-Berlin Young Researcher’s Meeting on Applied Stochastic Analysis, April 27–29, WIAS & TU Berlin, April 27.
29. ———, *American options under rough Heston*, 11th General AMaMeF Conference, June 26–30, Universität Bielefeld, Center for Mathematical Economics, June 30.
30. ———, *Pricing-path dependent options under rough Heston*, 18. Doktorand:innentreffen der Stochastik 2023, August 21–23, Universität Heidelberg, Fachbereich Mathematik, August 23.
31. ———, *Pricing-path dependent options under rough Heston*, CDT-IRTG Summer School 2023, September 3–8, Templin, September 3.
32. O. Butkovsky, *Stochastic equations with singular drift driven by fractional Brownian motion (online talk)*, Non-local Operators, Probability and Singularities (online event), researchseminars.org, April 4.

33. ———, *Stochastic equations with singular drift driven by fractional Brownian motion*, 17th Oxford-Berlin Young Researcher's Meeting on Applied Stochastic Analysis, April 27–29, WIAS & TU Berlin, April 28.

34. ———, *Regularization by noise for SDEs and SPDEs beyond the Brownian case*, Probability Seminar, Université Paris-Saclay, CentraleSupélec, France, May 25.

35. ———, *Strong rate of convergence of the Euler scheme for SDEs with irregular drift driven by Levy noise*, 14th Conference on Monte Carlo Methods and Applications, June 26–30, Sorbonne University, Paris, France, June 29.

36. ———, *Stochastic sewing, John–Nirenberg inequality, and taming singularities for regularization by noise: A very practical guide*, SDEs with Low Regularity Coefficients: Theory and Numerics, September 20–22, University of Torino, Department of Mathematics, Italy, September 22.

37. ———, *Stochastic sewing, John–Nirenberg inequality, and taming singularities for regularization by noise*, Mean Field, Interactions with Singular Kernels and their Approximations 2023, December 18, Institut Henri Poincaré, Paris, France, December 18.

38. P. Dvurechensky, *Hessian barrier algorithms for non-convex conic optimization*, 20th Workshop on Advances in Continuous Optimization, August 22–25, Corvinus University, Institute of Mathematical Statistics and Modelling, Budapest, August 25.

39. ———, *Decentralized local stochastic extra-gradient for variational inequalities*, Thematic Einstein Semester Conference on Mathematical Optimization for Machine Learning, September 13–15, Mathematics Research Cluster MATH+, Berlin, September 14.

40. ———, *Decentralized local stochastic extra-gradient for variational inequalities*, European Conference on Computational Optimization (EUCCO), Session "Optimization under Uncertainty", September 25–27, Universität Heidelberg, September 25.

41. M. Eigel, *Convergence of an empirical Galerkin method for parametric PDEs*, SIAM Conference on Computational Science and Engineering (CSE23), Minisymposium MS100 "Randomized Solvers in Large-Scale Scientific Computing", February 26 – March 3, Amsterdam, Netherlands, February 28.

42. ———, *Convergence of empirical Galerkin FEM for parametric PDEs with sparse TTs*, Universität Basel, Departement Mathematik und Informatik, Switzerland, May 12.

43. ———, *Accelerated interacting particle systems with low-rank tensor compression for Bayesian inversion*, 5th International Conference on Uncertainty Quantification in Computational Science and Engineering (UNCECOMP 2023), MS9 "UQ and Data Assimilation with Sparse, Low-rank Tensor, and Machine Learning Methods", June 12–14, Athens, Greece, June 14.

44. ———, *Convergence of adaptive empirical stochastic Galerkin FEM*, ECCOMAS Young Investigators Conference (YIC2023), Minisymposium CAM01 "Uncertainty Quantification of Differential Equations with Random Parameters: Methods and Applications", June 19–21, University of Porto, June 19.

45. ———, *Accelerated interacting particle transport for Bayesian inversion*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00966 "Theoretical and Computational Advances in Measure Transport", August 20–25, Waseda University, Tokyo, Japan, August 21.

46. ———, *Functional SDE approximation inspired by a deep operator network architecture*, Mini-Workshop "Nonlinear Approximation of High-dimensional Functions in Scientific Computing", October 15–20, Mathematisches Forschungsinstitut Oberwolfach, October 18.

47. Th. Eiter, *The concept of energy-variational solutions for hyperbolic conservation laws*, Seminar on Partial Differential Equations, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, March 28.

48. ———, *Artificial boundary conditions for time-periodic flow past a body*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00558 "Bifurcations, Periodicity and Stability in Fluid-structure Interactions", August 20–25, Waseda University, Tokyo, Japan, August 21.

49. A.H. Erhardt, *Mathematical modelling and simulation of cell-hydrogel interactions*, Leibniz MMS Days 2023, April 17–19, Leibniz-Institut für Agrartechnik und Bioökonomie (ATB), Potsdam, April 19.

50. ———, *Bifurcation analysis for axisymmetric capillary water waves*, 29th Nordic Congress of Mathematicians with EMS, July 3–7, Aalborg University, Department of Mathematical Sciences, Denmark, July 4.

51. P.K. Friz, *On rough stochastic differential equations*, SPDEs, Optimal Control and Mean Field Games – Analysis, Numerics and Applications, July 10–14, Universität Bielefeld, Center for Interdisciplinary Research (ZiF), July 11.

52. ———, *Rough paths for local (possibly rough) stochastic volatility*, Lie-Størmer Colloquium Analytic and Probabilistic Aspects of Rough Paths, November 27–29, Norwegian Academy of Science and Letters, Oslo, Norway, November 27.

53. J. Fuhrmann, *Voronoi finite volume methods for complex applications in Julia*, International Conference on Numerical Analysis of Partial Differential Equations (ANEDP 2023), October 16–18, Moulay Ismail University, Faculty of Sciences, Meknes, Morocco.

54. ———, *VORONOIFVM.JL – A multiphysics finite volume solver for elliptic and parabolic systems*, SIAM Conference on Computational Science and Engineering (CSE23), Minisymposium MS67 "Research Software Engineering with Julia", February 26 – March 3, Amsterdam, Netherlands, February 27.

55. C. Geiersbach, *Optimization with random uniform state constraints*, Optimal Control Theory and Related Fields, December 4–7, Universidad Tecnica Federico Santa Maria, Valparaiso, Chile, December 6.

56. ———, *Stochastic approximation for shape optimization under uncertainty*, Seminar in Numerical Analysis, Universität Basel, Switzerland, December 15.

57. M. Heida, *Diskrete Operatoren in Modellbildung und Numerik*, Universität der Bundeswehr München, Institut für Mathematik und Informatik, July 13.

58. R. Henrion, *Turnpike phenomenon in discrete-time optimal control with probabilistic constraint*, 2nd Vienna Workshop on Computational Optimization, March 15–17, Universität Wien, Austria, March 15.

59. ———, *Chance constraints in optimal control*, ALOP colloquium, Universität Trier, Graduiertenkolleg ALOP, April 24.

60. ———, *Probabilistic constraints in optimal control*, SIAM Conference on Optimization (OP23), MS 163 "Risk Models in Stochastic Optimization", May 31 – June 3, Seattle, USA, June 1.

61. ———, *Existence and stability in controlled polyhedral sweeping processes (online talk)*, International Workshop on Nonsmooth Optimization: Theory, Algorithms and Applications (NOTAA2023) (Online Event), June 7–8, University of Isfahan, Iran, June 8.

62. ———, *Optimality conditions for a PDE-constrained control problem with probabilistic and almost-sure state constraints*, Nonsmooth And Variational Analysis (NAVAL) Conference, June 26–28, Université de Bourgogne, Dijon, France, June 27.

63. ———, *A control problem with random state constraints in probabilistic and almost-sure form*, PGMO DAYS 2023, Session 10B "Stochastic Optimization", November 28–29, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF Lab Paris-Saclay, Palaiseau, France, November 29.

64. M. Hintermüller, *A descent algorithm for the optimal control of ReLU neural network informed PDEs based on approximate directional derivatives*, SIAM Conference on Computational Science and Engineering (CSE23), Minisymposium MS390 "Algorithms for Applications in Nonconvex, Nonsmooth Optimization", February 26 – March 3, Amsterdam, Netherlands, March 3.

65. ———, *A descent algorithm for the optimal control of ReLU neural network informed PDEs based on approximate directional derivatives*, SIAM Conference on Optimization (OP23), MS 35 "PDE-Constrained Optimization with Nonsmooth Structures or under Uncertainty", May 31 – June 3, Seattle, USA, May 31.

66. ———, *A descent algorithm for the optimal control of ReLU neural network Informed PDEs based on approximate directional derivatives*, FoCM 2023 – Foundations of Computational Mathematics, Session II.2: "Continuous Optimization", June 12–21, Sorbonne University, Paris, France, June 15.

67. ———, *Learning-informed and PINN-based multi scale PDE models in optimization*, Conference on Deep Learning for Computational Physics, July 4–6, UCL – London's Global University, UK, July 6.

68. ———, *Optimal control of (quasi)variational inequalities: Stationarity, risk-aversion, and numerical solution*, Workshop on Optimization, Equilibrium and Complementarity, August 16–19, The Hong Kong Polytechnic University, Department of Applied Mathematic, August 19.

69. ———, *PDE-constrained optimization with non-smooth learning-informed structures*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00711 "Recent Advances in Optimal Control and Optimization", August 20–25, Waseda University, Tokyo, Japan, August 21.

70. ———, *Short Course: Mathematics of PDE Constrained Optimization*, 2 talks, Recent Trends in Optimization and Control: Short Course and Workshop, September 18–22, University of Pretoria, Future Africa Campus, South Africa, September 19.

71. ———, *Optimal control of multiphase fluids and droplets (online talk)*, Workshop "Control Methods in Hyperbolic Partial Differential Equations" (Hybrid Event), November 5–10, Mathematisches Forschungsinstitut Oberwolfach, November 7.

72. D. Hömberg, *ODE-constrained optimal control*, 10 talks, preparatory winter school within the project "Ethiopian Norwegian Network in Computational Mathematics" (ENNCoMat), November 27 – December 1, Addis Ababa University, Ethiopia.

73. ———, *Two-scale topology optimization for 3D printing*, SIAM Conference on Computational Science and Engineering (CSE23), Minisymposium MS328 "ECMI: Perspectives and Successes of Mathematical Challenges in Industrial Applications", February 26 – March 3, Amsterdam, Netherlands, March 2.

74. ———, *Phase-field based topology optimization*, Norwegian Workshop on Mathematical Optimization, Nonlinear and Variational Analysis 2023, April 26–28, Norwegian University of Science and Technology, Trondheim, Norway, April 27.

75. ———, *Two-scale topology optimization – A phase field approach*, 22nd European Conference on Mathematics for Industry (ECMI2023), MS17 "ECMI SIG: Mathematics for the Digital Factory", June 26–30, Wrocław University of Science and Technology Congress Centre, Poland, June 26.

76. ———, *On two-scale topology optimization for AM*, The Fourth International Conference on Simulation for Additive Manufacturing (Sim-AM 2023), IS14 "Advanced Methods and Innovative Technologies for the Optimal Design of Structures and Materials II", July 26–28, Galileo Science Congress Center Munich-Garching, Garching, July 27.

77. K. Hopf, *The Cauchy problem for multi-component systems with strong cross-diffusion*, Johannes Gutenberg-Universität Mainz, Fachbereich Physik, Mathematik und Informatik, January 11.

78. ———, *Structure, dynamics, and approximation of cross-diffusive mixtures with incomplete diffusion*, Universität Hamburg, Fachbereich Mathematik, May 10.

79. ———, *Structure and approximation of cross-diffusive mixtures with incomplete diffusion*, Universität Kassel, Fachbereich Mathematik und Naturwissenschaften, September 21.

80. ———, *On cross-diffusive coupling of hyperbolic-parabolic type*, Variational and Geometric Structures for Evolution, October 9–13, Centro Internazionale per la Ricerca Matematica (CIRM), Levico Terme, Italy, October 13.

81. ———, *Normal form and the Cauchy problem for cross-diffusive mixtures*, Workshop "Variational Methods for Evolution", December 3–8, Mathematisches Forschungsinstitut Oberwolfach, December 4.

82. T. Iyer, *Properties of recursive trees with independent fitnesses (online talk)*, Seminar Complex Systems, Queen Mary University of London, School of Mathematical Sciences, London, UK, February 14.

83. B. Jahnel, *Continuum percolation in random environments*, 5 talks, SPP 2265 Summer School on Probability and Geometry on Configuration Spaces, July 17–21, WIAS Berlin (in Harnack House).

84. ———, *Stochastische Methoden für Kommunikationsnetzwerke*, Orientierungsmodul der Technischen Universität Braunschweig, Institut für Mathematische Stochastik, January 30.

85. ———, *Subcritical percolation phases for generalized weight-dependent random connection models*, BOS-Workshop on Stochastic Geometry, February 22–24, Universität Osnabrück, Institut für Mathematik, February 24.

86. ———, *The statistical mechanics of the interlacement point process*, Second Annual Conference of the SPP 2265, March 27–30, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, March 29.

87. ———, *Dynamical Gibbs variational principles and attractor properties*, Mathematisches Kolloquium, Universität zu Köln, Abteilung Mathematik, June 14.

88. ———, *Continuum percolation in random environment*, Oberseminar zur Stochastik, Otto-von-Guericke-Universität Magdeburg, Fakultät für Mathematik, June 22.

89. ———, *Subcritical percolation phases for generalized weight-dependent random connection models*, 21st INFORMS Applied Probability Society Conference, June 28–30, Centre Prouvé, Nancy, France, June 29.

90. ———, *Connectivity and chase-escape in mobile device-to-device networks in urban environments*, 29th Nordic Congress of Mathematicians with EMS, July 3–7, Aalborg University, Department of Mathematical Sciences, Denmark, July 5.

91. ———, *Subcritical percolation phases for generalized weight-dependent random connection models*, DMV Annual Meeting 2023, Minisymposium MS 12 “Random Graphs and Statistical Network Analysis”, September 25–28, Technische Universität Ilmenau, September 25.

92. ———, *Stochastische Methoden für Kommunikationsnetzwerke*, Seminar der Fakultät Informatik, Hochschule Reutlingen, October 6.

93. ———, *Stochastische Methoden für Kommunikationsnetzwerke*, Orientierungsmodul der Technischen Universität Braunschweig, Institut für Mathematische Stochastik, November 2.

94. ———, *Percolation*, Oberseminar, Technische Universität Braunschweig, Institut für Mathematische Stochastik, November 8.

95. V. John, *A SUPG-stabilized POD-ROM method for convection-diffusion-reaction problems (online talk)*, Numerical Analysis of Galerkin ROMs seminar series (Online Event), February 28.

96. ———, *On recent topics in the finite element analysis of convection-diffusion problems (online talk)*, Numerical Analysis Seminar (Hybrid Event), University of Waterloo, Applied Mathematics, Canada, April 11.

97. M. Kantner, *Modeling of semiconductor devices for quantum technologies: From single-photon sources to spin-qubit shuttles*, CASA Colloquium (Centre for Analysis, Scientific Computing and Applications), Eindhoven University of Technology, Netherlands, April 5.

98. J. Kern, *Mini Course: A unified approach to non-gradient systems*, 3 talks, Seminar Interacting Random Systems (Hybrid Event), WIAS Berlin, May 11–15.

99. ———, *Young measures and the hydrodynamic limit of asymmetric exclusion processes*, Seminar Stochastics, Technical University of Lisbon, Lisbon, Portugal, July 10.

100. N. Kliche, *A numerical approach for the optimal operation of mini-grids under uncertainty*, 22nd European Conference on Mathematics for Industry (ECMI2023), MS17 “ECMI SIG: Mathematics for the Digital Factory”, June 26–30, Wrocław University of Science and Technology Congress Centre, Poland, June 26.

101. W. König, *Spatial particle processes with coagulation: Large deviations and gelation*, Workshop MathMicS 2023: Mathematics and Microscopic Theory for Random Soft Matter Systems, February 13–15, Heinrich-Heine-Universität Düsseldorf, Institut für Theoretische Physik II – Soft Matter, February 15.

102. ———, *The statistical mechanics of the interlacement point process*, Second Annual Conference of the SPP 2265, March 27–30, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, March 30.

103. ———, *The interacting Bose gas in the semi-classical limit*, Workshop "Recent Advances in Bose–Einstein Condensation", August 30 – September 1, Technische Universität München, Department of Mathematics, August 31.

104. J. Köppl, *Dynamical Gibbs variational principles for irreversible interacting particle systems and applications to attractor properties*, Analysis and Probability Seminar Passau, Universität Passau, Fakultät für Informatik und Mathematik, January 17.

105. Th. Koprucki, *MaRDI – The Mathematical Research Data Initiative within the German National Research Data Infrastructure (NFDI)*, Kolloquium der AG "Modellierung, Numerik, Differentialgleichungen", Technische Universität Berlin, January 31.

106. ———, *MaRDI – The Mathematical Research Data Initiative within the German National Research Data Infrastructure (NFDI)*, SIAM Conference on Computational Science and Engineering (CSE23), Minisymposium MS301 "Interfaces, Workflows, and Knowledge Graphs for FAIR CSE", February 27 – March 3, Amsterdam, Netherlands, March 2.

107. ———, *Building research data services for the community*, Leibniz MMS Days 2023, April 17–19, Leibniz-Institut für Agrartechnik und Bioökonomie (ATB), Potsdam, April 17.

108. D. Korolev, *Physics-informed neural control of partial differential equations with applications to numerical homogenization*, Kaiserslautern Applied and Industrial Mathematics Days – KLAIM 2023, September 25–27, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, September 26.

109. A. Kroshnin, *Entropic Wasserstein barycenters*, Interpolation of Measures, January 24–25, Lagrange Mathematics and Computation Research Center, Huawei, Paris, France, January 24.

110. ———, *Robust k-means clustering in metric spaces*, Workshop on Statistics in Metric Spaces, October 11–13, Center for Research in Economics and Statistics (CREST), UMR 9194, Palaiseau, France, October 12.

111. ———, *Robust k-means clustering in metric spaces*, Rencontres de Statistique Mathématique, December 18–22, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 20.

112. M. Landstorfer, *Thermodynamic modeling of the electrode-electrolyte interface – Double-layer capacitance, solvation number, validation*, Van Marum Colloquia, Leiden University, Institute of Chemistry, Netherlands, November 14.

113. R. Lasarzik, *Energy-variational solutions for conservation laws*, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, February 7.

114. ———, *Analysis of an Allen–Cahn system in two scale topology optimization*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00874 "Recent Advances in the Analysis and Numerics for Phase-Field Models", August 20–25, Waseda University, Tokyo, Japan, August 22.

115. ———, *Energy-variational solutions for different viscoelastic fluid models*, Workshop "Energetic Methods for Multi-Component Reactive Mixtures Modelling, Stability, and Asymptotic Analysis", September 13–15, WIAS Berlin, September 15.

116. ———, *Energy-variational solutions for conservation laws*, CRC Colloquium, Freie Universität Berlin, Department of Mathematics and Computer Science, October 19.

117. L. Liang, *A squared smoothing Newton method for semidefinite programming*, SIAM Conference on Optimization (OP23), MS331 "A Newton-type Method for SDP", May 30 – June 3, Seattle, USA, June 3.

118. M. Liero, *On the geometry of the Hellinger–Kantorovich space (hybrid talk)*, Seminar "Modern Methods in Applied Stochastics and Nonparametric Statistics", WIAS Berlin, January 31.

119. ———, *Luminance inhomogeneities in large-area OLEDs due to electrothermal feedback*, Hybride Optoelektronische Materialsysteme (HYD Seminar), Integrative Research Institute for the Sciences (IRIS Adlershof), Hybrid Devices Group, Berlin, April 20.

120. ———, *EDP-convergence for evolutionary systems with gradient flow structure*, 29th Nordic Congress of Mathematicians with EMS, July 3–7, Aalborg University, Department of Mathematical Sciences, Denmark, July 4.

121. ———, *Variational modeling of biomechanical systems*, 10th International Conference on Computational Bioengineering (ICCB 2023), Minisymposium 22-3 "Continuum Biomechanics of Active Biological Systems", September 20–22, Technische Universität Wien, Austria, September 22.

122. L. Lüchtrath, *Evolving networks, their limits and global properties*, Oberseminar Stochastik, Universität Augsburg, Institut für Mathematik, January 25.

123. ———, *The emergence of a giant component in one-dimensional inhomogeneous networks with long-range effects*, 18th Workshop on Algorithms and Models for Web Graphs, May 23–26, The Fields Institute for Research in Mathematical Sciences, Toronto, Canada, May 25.

124. ———, *Euclidean diameter of the soft Boolean model*, 29th Nordic Congress of Mathematicians with EMS, July 3–7, Aalborg University, Department of Mathematical Sciences, Denmark, July 6.

125. ———, *The random cluster graph*, Probability Seminar, University of Sheffield, School of Mathematics and Statistics, Sheffield, UK, November 15.

126. ———, *The random cluster graph*, Probability and Financical Mathematics Seminar, University of Leeds, School of Mathematics, Leeds, UK, November 23.

127. Ch. Merdon, *Raviart–Thomas enriched Scott–Vogelius finite element methods for the Navier–Stokes equations (online talk)*, City University of Hong Kong, Department of Mathematics, Hong Kong, January 18.

128. A. Mielke, *Asymptotic self-similar behavior in reaction-diffusion systems on the real line*, Minisymposium "Interacting Particle Systems and Variational Methods", Einhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, February 3.

129. ———, *Viscoelastic fluid models for geodynamic processes in the lithosphere*, "SPP Meets TP" Workshop: Variational Methods for Complex Phenomena in Solids, February 21–24, Universität Bonn, Hausdorff Institute for Mathematics, February 24.

130. ———, *Non-equilibrium steady states and EDP-convergence for slow-fast gradient systems*, In Search of Model Structures for Non-equilibrium Systems, April 24–28, Westfälische Wilhelms-Universität Münster, April 25.

131. ———, *EDP-convergence for gradient systems and non-equilibrium steady states*, Nonlinear Diffusion and Nonlocal Interaction Models – Entropies, Complexity, and Multi-Scale Structures, May 28 – June 2, Universidad de Granada, Spain, May 30.

132. ———, *Balanced-viscosity solutions as limits in generalized gradient systems under slow loading*, 4 talks, Hausdorff School "Analysis of PDEs: Variational and Geometric Perspectives", July 10–14, Universität Bonn, Hausdorff School for Advanced Studies in Mathematics, July 10–13.

133. ———, *Variational and geometric structures for thermomechanical systems*, Variational and Geometric Structures for Evolution, October 9–13, Centro Internazionale per la Ricerca Matematica (CIRM), Levico Terme, Italy, October 11.

134. Ch. Miranda, *Approximating Langevin Monte Carlo with ResNet-like neural network architectures*, Mini-Workshop "Nonlinear Approximation of High-dimensional Functions in Scientific Computing", October 15–20, Mathematisches Forschungsinstitut Oberwolfach, October 18.

135. M. O'Donovan, *Tight binding simulations of localization in alloy fluctuations in nitride based LEDs*, Seminar zu Physik der Gruppe III-Nitrid-Halbleiter und nanophotonischer Bauelemente und Advanced III-Nitride Materials and Photonic Devices (IIIN-MPD), Technische Universität Berlin, AG Experimentelle Nanophysik und Photonik, May 17.

136. L. Pelizzari, *Rough PDEs for local stochastic volatility models*, 17th Oxford-Berlin Young Researcher's Meeting on Applied Stochastic Analysis, April 27–29, WIAS & TU Berlin, April 27.

137. ———, *Rough PDEs and local stochastic volatility*, Volatility is rough, Isle of Skye Workshop, May 21–25, Sabhal Mòr Ostaig, Sleat, Isle of Skye, UK, May 25.

138. D. Peschka, *Multiscale limits of thin-film models with moving support*, Kolloquium des SFB 1114, Freie Universität Berlin, April 20.

139. ———, *Multiscale limits of thin-film models with moving support*, In Search of Model Structures for Non-equilibrium Systems, April 24–28, Westfälische Wilhelms-Universität Münster, April 27.

140. L. Plato, *Existence of weak solutions to an anisotropic electrokinetic flow model*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00874 "Recent Advances in the Analysis and Numerics for Phase-Field Models", August 20–25, Waseda University, Tokyo, Japan, August 22.

141. J. Polzehl, *Smoothing techniques for quantitative MR*, colloquium, Marquette University, Department of Mathematical and Statistical Sciences, Milwaukee, USA, November 3.

142. M. Radziunas, *Modeling, simulation, and analysis of dynamics in semiconductor lasers: A brief overview of the WIAS-FBH collaboration*, Leibniz MMS Days 2023, April 17–19, Leibniz-Institut für Agrartechnik und Bioökonomie (ATB), Potsdam, April 18.

143. A. Rathsfeld, *Analysis of scattering matrix algorithm*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00297 "Wave Scattering Problems: Numerical Methods with Applications", August 20–25, Waseda University, Tokyo, Japan, August 22.

144. ———, *Analysis of scattering matrix algorithm for diffraction by periodic surface structures*, Chinese Academy of Sciences, Institute of Computational Mathematics and Scientific/Engineering Computing, Beijing, China, September 4.

145. ———, *Plane-wave scattering by biperiodic gratings and rough surfaces: Radiation condition and far-field model*, Nankai University, Department of Scientific and Engineering Computing, Tianjin, China, September 7.

146. ———, *Plane-wave scattering by biperiodic gratings and rough surfaces: Radiation condition and far-field model (online talk)*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, October 26.

147. ———, *Simulation and inverse problems for rough surfaces by numerical methods of periodic grating structures (online talk)*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, November 29.

148. L. Schmeller, *Gradient flows and moving contact lines*, Seminar Prof. Sebastian Aland, Technische Universität Bergakademie Freiberg, Institut für Numerische Mathematik und Optimierung, February 8.

149. J.G.M. Schoenmakers, *Primal-dual regression approach for Markov decision processes with general state and action spaces*, SPDEs, Optimal Control and Mean Field Games – Analysis, Numerics and Applications, July 11–14, Universität Bielefeld, Center for Interdisciplinary Research (ZiF), July 12.

150. ———, *Optimal stopping with randomly arriving opportunities*, Stochastische Analysis und Stochastik der Finanzmärkte, Humboldt-Universität zu Berlin, Institut für Mathematik, November 23.

151. J. Schütte, *Adaptive neural networks for parametric PDEs*, 5th International Conference on Uncertainty Quantification in Computational Science and Engineering (UNCECOMP 2023), MS9 "UQ and Data As-

simulation with Sparse, Low-rank Tensor, and Machine Learning Methods", June 12–14, Athens, Greece, June 14.

152. ———, *Adaptive multilevel neural networks for parametric PDEs with error estimation*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00960 "Hierarchical Low Rank Tensors and DNNs for High-dimensional Approximation", August 20–25, Waseda University, Tokyo, Japan, August 23.

153. ———, *Adaptive neural networks for parametric PDEs*, Mini-Workshop "Nonlinear Approximation of High-dimensional Functions in Scientific Computing, October 15–20, Mathematisches Forschungsinstitut Oberwolfach, October 20.

154. D. Sommer, *Computing log-densities of time-reversed diffusion processes through Hamilton–Jacobi–Bellman equations*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Minisymposium 00837 "Particle Methods for Bayesian Inference", August 20–25, Waseda University, Tokyo, Japan, August 24.

155. ———, *Computing log-densities of reverse-time diffusion processes through Hamilton–Jacobi–Bellman equations (online talk)*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, November 30.

156. V. Spokoiny, *Marginal Laplace approximation and Gaussian mixtures*, Optimization and Statistical Learning, OSL2023, January 15–20, Les Houches School of Physics, France, January 17.

157. ———, *Bayesian inference for complex models*, MIA 2023 – Mathematics and Image Analysis, February 1–3, Berlin, February 3.

158. ———, *Inference in error-in-operator model*, Tel Aviv University, Department of Statistics, Israel, March 30.

159. ———, *Estimation and inference for error-in-operator model*, Lecture Series Trends in Statistics, National University of Singapore, Department of Mathematics, Singapore, August 25.

160. ———, *Estimation and inference for error-in-operator model*, Massachusetts Institute of Technology, Department of Mathematics, Cambridge, USA, September 29.

161. ———, *Bayesian inference using mixed Laplace approximation with applications to error-in-operator models*, New York University, Courant Institute of Mathematical Sciences and Center for Data Science, USA, October 3.

162. A. Stephan, *Fast-slow chemical reaction systems: Gradient systems and EDP-convergence*, Oberseminar Dynamics, Technische Universität München, Department of Mathematics, April 17.

163. ———, *On time-splitting methods for gradient flows with two dissipation mechanisms*, In Search of Model Structures for Non-equilibrium Systems, April 24–28, Westfälische Wilhelms-Universität Münster, April 28.

164. ———, *Positivity and polynomial decay of energies for square-field operators*, Variational and Geometric Structures for Evolution, October 9–13, Centro Internazionale per la Ricerca Matematica (CIRM), Levico Terme, Italy, October 13.

165. ———, *Gradient systems and time-splitting methods (online talk)*, PDE & Applied Mathematics Seminar, University of California, Riverside, Department of Mathematics, USA, November 8.

166. ———, *On time-splitting methods for gradient flows with two dissipation mechanisms*, PDE Afternoon, Technische Universität Wien, Austria, December 13.

167. K. Tabelow, *Mathematical research data management in interdisciplinary research*, Workshop on Biophysics-based Modeling and Data Assimilation in Medical Imaging (Hybrid Event), WIAS Berlin, August 31.

168. ———, *MaRDI: Building research data infrastructures for mathematics and the mathematical science*, 1st Conference on Research Data Infrastructure (CoRDI), September 12–14, Karlsruhe Institute of Technology (KIT), September 12.

169. N. Tapia, *Stability of deep neural networks via discrete rough paths*, Oxford Stochastic Analysis and Mathematical Finance Seminar, University of Oxford, Mathematical Institute, UK, February 13.

170. ———, *Branched Itô formula*, SFI: Structural Aspects of Signatures and Rough Paths, August 28 – September 1, The Norwegian Academy of Science and Letters, Centre for Advanced Study (CAS), Oslo, Norway, August 31.

171. ———, *Branched Itô formula*, Imperial College London, Mathematical Institute, UK, November 7.

172. ———, *Branched Itô formula*, Mini-Workshop "Combinatorial and Algebraic Structures in Rough Analysis and Related Fields", November 26 – December 2, Mathematisches Forschungsinstitut Oberwolfach, November 30.

173. J.P. Thiele, *Competencies and responsibilities of an RSE and how to acquire them (in Germany)*, FG RSE 2023: Fachgruppentreffen, Gesellschaft für Informatik, October 10–11, Leibniz Universität Hannover, October 10.

174. M. Thomas, *Approximating dynamic phase-field fracture with a first-order formulation for velocity and stress*, Seminar für Angewandte Mathematik, Technische Universität Dresden, June 5.

175. ———, *Approximating dynamic phase-field fracture with a first-order formulation for velocity and stress*, Nonlinear PDEs: Recent Trends in the Analysis of Continuum Mechanics, July 17–21, Universität Bonn, Hausdorff School for Advanced Studies in Mathematics, July 17.

176. ———, *Approximating dynamic phase-field fracture with a first-order formulation for velocity and stress*, Annual Workshop of the GAMM Activity Group on Analysis of PDEs, September 18–20, Katholische Universität Eichstätt-Ingolstadt, September 20.

177. ———, *Damage in viscoelastic materials at finite strains*, Workshop "Variational Methods for Evolution", December 3–8, Mathematisches Forschungsinstitut Oberwolfach, December 7.

178. W. van Zuijlen, *Weakly self avoiding walk in a random potential*, iPOD Seminar, Leiden University, Institute of Mathematics, Leiden, Netherlands, May 4.

179. ———, *Weakly self avoiding walk in a random potential*, Probability Seminar, University of Warwick, Mathematics Institute, UK, June 14.

180. ———, *Weakly self avoiding walk in a random potential*, Seminar Dipartimento di Matematica e Applicazioni, Università degli Studi di Milano-Bicocca, Milano, Italy, September 7.

181. ———, *Anderson models, from Schrödinger operators to singular SPDEs*, Oberseminar Analysis und Theoretische Physik, Leibniz Universität Hannover, Institut für Angewandte Mathematik, December 12.

182. A.G. Vladimirov, *Neutral delay differential equation Kerr cavity model*, Dissipative Solitons, Turbulence and Extreme Events in Nonlinear Photonics, September 6–8, International Solvay Institutes, Brussels, Belgium, September 8.

183. M. Wolfrum, *Bumps, chimera states, and Turing patterns in systems of coupled active rotators*, Mini-Workshop: Developing a Mathematical Theory for Co-evolutionary Dynamical Networks, Centre for Mathematical Science at Lund University, Lund, Sweden, May 30.

184. ———, *Dynamics of localized structures in DDEs with large delay*, 12th Colloquium on the Qualitative Theory of Differential Equations, June 19–23, Bolyai Institute, University of Szeged, Hungary, June 21.

185. ———, *Bumps, chimera states, and Turing patterns in systems of coupled active rotators (online talk)*, Workshop Complex Dynamical Systems – 2023 (Hybrid Event), October 2–4, Institute of Mathematics of the National Academy of Sciences of Ukraine, Kyiv, Ukraine, October 4.

186. C. Zarco-Romero, *Wilson's current idea using Markov Chains (online talk)*, 56th National Congress of the Mexican Mathematical Society, Autonomous University of San Luis Potosí, San Luis Potosí, Mexico, October 9.

187. J.-J. Zhu, *Principled robust machine learning in new geometries*, Leibniz MMS Days 2023, April 17–19, Leibniz-Institut für Agrartechnik und Bioökonomie (ATB), Potsdam, April 17.

188. ———, *From gradient flow force-balance to distributionally robust machine learning*, Universität Bonn, Mathematisch-Naturwissenschaftliche Fakultät, May 23.

189. ———, *From gradient flow to distributionally robust optimization*, Seminar of the Computer Science Department, University of British Columbia, Vancouver, Canada, June 5.

190. ———, *Duality from distributionally robust learning to gradient flow force-balance*, ICML 2023 Workshop on Duality Principles for Modern Machine Learning, July 27–29, Honolulu, USA, July 29.

191. ———, *Optimization and dynamics: From Euclidean gradient descent to Wasserstein gradient flow*, International Workshop of Intelligent Autonomous Learning Systems 2023, August 14–17, Technische Universität Darmstadt, Intelligent Autonomous Systems, Computer Science Department, August 15.

192. ———, *Learning with kernel gradient flow*, Thematic Einstein Semester Conference on Mathematical Optimization for Machine Learning, September 13–15, Mathematics Research Cluster MATH+, Berlin, September 15.

193. ———, *From gradient flow force-balance to distributionally robust learning*, European Conference on Computational Optimization (EUCCO), Minisymposium ML3 "Optimization and Machine Learning", September 25–27, Universität Heidelberg, September 26.

194. ———, *From gradient flow force-balance to robust machine learning*, Basque Center for Applied Mathematics, Bilbao, Spain, October 31.

A.8.3 Talks for a More General Public

1. Th. Eiter, *Interview* (`https://cloud.uni-jena.de/s/waTqNXWrrXJpZtD`), Episode 6 of podcast of Prof. Jonas Sauer who interviews mathematicians working in Analysis, November 17.

2. L. Ermoneit, *Computer presentation on "The quantum bit bus shuttle to solve the space problem of a quantum computer"*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2023, WIAS at Leibniz Association Headquarters, Berlin, June 17.

3. J. Fuhrmann, *Wieviel Energie "passt" in Batterien und andere Speicher?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2023, WIAS at Leibniz Association Headquarters, Berlin, June 17.

4. C. Geiersbach, *Representation of the interactive topic "Energy and Mathemactics"*, Crossing Boundaries – A Networking Event of the Berlin University Alliance, Kulturbrauerei, Berlin, November 22.

5. A. Glitzky, *Elektrothermik von organischen Halbleitern*, Girls' Day 2023, WIAS Berlin, April 27.

6. B. Jahnel, *Die Poesie der Logik*, 26. Berliner Tag der Mathematik (26th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, May 6.

7. J. Kern, *Wer wird Haribillionär?*, 26. Berliner Tag der Mathematik (26th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, May 6.

8. ———, *What is... an Interacting Particle System?*, What is... ?-Seminar der Berlin Mathematical School (BMS), Technische Universität Berlin, May 26.

9. ———, *Workshop "Wie funktionieren eigentlich Fotos?"*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2023, WIAS at Leibniz Association Headquarters, Berlin, June 17.

10. W. König, *Wird ein Gigant erscheinen oder nicht?*, Mathematische Forschung verstehen, Freie Universitat Berlin, January 5.

11. ———, *Paradoxa der Wahrscheinlichkeitsrechung*, MINT-Tag am Primo-Levi-Gymnasium 2023, Primo-Levi-Gymnasium, January 25.

12. ———, *Stochastische Geometrie in der Telekommunikation*, 2 talks, Tag der Wissenschaften 2023, Weinberg-Gymnasium Kleinmachnow, February 24.
13. ———, *Der fünfte Aggregatzustand: Eine kleine Geschichte der Bose-Einstein-Kondensation*, MathInside — am Pi Day 2023, Technische Universität Berlin, Institut für Mathematik, Berlin, March 14.
14. ———, *Das interagierende Bosegas im Lichte der Wahrscheinlichkeitstheorie*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2023, WIAS at Leibniz Association Headquarters, Berlin, June 17.
15. L. Lüchtrath, *Perkolationstheorie — der Kaffeefilter aus Sicht der Stochastik*, 26. Berliner Tag der Mathematik (26th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, May 6.
16. A. Stephan, *Wie kann man mit Billard Pi berechnen?*, 26. Berliner Tag der Mathematik (26th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, May 6.
17. H. Stephan, *Die mathematischen Grenzen der künstlichen Intelligenz*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2023, WIAS at Leibniz Association Headquarters, Berlin, June 17.
18. M. Thomas, *Wie Spaghetti zerbrechen — eine mathematische Untersuchung*, 9. BMG-Tag, Freie Universität Berlin, November 9.

A.8.4 Posters

1. D. Abdel, N.E. Courtier, P. Farrell, *Modelling and simulation of charge transport in Perovskite solar cells*, SIAM Conference on Computational Science and Engineering (CSE23), Amsterdam, Netherlands, February 26 – March 3.
2. Ch. Bayer, P. Friz, J.G.M. Schoenmakers, V. Spokoiny, N. Tapia, L. Pelizzari, *Optimal control in energy markets using rough analysis and deep networks*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
3. Ch. Bayer, D. Kreher, M. Landstorfer, W. Kenmoe Nzali, *Volatile electricity markets and battery storage: A model-based approach for optimal control*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
4. S. Breneis, *Pricing American options under rough Heston*, Stochastic Numerics and Statistical Learning: Theory and Applications Workshop 2023, Thuwal, Saudi Arabia, May 21 – June 1.
5. ———, *Path-dependent options under rough Heston*, 4th Workshop on Stochastic Methods in Finance and Physics, Heraklion, Kreta, Greece, July 17–21.
6. C. Cárcamo Sanchez, F. Galarce Marín, A. Caiazzo, I. Sack, K. Tabelow, *Quantitative tissue pressure imaging via PDE-informed assimilation of MR-data*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
7. P. Dvurechensky, C. Geiersbach, M. Hintermüller, A. Kannan, St. Kater, *Equilibria for distributed multi-modal energy systems under uncertainty*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
8. M. Eigel, M. Heida, M. Landstorfer, A. Selahi, *Recovery of battery ageing dynamics with multiple timescales*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
9. Th. Eiter, R. Lasarzik, *Analysis of energy-variational solutions for hyperbolic conservation laws*, Presentation of project proposals in SPP 2410 “Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness”, Bad Honnef, April 28.
10. L. Ermoneit, M. Kantner, Th. Koprucki, B. Schmidt, *Coherent spin-qubit shuttling for scalable quantum processors: Modeling, simulation and optimal control*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
11. L. Ermoneit, B. Schmidt, J. Fuhrmann, Th. Koprucki, M. Kantner, *Coherent spin-qubit shuttling in a SiGe quantum bus: Device-scale modeling, simulation and optimal control*, Leibniz MMS Days 2023, Potsdam, April 17–19.

12. P. Farrell, *Modeling and numerical simulation of two-dimensional TMDC memristive devices*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Tokyo, Japan, August 20–25.
13. J. Fuhrmann, Ch. Keller, M. Landstorfer, B. Wagner, *Development of an ion-channel model-framework for in-vitro assisted interpretation of current voltage relations*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
14. M. Heida, *Finite volumes for simulation of large molecules*, Finite Volumes for Complex Applications (FVCA10), Strasbourg, France, October 30 – November 3.
15. R. Henrion, D. Hömberg, N. Kliche, *Modeling and simulation of mini-grids under uncertainty*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Tokyo, Japan, August 20–25.
16. D. Hömberg, R. Henrion, N. Kliche, *Modeling and simulation of weakly coupled mini-grids under uncertainty*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
17. M. Kantner, *Wiener filter enhanced estimation of the intrinsic laser linewidth from delayed self-heterodyne beat note measurements*, 2023 Conference on Lasers and Electro-Optics/Europe-European Quantum Electronics Virtual Conferences, Munich, June 26–30.
18. M. Kantner, L. Ermoneit, B. Schmidt, J. Fuhrmann, A. Sala, L.R. Schreiber, Th. Koprucki, *Optimal control of a SiGe-quantum bus for coherent electron shuttling in scalable quantum computing architectures*, Silicon Quantum Electronics Workshop 2023, Kyoto, Japan, October 31 – November 2.
19. Ch. Keller, *Continuum-based modeling of biological ion channels*, Energetic Methods for Multi-Component Reactive Mixtures Modelling, Stability, and Asymptotic Analysis (EMRM 2023), Berlin, September 13–15.
20. J. Köppl, *The long-time behaviour of interacting particle systems: A Lyapunov functional approach*, In Search of Model Structures for Non-equilibrium Systems, Münster, April 24–28.
21. ———, *The long-time behaviour of interacting particle systems*, Stochastic Processes and Related Fields, Kyoto, September 4–8.
22. D. Korolev, *Machine learning for simulation intelligence in composite process design*, Leibniz MMS Days 2023, Potsdam, April 17–19.
23. M. Liero, *Analysis for thermo-mechanical models with internal variables*, Presentation of project proposals in SPP 2256 “Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials”, Bad Honnef, March 27.
24. L. Lüchtrath, *Percolation in weight-dependent random connection models*, Workshop on Random Discrete Structures, Münster, March 20–24.
25. E. Magnanini, *Gelation in a spatial Marcus–Lushnikov process*, Workshop MathMicS 2023: Mathematics and Microscopic Theory for Random Soft Matter Systems, Düsseldorf, February 13–15.
26. ———, *Gelation and hydrodynamic limits in a spatial Marcus–Lushnikov process*, In Search of Model Structures for Non-equilibrium Systems, Münster, April 24–28.
27. ———, *Spatial coagulation and gelation*, SPP2265-Reviewer-Kolloquium, Köln, August 29.
28. A. Maltsi, *Symmetries in transmission electron microscopy imaging of crystals with strain*, 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023), Tokyo, Japan, August 20–25.
29. O. Pártl, *A computational framework for sustainable geothermal energy production in fracture-controlled reservoir based on well placement optimization*, Leibniz MMS Days 2023, Potsdam, April 17.
30. L. Pelizzari, *Primal-dual optimal stopping with signatures*, Stochastic Numerics and Statistical Learning: Theory and Applications Workshop 2023, Thuwal, Saudi Arabia, May 26 – June 1.
31. L. Plato, R. Lasarzik, D. Hömberg, E. Emmrich, *Nonlinear electrokinetics in anisotropic microfluids – Analysis, simulation, and optimal control*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.

32. L. Schütz, *Towards stochastic homogenization of a rate-independent delamination model*, Hausdorff School "Analysis of PDEs: Variational and Geometric Perspectives", Bonn, July 10–14.
33. L. Schütz, M. Heida, M. Thomas, *Materials with discontinuities on many scales*, SCCS Days 2023 of the Collaborative Research Center – CRC 1114 "Scaling Cascades in Complex Systems", November 13–15.
34. A. Selahi, *A finite-element-solver for coupled domains in rust*, SIAM Conference on Computational Science and Engineering (CSE23), Amsterdam, Netherlands, February 26 – March 3.
35. M. Thomas, *Nonlinear fracture dynamics: Modeling, analysis, approximation, and applications*, Presentation of project proposals in SPP 2256 "Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials", Bad Honnef, March 27.
36. A.D. Vu, *Percolation on the Manhattan grid*, Stochastic Processes and Related Fields, Kyoto, Japan, September 4–8.
37. B. Wagner, *On disordered regions driving phase separation of proteins under variable salt concentration*, Cellular Matters Conference 2023, Ascona, Switzerland, June 4–7.
38. Q. Wang, *Robust multilevel training of artificial neural networks*, MATH+ Day, Humboldt-Universität zu Berlin, October 20.
39. M. Wolfrum, *Phase sensitive excitability of a limit cycle*, Conference on Nonlinear Data Analysis and Modeling: Advances, Appilcations, Perspective, Potsdam, March 15–17.

A.9 Visits to other Institutions[6]

1. J. Rehberg, Universität Duisburg-Essen, Fakultät für Mathematik, May 2–5.
2. J. Sprekels, Università degli Studi di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, April 11–20.
3. Ch. Bayer, King Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences, Thuwal, Saudi Arabia, August 1–10.
4. M. Bongarti, Polish Academy of Sciences, Systems Research Institute, Warsaw, Poland, June 26–29.
5. S. Breneis, King Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences, Thuwal, Saudi Arabia, August 6–10.
6. D. Dolinina, Institut de Physique de Nice, France, October 21–27.
7. P. Dvurechensky, Universität Mannheim, Fakultät für Wirtschaftsinformatik und Wirtschaftsmathematik, August 15–18.
8. M. Eigel, Centrale Nantes, Laboratoire de Mathématiques Jean Leray, France, June 26–29.
9. Th. Eiter, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, March 26–31.
10. ———, June 26–30.
11. D. Hömberg, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, March 13 – April 1.
12. ———, October 2–6.
13. V. John, Universidad Autonoma de Madrid, Departamento de Matemáticas, Spain, March 13–17.
14. ———, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, December 3–8.
15. M. Kantner, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications, Netherlands, April 3–6.
16. J. Kern, University of Lisbon, Instituto Superior Técnico, Department of Mathematics, Portugal, March 13–24.
17. ———, July 1–12.
18. W. König, University of California, Department of Mathematics, Los Angeles, USA, April 5–15.
19. R. Lasarzik, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, February 6–9.
20. V. Laschos, Aristotle University of Thessaloniki, Department of Mathematics, Greece, May 12 – August 21.
21. L. Lüchtrath, University of Leeds, School of Mathematics, Leeds, UK, November 15–24.
22. L. Mertenskötter, Technical University of Denmark-DTU, Copenhagen, Denmark, November 13–16.
23. A. Mielke, Eindhoven University of Technology, Department of Mathematics and Computer Science, Netherlands, January 30 – February 4.
24. ———, Universität Bonn, Hausdorff Research Institute for Mathematics, February 20 – March 3.
25. ———, Technische Universität München, Institute for Advanced Study, March 13–17.
26. A. Quitmann, Università di Roma “La Sapienza”, Dipartimento di Matematica, Italy, January 15 – February 3.
27. D. Sommer, Centrale Nantes, Laboratoire de Mathématiques Jean Leray, France, June 26–29.
28. V. Spokoiny, National Academy of Sciences, Institute of Mathematics, Yerevan, Armenia, July 8–12.
29. ———, National University of Singapore, Department of Mathematics, Singapore, August 23–30.

[6] Only stays of more than three days are listed.

30. ———, Massachusetts Institute of Technology, Department of Mathematics, Cambridge, USA, September 25–30.
31. ———, New York University, Courant Institute of Mathematical Sciences and Center for Data Science, USA, October 2–6.
32. N. Tapia, The Norwegian Academy of Science, Centre for Advanced Study (CAS), Oslo, Norway, August 21–27.
33. M. Theiss, Simula Research Laboratory, Oslo, Norway, February 14–17.
34. W. van Zuijlen, Radboud University Nijmegen, Department of Mathematics, Nijmegen, Netherlands, December 21, 2022 – January 3, 2023.
35. ———, University of Warwick, Mathematics Institute, UK, June 12–16.
36. ———, Università degli Studi di Milano-Bicocca, Dipartimento di Matematica e Applicazioni, Milano, Italy, September 4–8.
37. ———, Radboud University Nijmegen, Department of Mathematics, Nijmegen, Netherlands, October 13 – November 2.
38. B. Wagner, University of Oxford, Mathematical Institute, UK, May 1–8.
39. J.-J. Zhu, Basque Center for Applied Mathematics, Bilbao, Spain, October 29 – November 1.

A.10 Academic Teaching[7]

Winter Semester 2022/2023

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. Th. Eiter, M. Liero, *Mehrdimensionale Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
3. J. Fuhrmann, *Advanced Topics from Scientific Computing* (lecture), Technische Universität Berlin, 2 SWS.
4. A. Glitzky, A. Mielke, M. Thomas, B. Zwicknagl, *Online and Hybrid: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin/Freie Universität Berlin, 2 SWS.
5. M. Hintermüller, *Online: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
6. D. Hömberg, *Online and on site: Optimization II – PDE-Constrained Optimal Control (9 two-hour lectures from Jan. 1 to May 4, 2023)* (lecture), Norwegian University of Science and Technology, Trondheim, – SWS.
7. K. Hopf, *Nichtlineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
8. ———, *Nichtlineare partielle Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
9. B. Jahnel, *Introduction to Probability Theory* (lecture), Technische Universität Braunschweig, 4 SWS.
10. ———, *Probabilistic Methods in Telecommunications* (lecture), Technische Universität Braunschweig, 3 SWS.
11. V. John, *Basismodul: Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
12. Ch. Merdon, *Numerik gewöhnlicher Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
13. ———, *Numerik gewöhnlicher Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
14. A. Mielke, *Ausgewählte Themen der angewandten Analysis: Gradientensysteme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
15. R.I.A. Patterson, *Mathematik für Geowissenschaftler* (lecture), Freie Universität Berlin, 2 SWS.
16. V. Spokoiny, *Nonparametric Statistics (M29)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
17. ———, *Nonparametric Statistics (M29)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
18. V. Spokoiny, M. Reiss, S. Greven, W. Härdle, A. Carpentier, *Online and Hybrid: Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
19. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
20. H. Stephan, *Funktionalanalytische Methoden in der klassischen Physik (nichtlineare Theorie)* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
21. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
22. M. Thomas, *Analysis I* (lecture), Freie Universität Berlin, 4 SWS.
23. ———, *Variational methods and Gamma-convergence* (seminar), Freie Universität Berlin, 2 SWS.

[7] SWS = semester periods per week

24. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Online: Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/Technische Universität Berlin, 2 SWS.

Summer Semester 2023

1. U. Bandelow, S. Amiranashvili, *Nichtlineare Dynamik in der Photonik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
2. A. Glitzky, A. Mielke, M. Thomas, B. Zwicknagl, *Hybrid: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin/Freie Universität Berlin, 2 SWS.
3. M. Hintermüller, *Online: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
4. D. Hömberg, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
5. ———, *Online and on site: Optimization II – PDE-Constrained Optimal Control (9 two-hour lectures from Jan. 1 to May 4, 2023)* (lecture), Norwegian University of Science and Technology, Trondheim, – SWS.
6. B. Jahnel, *RampUp for Data Scientists: Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
7. W. König, *Wahrscheinlichkeitstheorie I* (lecture), Technische Universität Berlin, 4 SWS.
8. D. Peschka, *Lineare Algebra I* (lecture), Freie Universität Berlin, 4 SWS.
9. ———, *Numerical Methods for Fluid Flows* (seminar), Freie Universität Berlin, 2 SWS.
10. ———, *Zentralübung zu Lineare Algebra I* (practice), Freie Universität Berlin, 2 SWS.
11. V. Spokoiny, M. Reiss, S. Greven, W. Härdle, A. Carpentier, *Online and Hybrid: Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
12. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
13. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
14. M. Thomas, *Analysis II* (lecture), Freie Universität Berlin, 4 SWS.
15. ———, *Konvexe Analysis* (seminar), Freie Universität Berlin, 2 SWS.
16. ———, *Zentralübung zu Analysis II* (practice), Freie Universität Berlin, 1 SWS.

Winter Semester 2023/2024

1. M. Kniely, *Ausgewählte Themen der angewandten Analysis (M38): Reaction-Diffusion Equations* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
2. ———, *Ausgewählte Themen der angewandten Analysis (M38): Reaction-Diffusion Equations* (practice), Humboldt-Universität zu Berlin, 1 SWS.
3. A. Alphonse, *Ausgewählte Themen der Optimierung (M21): Obstacle Problems and Optimal Control* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
4. ———, *Ausgewählte Themen der Optimierung (M21): Obstacle Problems and Optimal Control* (practice), Humboldt-Universität zu Berlin, 1 SWS.
5. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
6. Th. Eiter, *Funktionalanalysis* (lecture), Universität Kassel, 4 SWS.
7. ———, *Fachwissenschaftliches Seminar für Lehramt Grundschule* (seminar), Universität Kassel, 2 SWS.
8. ———, *Fachwissenschaftliches Seminar I für Lehrämter L2* (seminar), Universität Kassel, 2 SWS.

9. J. Fuhrmann, *Advanced Topics from Scientific Computing* (lecture), Technische Universität Berlin, 2 SWS.
10. C. Geiersbach, *Stochastische Optimierung (M20)* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. ———, *Stochastische Optimierung (M20)* (practice), Humboldt-Universität zu Berlin, 1 SWS.
12. A. Glitzky, M. Liero, A. Mielke, M. Thomas, B. Zwicknagl, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin/Freie Universität Berlin, 2 SWS.
13. M. Hintermüller, *Ausgewählte Kapitel der Mathematik (M40): Semismooth Newton Method* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
14. ———, *Hybrid: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
15. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
16. B. Jahnel, *Bachelor Seminar Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
17. ———, *Einführung in die Stochastik* (lecture), Technische Universität Braunschweig, 4 SWS.
18. ———, *Markov Processes* (lecture), Technische Universität Braunschweig, 4 SWS.
19. ———, *RampUp for Data Scientists: Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
20. W. König, *Wahrscheinlichkeitstheorie II* (lecture), Technische Universität Berlin, 4 SWS.
21. R. Lasarzik, *Partielle Differentialgleichungen II* (lecture), Freie Universität Berlin, 4 SWS.
22. ———, *Sobolev- und BV-Räume* (seminar), Freie Universität Berlin, 1 SWS.
23. ———, *Partielle Differentialgleichungen II* (practice), Freie Universität Berlin, 2 SWS.
24. J. Ginster, M. Liero, *Mathematische Prinzipien der Kontinuumsmechanik (M1)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
25. ———, *Mathematische Prinzipien der Kontinuumsmechanik (M1)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
26. B. Moreau, *Computational Fluid Dynamics* (lecture), Beuth Hochschule für Technik Berlin, 4 SWS.
27. B. Keller, B. Schmidt, *Einführung in die Theoretische Chemie* (lecture), Freie Universität Berlin, 2 SWS.
28. C. Sirotenko, *Ausgewählte Kapitel der Mathematik (M40): Semismooth Newton Method* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
29. ———, *Ausgewählte Kapitel der Mathematik (M40): Semismooth Newton Method* (practice), Humboldt-Universität zu Berlin, 2 SWS.
30. V. Spokoiny, M. Reiss, S. Greven, W. Härdle, A. Carpentier, *Online and Hybrid: Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
31. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
32. V. Spokoiny, J.-J. Zhu, *Nonparametric Statistics (M29)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
33. ———, *Nonparametric Statistics (M29)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
34. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
35. M. Thomas, *Analysis III* (lecture), Freie Universität Berlin, 4 SWS.
36. ———, *Sobolev- und BV-Räume* (seminar), Freie Universität Berlin, 2 SWS.
37. ———, *Zentralübung zu Analysis III* (practice), Freie Universität Berlin, 1 SWS.

A.11 Visiting Scientists[8]

A.11.1 Guests

1. A. Acharya, Carnegie Mellon University, Civil and Environmental Engineering, Pittsburgh, USA, May 14–27.
2. A. Agosti, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 22–25.
3. L. Andreis, Politecnico di Milano, Departimento di Mathematica (DMAT) D, Milano, Italy, April 30 – May 5.
4. L. Andreis, Politecnico di Milano, Departimento di Mathematica (DMAT), Milano, Italy, July 27 – August 4.
5. L. Araujo, Technische Universität München, Fakultät für Mathematik, September 18–30.
6. R.J. Baraldi, Sandia National Laboratories, Optimization & Uncertainty Quantification, Albuquerque, USA, August 28 – September 1.
7. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, March 20–31.
8. Th. Belin, CentraleSupélec, Mathematics and Computer Science Laboratory for Complexity and Systems – MICS (EA 4037), Gif-sur-Yvette, France, April 11 – August 18.
9. D. Belomestny, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, May 10–19.
10. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, December 11–18.
11. Z. Bian, University of São Paulo, Instituto de Ciências Matemáticas e de Computação, São Carlos, Brazil, November 18 – December 16.
12. M. Biskup, University of California, Los Angeles, Department of Mathematics, Los Angeles, USA, December 3–8.
13. R. Blossey, University of Lille 1 & CNRS, Unité de Glycobiologie Structurale et Fonctionnelle (UGSF) CNRS UMR 8576, Villeneuve-d'Ascq, France, June 26–30.
14. M. Brokate, Technische Universität München, Department of Mathematics, Garching, January 1 – December 31.
15. D. Brust, Deutsches Zentrum für Luft- und Raumfahrt (German Aerospace Center) DLR, Institute of Future Fuels, Juelich, July 17–21.
16. M. Bulíček, Charles University, Mathematical Institute, Prague, Czech Republic, September 5–15.
17. O. Burylko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, Ukraine, May 1 – December 31.
18. C. Christof, Technische Universität München, Lehrstuhl für Optimalsteuerung, Zentrum Mathematik, M17, Garching, March 19–24.
19. P. Colli, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, April 20–28.
20. A. Drewitz, Universität zu Köln, Mathematisches Institut, Köln, January 23–27.
21. C. Erignoux, Centre INRIA Lille Nord-Europe, Equipe PARADYSE, Villeneuve-d'Ascq, France, May 11–17.
22. E. Ferrucci, University of Oxford, Mathematical Institute, Oxford, UK, March 12–18.
23. R. Finn, Tyndall National Institute, Photonics, Cork, Ireland, December 11–15.
24. S. Fischer, Ludwig-Maximilians-Universität München, Institut für Statistik, München, October 1, 2023 – September 30, 2024.

[8] Only stays of more than three days are listed.

25. S. Floreani, Rheinische Friedrich-Wilhelms-Universität Bonn, Mathematisch-Naturwissenschaftliche Fakultät, Bonn, October 17–20.
26. B. Gaudeul, Université Paris-Saclay, Faculté des Sciences d'Orsay, France, July 17–28.
27. H. Harbrecht, Universität Basel, Departement Mathematik und Informatik, Switzerland, July 16–21.
28. G. Hu, Nankai University, School of Mathematical Sciences, Tianjin, China, June 30 – July 4.
29. G. Huyet, Université Côte d'Azur, Institut de Physique de Nice, Nice, France, October 9–15.
30. B. Keith, Brown University, Division of Applied Mathematics, Providence, Rhode Island, USA, May 21–27.
31. C. Kerriou, Universität zu Köln, Mathematisches Institut, Köln, June 27–30.
32. J. King, University of Nottingham, School of Mathematical Sciences, UK, August 17–24.
33. P. Krejčí, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, Czech Republic, May 22–26.
34. G. Last, Karlsruher Institut für Technologie, Institut für Stochastik, Karlsruhe, June 6–9.
35. T.Y. Lo, Uppsala University, Department of Mathematics, Uppsala, Sweden, October 3–7.
36. B. Lodewijks, Universität Augsburg, Mathematisch-Naturwissenschaftlich-Technische Fakultät, October 7–13.
37. H. Meinlschmidt, Friedrich-Alexander Universität Erlangen-Nürnberg, Dynamics, Control, Machine Learning and Numerics, October 31 – November 3.
38. Ch. Miranda, Université de Nantes, Laboratoire de Mathématiques Jean Leray, France, April 3 – September 30.
39. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, June 28 – July 14.
40. ———, August 17 – September 15.
41. F. Oschmann, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, January 16–20.
42. M. Oster, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, December 18–22.
43. T. Pereira, University of São Paulo, Departamento de Matematica Aplicada e Estatistica, São Paulo, Brazil, March 13–23.
44. ———, November 17, 2023 – February 5, 2024.
45. P. Pérez-Aros, Universidad de O'Higgins, Instituto de Ciencias de la Ingeniería, Rancagua, Chile, October 3–7.
46. M. Renger, Technische Universität München, Fachbereich Mathematik, Garching, September 25–29.
47. E. Rocca, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 22–26.
48. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, September 5–9.
49. A. Rossier, University of Oxford, Mathematical Institute, Oxford, UK, February 6–17.
50. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, October 18 – November 18.
51. B. Salvador, Technical University of Lisbon, Mathematics Department, Portugal, December 11–14.
52. L. Schmitz, Universität Greifswald, Institut für Mathematik und Informatik, Greifswald, October 1, 2023 – March 17, 2024.

53. H. Si, Cadence Austin Office, Texas, USA, October 11–27.
54. A.L. Silvestre, University of Lisbon, School of Engineering, Portugal, June 7–15.
55. M. Slowik, Universität Mannheim, Fakultät für Wirtschaftsinformatik und Wirtschaftsmathematik, July 3–12.
56. R. Soares dos Santos, Universidade Federal de Minas Gerais (UFMG), Departamento de Matemática, Pampulha – Belo Horizonte, Brazil, May 20–30.
57. A. ter Elst, University of Auckland, Department of Mathematics, New Zealand, February 1 – March 1.
58. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, Romania, October 30 – November 3.
59. M. Tlidi, Université Libre de Bruxelles, Physics, Belgium, July 2–6.
60. P. Tolksdorf, Johannes Gutenberg-Universität Mainz, FB 08: Physik, Mathematik und Informatik, February 6–9.
61. O. Tse, Eindhoven University of Technology, Mathematics and Computer Science, Eindhoven, Netherlands, January 8–13.
62. S.K. Turitsyn, Aston University, Institute of Photonic Technology, Birmingham, UK, July 2–6.
63. B. Walker, University of Oxford, Mathematical Institute, Radcliffe Observatory Quarter, Oxford, UK, November 6, 2023 – January 19, 2024.
64. K. Welker, TU Bergakademie Freiberg, Mathematische Optimierung, Freiberg, May 1–5.
65. K. Wiśniewski, Warsaw University of Technology, Faculty of Physics, Warsaw, Poland, January 30 – February 4.

A.11.2 Scholarship Holders

1. O. Burylko, National Academy of Sciences of Ukraine, Kiev, MATH+ Fellowship for Mathematicians from Ukraine, November 1, 2022 – April 30, 2023.
2. M. Kniely, Universität Graz, Austria, Erwin Schrödinger-Auslandsstipendium, March 1, 2022 – February 29, 2024.
3. H. Liang, Shandong University, Jinan, China, Freie Universität Berlin – China Scholarship Council Program for Doctoral Researchers (FUB-CSC Program), September 15, 2023 – September 15, 2027.
4. I. Papadopoulos, Imperial College London, UK, MATH+ Dirichlet-Fellowship, November 15 – December 31.
5. Ch.P. Papanikas, University of Cyprus, Nicosia, Cyprus, Erasmus+ Traineeship, September 1 – December 31.
6. M. Tsopanopoulos, Humboldt-Universität zu Berlin, Institut für Mathematik, Phase II Scholarship of the Berlin Mathematical School, July 1, 2023 – June 30, 2026.

A.11.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. E. Gladin, Humboldt-Universität zu Berlin, supervisor: Prof. Dr. V. Spokoiny, BMS, doctoral candidate, January 1 – December 31.
2. M. Reiter, Technische Universität Berlin, Institut für Mathematik, supervisor: Dr. R. Lasarzik, doctoral candidate, January 1 – December 31.

A.12 Guest Talks

1. E. Aamari, Université Paris Diderot, Laboratoire de Probabilités, Statistiques et Modélisation, France, *Minimax manifold estimation: Boundary, noise and computational constraints*, June 21.
2. A. Acharya, Carnegie Mellon University, Civil and Environmental Engineering, Pittsburgh, USA, *Slow time-scale behavior of fast microscopic dynamics (hybrid talk)*, May 16.
3. G. Adelfio, Università degli Studi di Palermo, Scienze Economiche, Aziendali e Statistiche, Italy, *Spatio-temporal point processes: Local second-order statistics for estimation and diagnostics (hybrid talk)*, July 19.
4. A. Agosti, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, *A Cahn–Hilliard phase field model coupled to viscoelasticity at large strains*, May 24.
5. M. Ali, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Strömungs- und Materialsimulation, Kaiserslautern, *Quantum computing for differential equations and surrogate modeling*, October 12.
6. R. Altmeyer, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, *Statistics for stochastic PDEs: Optimal rates and a nonparametric LAN expansion (hybrid talk)*, May 31.
7. L. Andreis, Politecnico di Milano, Dipartimento di Matematica (DMAT), Italy, *Rare events for sparse random graphs and some new large deviation result*, May 3.
8. L. Araujo, Technische Universität München, Fakultät für Mathematik, *Beyond the Born–Oppenheimer approximation by surface hopping trajectories methods*, September 25.
9. R.J. Baraldi, Sandia National Laboratories, Optimization & Uncertainty Quantification, Albuquerque, USA, *A proximal trust–region method for nonsmooth optimization with inexact function and gradient evaluations*, August 29.
10. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Positivity-preserving discretisations in general meshes*, March 23.
11. Th. Belin, CentraleSupélec, Mathematics and Computer Science Laboratory for Complexity and Systems – MICS (EA 4037), Gif-sur-Yvette, France, *An entropic finite volume scheme for a fully non-linear forward-backward parabolic equation*, May 11.
12. D. Belomestny, Universität Duisburg-Essen, Fakultät für Mathematik, *Provable benefits of policy learning from human preferences (hybrid talk)*, October 25.
13. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, *Asymptotic stability in a free boundary PDE model of active matter*, December 12.
14. F. Besold, Humboldt-Universität zu Berlin, Institut für Mathematik, *Adaptive weights community detection*, January 4.
15. G. Blanchard, Université Paris Saclay, Institut de Mathématiques d'Orsay, France, *Stein effect for estimating many vector means: A "blessing of dimensionality" phenomenon*, May 3.
16. D. Brust, Deutsches Zentrum für Luft- und Raumfahrt (German Aerospace Center) DLR, Institute of Future Fuels, Juelich, *Modelling study of a photo-thermal catalytic reactor for rWGS reaction under concentrated irradiation*, July 20.
17. B. Buchmann, Australian National University, Research School of Finance, Actuarial Studies & Statistics, Canberra, Australia, *Weak subordination of multivariate Levy processes (hybrid talk)*, December 13.
18. L. Bungert, Technische Universität Berlin, Institut für Mathematik, *Polarized consensus based particle dynamics (hybrid talk)*, June 20.
19. ———, *The geometry of adversarial machine learning*, June 21.

20. A. Callegaro, Technische Universität München and Johannes Gutenberg-Universität Mainz, Department of Mathematics and Institut für Mathematik, *Survival and complete convergence for a branching annihilating random walk*, February 1.
21. A. Caponera, University of Milano-Bicocca, Department of Economics, Management and Statistics (DEMS), Italy, *Functional estimation of anisotropic covariance and autocovariance operators on the sphere (hybrid talk)*, June 28.
22. C. Christof, Technische Universität München, Lehrstuhl für Optimalsteuerung, Zentrum Mathematik, M17, Garching, *On the identification and optimization of nonsmooth superposition operators in semilinear elliptic PDEs*, March 22.
23. P. Colli, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, *The Cahn–Hilliard–Oono system with control in the mass term (hybrid talk)*, April 26.
24. J.-Y. Dai, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Exploring a new mechanism of periodic orbits: Dynamics of two predators competing for a prey*, June 27.
25. É. de Panafieu, Nokia Bell Labs, Nozay, France, *Active clustering of a set using pairwise comparisons*, February 23.
26. V. Didelez, Universität Bremen, Fachbereich 3 – Mathematik und Informatik, *Causal reasoning and causal discovery with applications in epidemiology*, February 8.
27. A. Drewitz, Universität zu Köln, Mathematisches Institut, *Percolation, long-range correlations and critical exponents on transient graphs*, January 25.
28. C. Erignoux, Centre INRIA Lille Nord-Europe, Villeneuve-d'Ascq, France, *Symmetric and asymmetric hydrodynamics for the facilitated exclusion process via mapping*, May 17.
29. T. Fastovska, Karazin Kharkiv National University and Humboldt-Universität zu Berlin, School of Mathematics and Computer Sciences and Institut für Mathematik, Ukraine, *Asymptotic behaviour of solutions to transmission problems for elastic beams (hybrid talk)*, February 1.
30. R. Finn, Tyndall National Institute, Photonics, Cork, Ireland, *UV light emitters: From alloy microstructure to carrier transport*, December 14.
31. S. Floreani, Rheinische Friedrich-Wilhelms-Universität Bonn, Mathematisch-Naturwissenschaftliche Fakultät, Bonn, *Universal properties of non-equilibrium steady states of boundary-driven symmetric systems*, October 18.
32. H. Frankowska, Sorbonne Université, Institut de Mathématiques de Jussieu, Paris, France, *Differential inclusions and optimal control on Wasserstein spaces*, November 13.
33. B. Gaudeul, Université Paris-Saclay, Faculté des Sciences d'Orsay, France, *Building thermodynamically consistent models using variational modelling*, July 18.
34. P. Gelss, Zuse-Institut Berlin, Interactive Optimization and Learning (IOL), *Fredholm integral equations for the training of shallow neural networks*, July 12.
35. P.P. Ghosh, Technische Universität Braunschweig, Institut für Mathematische Stochastik, *A last progeny modified branching random walk*, March 1.
36. S. Ghosh, National University of Singapore, Department of Mathematics, Singapore, *Rigidity phenomena in strongly correlated random point fields and the emergence of forbidden regions*, October 4.
37. P. Gladbach, Universität Bonn, Institut für Angewandte Mathematik, *Homogenization and mean-field limits of transport costs (hybrid talk)*, June 28.
38. E. Gladin, Humboldt-Universität zu Berlin, Berlin Mathematical School, *Accuracy certificates for convex minimization with inexact oracle (hybrid talk)*, August 15.

39. M. Grith, Erasmus University Rotterdam, School of Economics, Netherlands, *The block-autoregressive model in non-standard bases (hybrid talk)*, January 25.
40. E. Hansen, Lund University, Mathematics (Faculty of Engineering), Lund, Sweden, *Convergence analysis of the nonoverlapping Robin–Robin method for nonlinear elliptic equations*, May 4.
41. H. Harbrecht, Universität Basel, Departement Mathematik und Informatik, Switzerland, *Low-rank tensor approximation of continuous functions*, July 18.
42. D. Hauer, The University of Sidney, School of Mathematics and Statistics, Australia, *The fundamental gap conjecture (hybrid talk)*, April 19.
43. E. Herberg, Universitat Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen (IWR), *Deep learning with variable time stepping (online talk)*, June 20.
44. M.F. Herbst, Rheinisch-Westfälische Technische Hochschule Aachen, Applied and Computational Mathematics, *Black-box algorithms and robust error control for density-functional theory*, January 16.
45. Ch. Hirsch, Aarhus University, Department of Mathematics, Aarhus, Denmark, *On the topology of higher-order age-dependent random connection models*, May 16.
46. M. Hoffmann, Université Paris-Dauphine, Department of Mathematics and Information Technologies, France, *On estimating multidimensional diffusions from discrete data (hybrid talk)*, November 22.
47. G. Hu, Nankai University, School of Mathematical Sciences, Tianjin, China, *Time-harmonic scattering by periodic structures with Dirichlet and Neumann boundary conditions*, July 4.
48. Ch. Huang, Aarhus University, Department of Economics and Business Economics, Denmark, *Arellano–Bond LASSO estimator for long panel dynamic linear models*, April 19.
49. D. Jacobi, Technische Universität Berlin, Berlin-Oxford IRTG 2544 "Stochastic Analysis in Interaction", *Super-Brownian motion with dormancy*, February 8.
50. T. Jahn, Universität Bonn, Institut für Numerische Simulation, *Discretisation-adaptive regularisation of statistical inverse problems (hybrid talk)*, January 18.
51. N. Kajino, Kyoto University, Research Institute for Mathematical Sciences, Japan, *Two-sided bounds on tail probabilities of the number of collisions of random walks*, July 6.
52. B. Keith, Brown University, Division of Applied Mathematics, Providence, Rhode Island, USA, *The entropic finite element method*, May 25.
53. C. Kerriou, Universität zu Köln, Mathematisches Institut, *Condensation in scale-free geometric graphs with excess edges*, June 28.
54. R. Klein, Freie Universität Berlin, Institut für Mathematik, *Thoughts on machine learning*, November 9.
55. A. Klippel, Technische Universität Darmstadt, Fachbereich Mathematik, Darmstadt, *Comparison of the random loop model to percolation and infinite loops in the random link mode*, July 12.
56. D. Knees, Universität Kassel, FB 10, Institut für Mathematik, *Regularity results for a static relaxed micromorphic model*, October 4.
57. A. Korba, École Nationale de la Statistique et de l'Administration Économique (ENSAE), Statistics Department, Palaiseau, France, *Sampling with mollified interaction energy descent*, July 24.
58. J. Kowal, Technische Universität Berlin, Institut für Energie und Automatisierungstechnik, *Working principle and ageing of batteries*, February 13.
59. P. Krejči, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, *Degenerate hysteresis in partially saturated porous media (hybrid talk)*, May 24.
60. Ch. Külske, Ruhr-Universität Bochum, Fakultät für Mathematik, *New states with non-singleton localization sets for gradient models on trees*, March 15.

61. P. Lappicy, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *On the exceptional Bianchi models*, June 27.
62. G. Last, Karlruher Institut für Technologie, Institut für Stochastik, Karlsruhe, *A Palm approach to tail processes and tail measures*, June 7.
63. T. Laux, Universität Bonn, Hausdorff Center for Mathematics, Bonn, *The large-data limit of the MBO scheme for data clustering*, February 14.
64. C. Le Bris, École des Ponts ParisTech & INRIA, Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique & Mathematics for Materials, France, *Defects in homogenization theory and related computational issues (hybrid talk)*, February 15.
65. P. Lewintan, Universität Duisburg-Essen, Fakultät für Mathematik, *Optimal Korn–Maxwell–Sobolev inequalities (hybrid talk)*, June 28.
66. B. Lodewijks, Universität Augsburg, Mathematisch-Naturwissenschaftlich-Technische Fakultät, *Long-range first-passage percolation on the complete graph*, October 11.
67. E. Mammen, Universität Heidelberg, Mathematikon, Heidelberg, *Random planted forest: A directly interpretable tree ensemble (hybrid talk)*, May 17.
68. D.J. Mankowitz, Google Deepmind, London, UK, *AlphaDev: Faster sorting algorithms discovered using deep reinforcement learning (hybrid talk)*, July 18.
69. J.L. Matic, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *Global sensitivity analysis in the presence of missing values*, February 15.
70. H. Meinlschmidt, Friedrich-Alexander-Universität Erlangen-Nürnberg, Dynamics, Control, Machine Learning and Numerics, *Renormalized solutions for optimal control of the drift in Fokker–Planck equations*, November 3.
71. M. Mittnenzweig, Weizmann Institute of Science, Department of Computer Science and Applied Mathematics, Rehovot, Israel, *From an egg to an embryo – Inferring the temporal dynamics of cells during embryonic development (hybrid talk)*, April 6.
72. Ch. Mukherjee, Westfälische Wilhelms-Universität Münster, Institut für Mathematische Stochastik, *Homogenization of Hamilton–Jacobi–Bellman equations on continuum percolation clusters*, January 11.
73. D. Nieman, Vrije Universiteit Amsterdam, Faculty of Science, Mathematics, Netherlands, *Frequentist guarantees for variational Gaussian process regression*, December 6.
74. J. Niles-Weed, New York University, Courant Institute of Mathematical Sciences and Center for Data Science, USA, *Optimal transport map estimation in general function spaces (online talk)*, May 24.
75. Th. O'Leary Roseberry, University of Texas, Oden Institute, Austin, USA, *Enabling efficient UQ and optimization with derivative-informed neural operators (hybrid talk)*, March 9.
76. F. Oschmann, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, *Stratified fluids: On pancakes and non-local temperatures (hybrid talk)*, January 18.
77. M. Oster, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, *Going deep with dictionaries: ODE-based models*, December 19.
78. D. Padilla-Garza, Technische Universität Dresden, Institut für Wissenschaftliches Rechnen, *Mathematical challenges and developments in the nonlinear bending theory for plates (hybrid talk)*, July 12.
79. V. Panaretos, École Polytechnique Fédérale de Lausanne, Institute of Mathematics, Lausanne, Switzerland, *Optimal transport for covariance operators*, November 1.
80. Ch. Parkinson, University of Arizona, Department of Mathematics, Tucson, USA, *The Hamilton–Jacobi formulation of optimal path planning for autonomous vehicles (online talk)*, February 16.

81. P. Pérez-Aros, Universidad de O'Higgins, Instituto de Ciencias de la Ingeniería, Rancagua, Chile, *Coderivative-based semi-Newton method in nonsmooth difference programming*, October 4.
82. C. Poon, University of Warwick, Mathematics Institute, Coventry, UK, *Super-resolved Lasso (hybrid talk)*, December 18.
83. M. Pütz, Brandenburgische Technische Universität, Fachgebiet Numerische Mathematik und Wissenschaftliches Rechnen, Cottbus-Senftenberg, *Quadrature-based moment methods for the solution of population balance equations*, January 19.
84. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *A common approach to singular perturbation and homogenization*, November 15.
85. M. Renger, Technische Universität München, Fachbereich Mathematik, *Collisions in the exclusion process*, September 27.
86. St. Ringe, Korea University, Department of Chemistry, Seongbuk-gu, Seoul, Korea (Republic of), *First-principles multi-scale modeling of electrochemical CO2 reduction*, July 26.
87. A. Rossier, University of Oxford, Mathematical Institute, Oxford, UK, *Asymptotic analysis of deep residual networks (hybrid talk)*, February 7.
88. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, *Some gradient theories in linear visco-elastodynamics towards dispersion and attenuation of waves in relation to large-strain models*, November 8.
89. Ch. Roux, Zuse-Institut Berlin and Technische Universität Berlin, Interactive Optimization and Learning Lab, *Bounding geometric penalties in first-order Riemannian optimization*, November 28.
90. B. Salvador, Technical University of Lisbon, Mathematics Department, Portugal, *From duality to correlations: Application to the partial exclusion process SEP*, December 13.
91. A. Salvadori, Università degli Studi di Brescia, Dipartimento di Ingegneria Meccanica e Industriale, Italy, *Modeling and simulations towards the design of high performance batteries*, February 21.
92. L. Sangalli, Politecnico di Milano, Dipartimento di Matematica, Italy, *Physics-informed spatial and functional data analysis*, December 15.
93. R.P. Schaerer, Zürcher Hochschule für Angewandte Wissenschaften (ZHAW), Institute of Computational Physics (ICP), Winterthur, Switzerland, *A non-isothermal cell performance model for organic flow batteries*, July 18.
94. L. Schmitz, Universität Greifswald, Institut für Mathematik und Informatik, Greifswald, *Two-parameter sums signatures and corresponding quasisymmetric functions (hybrid talk)*, November 14.
95. I. Schneider, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *From Pythagoras to differential equations: Uncovering the mysteries of musical sound*, May 25.
96. R. Scholz, Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, *Simulation amphiphiler Polymernetzwerke*, October 4.
97. H. Si, Cadence Austin Office, Texas, USA, *Perspectives of anisotropic Delaunay mesh adaptation*, October 12.
98. A.L. Silvestre, University of Lisbon, School of Engineering, Portugal, *Optimal boundary control for the steady Navier–Stokes equations with directional do-nothing boundary conditions (hybrid talk)*, June 14.
99. R. Soares dos Santos, Universidade Federal de Minas Gerais (UFMG), Departamento de Matemática, Brazil, *Ballistic random walk on the zero-range process*, May 24.
100. M. Spindler, Universität Hamburg, Fakultät BWL, *High-dimensional L2-boosting: Rate of convergence (hybrid talk)*, November 29.

101. R. Stoica, Université de Lorraine, Faculté des Sciences et Technologies, Nancy, France, *Random structures and patterns in spatio-temporal data: probabilistic modelling and statistical inference (hybrid talk)*, February 1.

102. Th. Tenzler, Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, *Simulation of the generation of entangled photons through spontaneous parametric down conversion in Bragg-reflection-waveguide lasers based on AlGaA*, November 30.

103. A. ter Elst, University of Auckland, Department of Mathematics, New Zealand, *Kato's inequality and degenerate elliptic operators (hybrid talk)*, February 22.

104. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, Romania, *Topology optimization and boundary observation for clamped plates*, October 31.

105. E.S. Titi, University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK, *The inviscid primitive equations and the effect of fast rotation (hybrid talk)*, July 7.

106. Y. Tokushige, The University of Manchester, Department of Mathematics, UK, *Scaling Limits of SRWs on the long-range percolation cluster*, July 6.

107. P. Tolksdorf, Johannes Gutenberg-Universität Mainz, FB 08: Physik, Mathematik und Informatik, L^p *-extrapolation of the generalized Stokes operator (hybrid talk)*, February 8.

108. F. Tröltzsch, Technische Universität Berlin, Institut für Mathematik, *Optimal control of partial differential equations – Selected results and recent trends*, November 1.

109. O. Tse, Eindhoven University of Technology, Mathematics and Computer Science, Netherlands, *Scharfetter–Gummel for aggregation-diffusion equations: Gradient structures and their limits (hybrid talk)*, January 11.

110. D. Turaev, Imperial College London, Faculty of Natural Sciences, Department of Mathematics, London, UK, *Chaos in reversible homoclinic tangles*, August 3.

111. R.A. Vandermeulen, Technische Universität Berlin, Berlin Institute for the Foundations of Learning and Data (BIFOLD), *Beating the nonparametric curse of dimensionality using multi-view density estimators (hybrid talk)*, April 4.

112. M. Vetter, Christian-Albrechts-Universität zu Kiel, Sektion Mathematik, *On goodness-of-fit testing for point processes*, July 12.

113. I. Voulis, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *Optimality of adaptive stochastic Galerkin methods for affine-parametric elliptic PDEs*, January 26.

114. K. Waghmare, École Polytechnique Fédérale de Lausanne, Chaire de Statistique Mathématique, Switzerland, *Functional graphical lasso (hybrid talk)*, June 28.

115. D. Walter, Humboldt-Universität zu Berlin, Institut für Mathematik, *Nonsmooth minimization in infinite dimensional spaces meets sparse dictionary learning (hybrid talk)*, May 23.

116. S. Wang, Humboldt-Universität zu Berlin, Institut für Mathematik, *Statistical convergence rates for transport- and ODE-based generative models*, November 8.

117. F. Yang, Eidgenössische Technische Hochschule Zürich, Computer Science Department (D-INFK), Switzerland, *Surprising failures of standard practices in ML when the sample size is small (hybrid talk)*, July 11.

A.13 Software

ALEA – Framework for high-dimensional functional Uncertainty Quantification (contact: M. Eigel, phone: +49 30/20372-413, e-mail: martin.eigel@wias-berlin.de)

ALEA is an open source library for research in new methods for Uncertainty Quantification (UQ). Its focus lies on functional spectral methods on the basis of polynomial chaos expansions and the treatment of high-dimensional discretizations. For this, adaptive sparse grid techniques and tensor-based low-rank formats are incorporated. Apart from stochastic forward problems (PDEs with random data), methods for (sample-free) Bayesian inverse problems are available.

AWS – Adaptive Weights Smoothing (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@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/

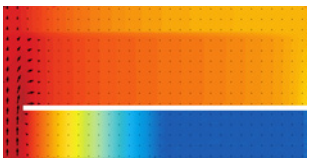
BALaser (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.radziunas@wias-berlin.de)

`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. When required, the traveling-wave-model-based solver is self-consistently coupled to the quasi-three-dimensional inhomogeneous current-spreading and heat-flow solvers, both developed using the WIAS `pdelib` toolkit.

More information: https://www.wias-berlin.de/software/balaser/

ddfermi (contact: 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, P. Farrell, phone: +49 30/20372-401, e-mail: patricio.farrell@wias-berlin.de)

`ddfermi` is an open-source software prototype that simulates the carrier transport in classical or organic semiconductor devices based on drift-diffusion models.



Current density for single photon system

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/.

ParMooN (contact: A. Caiazzo, phone: +49 30/20372-332, e-mail: alfonso.caiazzo@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 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.

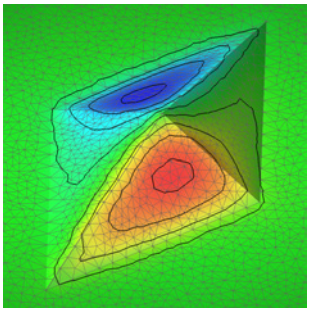
ParMooN is a joint development with the group of Prof. S. Ganesan (IISc Bangalore) and the group of Prof. G. Matthies (TU Dresden).

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, T. Streckenbach, phone: +49 30/20372-476, e-mail: timo.streckenbach@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/.



Displacement (y-component) from FEM simulation of elastic relaxation of a pyramidal InAs quantum dot with a rhomboidal base in GaAs matrix. Used as input for TEM image simulation.

PDELib.jl (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, T. Streckenbach, phone: +49 30/20372-476, e-mail: timo.streckenbach@wias-berlin.de, Ch. Merdon, phone: +49 30/20372-452, e-mail: christian.merdon@wias-berlin.de)

PDELib.jl is being developed as the successor of pdelib in the Julia programming language. It is a collection of open source Julia packages dedicated to the handling of sparse matrices, mesh generation, and visualization. It wraps the Julia package VoronoiFVM.jl that implements the Voronoi box-based finite volume method for nonlinear systems of partial differential equations and the Julia package GradientRobustMultiPhysics.jl implementing gradient-robust finite element methods in Julia.

Please see also https://github.com/wias-berlin/pdelib.jl.

TetGen (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@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. Based on recent research on fundamental algorithms for the generation of tetrahedral meshes, the new version 1.6 provides improvements with respect to the quality of the created meshes and the speed for their creation.

More information is available at https://www.wias-berlin.de/software/tetgen/.

WavePacket (contact: B. Schmidt, phone: +49 30/20372-536, e-mail: burkhard.schmidt@wias-berlin.de)

WavePacket is an open-source MatLab program package for numerical quantum mechanics. It can be used to solve single or coupled time-independent or time-dependent (linear) Schrödinger and Liouville–von Neumann equations, as well as classical or quantum-classical Liouville equations. Optionally accounting for the interaction

with external electric fields within the semiclassical dipole approximation, WavePacket can be used to simulate modern experiments involving ultrashort light pulses in photo-induced physics or chemistry, including quantum optimal control. WavePacket offers visualization of quantum dynamics generated "on the fly," and it comes with numerous demonstration examples.

Please see also https://sourceforge.net/projects/wavepacket/.

WaveTrain (contact: B. Schmidt, phone: +49 30/20372-536, e-mail: burkhard.schmidt@wias-berlin.de)

WaveTrain is an open-source Python software for numerical simulations of chain-like quantum systems with nearest-neighbor (NN) interactions only. It is centered around tensor train (TT, or matrix product) representations of quantum-mechanical Hamiltonians and (stationary or time-evolving) state vectors. WaveTrain builds on the Python tensor train toolbox scikit_tt, which provides efficient construction methods, storage schemes, as well as solvers for eigenvalue problems and linear differential equations in the TT format. Those are used in WaveTrain to solve the time-independent and time-dependent Schrödinger equations employing low-rank TT representations, thus mitigating the curse of dimensionality.

Please see also https://github.com/PGelss/wave_train/.

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 were 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 the new code and the support of running projects.

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 and or with an inversion recovery sequence, including 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).