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Intelligent solutions for complex problems

Annual Research Report 2024

Cover figure: The plot shows a top-down view of the pointwise error between a neural network–based solution of a 2D obstacle problem and the exact solution. The underlying method relies on a novel min–max optimization strategy that in particular enables the derivation of rigorous error bounds. The approach illustrates the potential of neural network methodologies to deliver certified solutions for variational inequality problems.

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The Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Leibniz Institute within the Forschungsverbund Berlin e.V. (FVB), a member of the Leibniz Association, presents its annual research report for 2024.

Prof. Michael Hintermüller, Director

A landmark event for WIAS in 2024 was the Evaluation by the Leibniz Association. It culminated in an on-site visit of an international review board including representatives from the funding bodies in June. After two intense days of presentations, discussions, and interviews, the board appeared impressed by the overall development of WIAS since the last routine Evaluation in 2017, as well as by the research and administrative excellence of the institute. The official decision by the corresponding Leibniz Senate on the Evaluation outcome including a recommendation for future funding came on March 18, 2025, and the Evaluation report was very positive.

In 2024, WIAS also renewed its Research Program for the upcoming three-years period by passing a corresponding document through the institute's Scientific Advisory Board. Building on WIAS's strengths in conducting cutting-edge, project-oriented research in applied mathematics inspired by pressing problems of our times, particularly data-driven approaches including machine learning and artificial intelligence gain more and more traction.

Based on the research strategy emanating from the WIAS Research Program, numerous third-party-funded projects could be secured. WIAS is a central partner of the newly established Collaborative Research Center / Transregio 388 *Rough Analysis, Stochastic Dynamics and Related Fields*. The Funding Atlas 2024 of the German Science Foundation DFG displays WIAS on top of the ranking in the natural sciences among all Leibniz, Max Planck, and Fraunhofer institutions in terms of participation in DFG-funded collaborative programs. The DFG supported WIAS's projects with an amount of 11.1 million euros in the period 2020–2022, which constitutes rank 5 among all Leibniz institutions. In 2024, funded by the Einstein Foundation Berlin, the WIAS co-organized the Thematic Einstein Semester "Mathematics for Quantum Technologies" that shed light on the mathematical aspects of the rapidly developing fields of quantum information processing, quantum cryptography, and quantum metrology. In the course of this six-months-long program, young researchers and experienced scientists from mathematics, theoretical physics, engineering, and related disciplines met and exchanged ideas in a number of workshops, a summer school, and further activities. Finally, the follow-up application of the Cluster of Excellence MATH+, Berlin's Mathematics Research Center, was submitted in cooperation with the Freie Universität Berlin, Humboldt-Universität zu Berlin, Technische Universität Berlin, and the Zuse Institute Berlin. The decision on continued funding is expected for May 2025.

WIAS hosts the Secretariat of the International Mathematical Union (IMU), which supported the organization of the 15th International Congress on Mathematics Education (ICME), which took place in Sydney in July 2024 in a major event with around 3,000 participants.

Among the many outstanding scientists at WIAS, it was a pleasure to see that Dr. Alexandra Quitmann (formerly Research Group 5 *Interacting Random Systems*) received the Marthe Vogt Award of the FVB for outstanding young female scientists. In her dissertation "Phase transitions in random loop models," she addressed Bose–Einstein condensates, an important problem class in statistical physics. Moreover, the International Society for the Interaction of Mechanics and Mathematics (ISIMM) awarded its 2024 Medal to Prof. Dr. Alexander Mielke, the former head of the Research Group 1 *Partial Differential Equations* and Honorary Member of WIAS.

Another wonderful occasion for celebration was the inauguration of the Iris Runge Program in March 2024. Under its umbrella, various equality measures at WIAS are bundled to promote the career of female scientists.

Unfortunately, also the sad side of life overshadowed the institute's community in 2024: We mourned the loss of the former head of the WIAS Research Group 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, Prof. Dr. Wolfgang Dreyer. His wonderful personality and his scientific spirit live on in our memories and in the science of WIAS.

Berlin, in May 2025

M. Hintermüller

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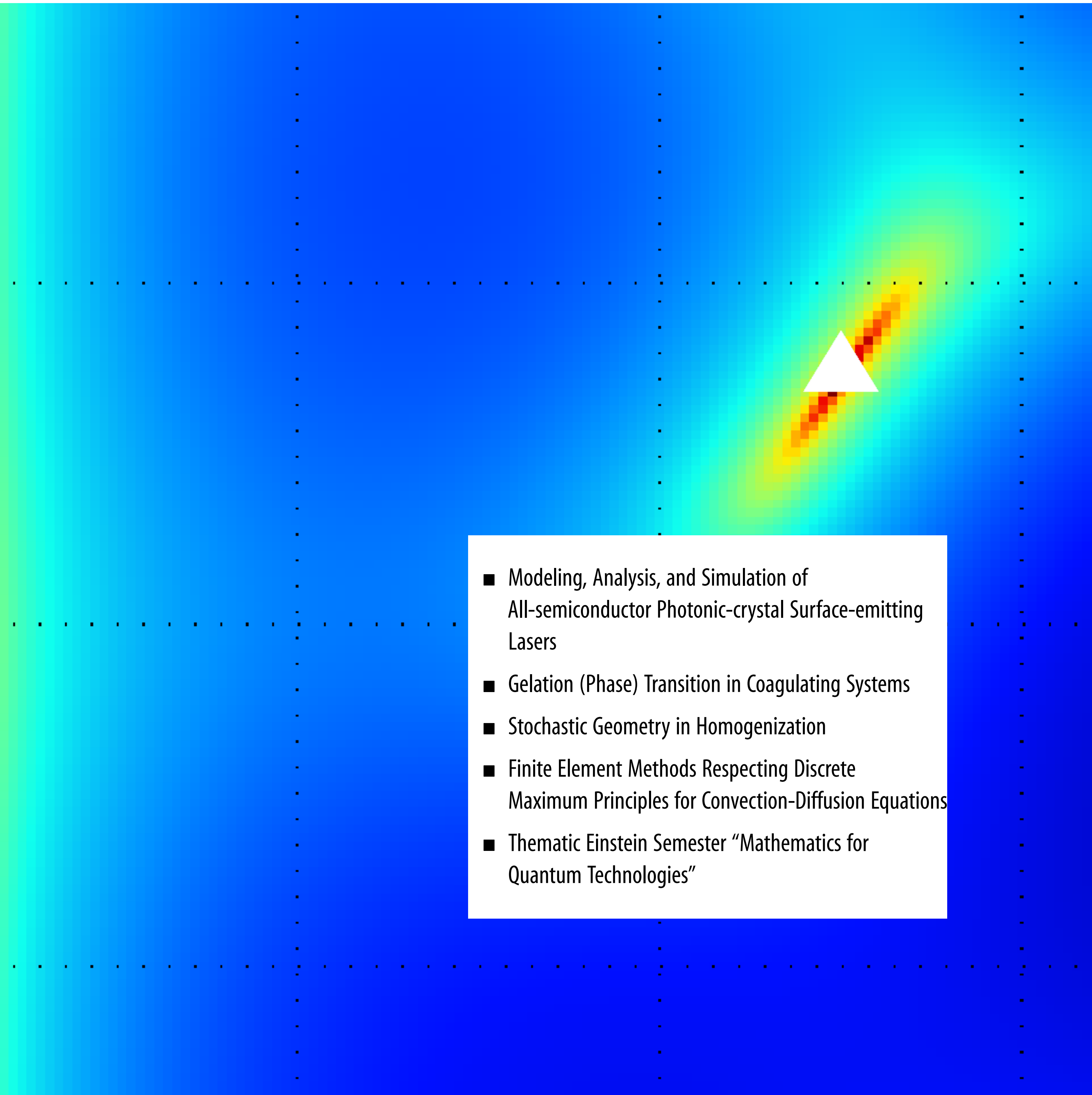
1 Scientific Highlights



- Modeling, Analysis, and Simulation of All-semiconductor Photonic-crystal Surface-emitting Lasers
- Gelation (Phase) Transition in Coagulating Systems
- Stochastic Geometry in Homogenization
- Finite Element Methods Respecting Discrete Maximum Principles for Convection-Diffusion Equations
- Thematic Einstein Semester “Mathematics for Quantum Technologies”

1.1 Modeling, Analysis, and Simulation of All-semiconductor Photonic-crystal Surface-emitting Lasers

Mindaugas Radziunas and Eduard Kuhn

Semiconductor lasers (SLs) are compact, efficient, durable, and cost-effective devices used in various modern applications. Among these, material processing often demands optical power up to several kilowatts. High-power edge-emitting SLs, commonly used for such purposes, face challenges like large asymmetric beam divergence and poor lateral beam quality due to multiple lateral optical modes contributing to laser emission. In 1999, Prof. Susumu Noda (Kyoto University) proposed the Photonic-Crystal (PC) surface-emitting laser (SEL), shown schematically in Figure 1. These SLs consist of multiple thin layers, most of which are uniform in two lateral directions. The vertical structure ensures the selection of a single vertical transverse-electric optical mode. Near the active zone, a PC layer induces a two-dimensional (2D) band-edge resonant effect, enabling both light amplification and surface emission. PCSELs are remarkable for their large-area, low-divergence emission ($< 1^\circ$) defined by a single or few optical modes. High-power PCSELs can achieve emission levels of several tens of watts, rivaling the best single high-power *edge-emitting* SLs. Modern PCSELs utilize PCs formed by periodic air voids in both lateral directions within the semiconductor material. As a part of the Leibniz Collaborative Excellence project PCSELence, we are collaborating with the Ferdinand Braun Institute (FBH) in Berlin to design a comparable PCSEL with an all-semiconductor PC layer. This innovation could significantly enhance both the efficiency and manufacturability of PCSELs.

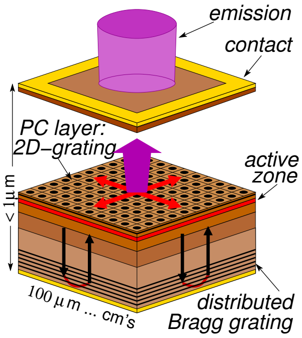


Fig. 1: *Schematics of photonic-crystal surface-emitting semiconductor laser*

Dynamic model, spectral problem, and numerical challenges

Model equations. The above-threshold behavior of PCSELs is described by a dynamic model based on three-dimensional coupled-wave theory. The field equations are represented by a system of four linear partial differential equations (PDEs) in one temporal and two spatial dimensions within the lateral domain $Q_{\mathrm{L}} = [0, L] \times [0, L]$:

$$\partial_t \Psi(x, y, t) = v_{\mathrm{g}}\Big[i(\mathbf{C} - \Delta\beta) - \begin{pmatrix} \sigma\partial_x & 0 \\ 0 & \sigma\partial_y \end{pmatrix}\Big]\Psi + \mathbf{F}_{\mathrm{sp}}, \quad (x, y) \in Q_{\mathrm{L}}, \quad \sigma \overset{\mathrm{def}}{=} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

These equations are derived using lateral Fourier expansions of the transverse-electric polarized field $\mathbf{E}(\mathbf{r}) = (E_x(\mathbf{r}), E_y(\mathbf{r}), 0)^T$ and the squared refractive index, $n^2(\mathbf{r}) = \sum_{\mathbf{s}\in\mathbb{Z}^2} \xi_{\mathbf{s}}(z) e^{-i2\pi(s_1x+s_2y)/a}$, where a is the lattice constant of the PC. Four basic Fourier modes, $E_{y,(\pm1,0)}$ and $E_{x,(0,\pm1)}$, define the complex, slowly varying field amplitudes (Ψ_1, Ψ_2) and (Ψ_3, Ψ_4). These functions satisfy non-reflecting boundary conditions (BCs) at the edges of Q_{L} and form the vector function Ψ. L, v_{g}, $\Delta\beta$, $\mathbf{C}$, and $\mathbf{F}_{\mathrm{sp}}$ in (1) are the lateral size, group velocity, local change of the propagation factor, field coupling matrix, and stochastic spontaneous emission term, respectively [1]. In hot-cavity PCSELs, $\Delta\beta(x, y, t) = \frac{i}{2}[g - \alpha] + \Delta_n$ is a complex spatially distributed function. It accounts for the instantaneous local values of optical gain g, losses α, and refractive index-induced correction Δ_n, all of which depend on the local carrier density, governed by a diffusive carrier rate equation [1, 2]. More advanced models should also account for the gain dispersion, with additional equations to model the frequency dependence of g and Δ_n [WIAS Preprint no. 809], self-heating effects, including three-dimensional heat transport equations for the entire PCSEL structure [WIAS Preprint no. 2558], and current spreading, defined by a three-dimensional Laplace equation with inhomogeneous BCs [WIAS Preprint no. 2421].

Construction of the field coupling matrix. The coupling of counter- and cross-propagating fields in (1) is realized through a complex (4×4) field coupling matrix, $\mathbf{C} = \mathbf{C}^{(1D)} + \mathbf{C}^{(RD)} + \mathbf{C}^{(2D)}$. The Hermitian submatrices $\mathbf{C}^{(1D)}$ and $\mathbf{C}^{(2D)}$ define one-dimensional coupling of basic waves and two-dimensional coupling from higher-order Fourier modes. The non-Hermitian $\mathbf{C}^{(RD)}$ represents the out-of-plane coupling to radiative waves, $E_{x,\mathbf{0}}$ and $E_{y,\mathbf{0}}$, determining laser emission. To define these matrices, we use i) the complex Fourier coefficients $\xi_{\mathbf{s}}(z)$ of the PC features (see, e.g., Figure 2(a)–(c)); ii) the vertical mode $\Theta(z)$ and respective effective refractive index (solid violet and black dashed lines in Figure 2(d), both defined by the vertical structure, red dots in the same panel); iii) the Green's functions $G_{\mathbf{s}}(z,z')$, which solve inhomogeneous Helmholtz problems and represent Fourier modes $E_{x,\mathbf{s}}$ and $E_{y,\mathbf{s}}$.

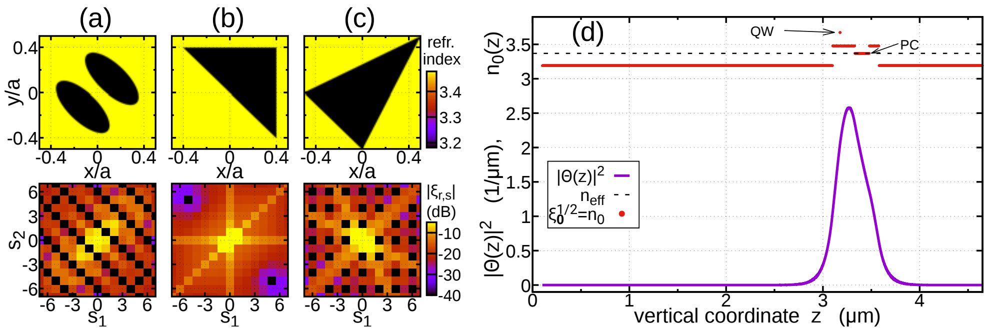


Fig. 2: Defining structure of PCSELs. (a)–(c): Refractive indices within a unit PC cell (top) and $|\xi_{\mathbf{s}}|$ of leading Fourier coefficients (bottom). (d): Laterally-averaged (red) and effective (black dashed) refractive index, and vertical mode intensity (violet) along the vertical direction.

We cannot use fully numerical algorithms to construct the submatrix $\mathbf{C}^{(2D)}$ because integrating the rapidly growing/decaying parts of $G_{\mathbf{s}}$ with moderate $|\mathbf{s}| \approx 10$ requires very fine numerical meshes, leading to huge computational times. Fortunately, within vertical layers, $G_{\mathbf{s}}$ and Θ can be represented by exponentials, allowing all required integrals to be solved analytically. However, direct use of analytic formulas can cause large- and small-number-related arithmetic issues, even at moderate $|\mathbf{s}| \approx 25$, and more so at ≈ 200. After resolving these problems [3], we can construct $\mathbf{C}$ for typical PCSELs using Fourier modes with $|\mathbf{s}| \leq 500$ in just a few seconds.

Spectral problem. The substitution of $\Psi = \Theta(x,y)e^{i\Omega t}$ into (1) yields the spectral problem

$$\begin{pmatrix} \sigma\partial_x & 0 \\ 0 & \sigma\partial_y \end{pmatrix}\Theta(x,y) = i[\mathbf{C} - (\Delta\beta + \tfrac{\Omega}{v_g})]\Theta, \quad (x,y) \in Q_L, \quad \textbf{+ BCs}. \tag{2}$$

For cold-cavity PCSELs with vanishing $\Delta\beta$, the imaginary and real parts of complex eigenfrequencies, $\Im\Omega$ and $\Re\Omega$, respectively, provide key information on the optical gain needed to excite the corresponding mode and its relative frequency. The enhanced threshold gain separation $\frac{2\Im(\Omega_1-\Omega_0)}{v_g}$ between the fundamental mode with smallest $\Im\Omega$ and the first higher-order mode (second smallest $\Im\Omega$) suggests potential single-mode operation in well pumped (hot-cavity) PCSELs. In contrast to the spectral problems in narrow-waveguide edge-emitting lasers [WIAS Preprint no. 939], exact

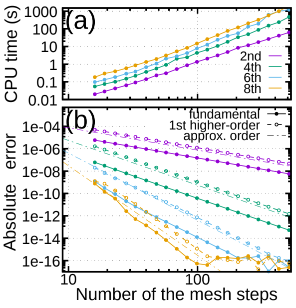


Fig. 3: *CPU time (a) and main mode precision (b) as functions of the mesh step number for various precision order schemes*

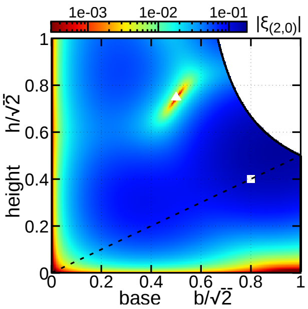


Fig. 4: *Factors $|\xi_{(2,0)}|$ in all non-overlapping isosceles triangles. Dashed: RITs. White box and triangle: Cases shown in Figure 2(b) and (c).*

solutions of (2) are not available. To approximate the most important modes, we replace the continuous problem with a finite difference scheme [3]. In [3, 4, 5], we showed that relatively coarse numerical meshes and simple second-precision-order schemes can provide good approximations of the most important eigenfrequencies. Precision can be improved by using higher-order precision schemes and/or refining the meshes for a few selected modes, as shown in Figure 3 and [3].

Tailoring all-semiconductor PCSELs

Compared to the air-void-based PCs in modern PCSELs, all-semiconductor PCs have a lower refractive index contrast. This results in relatively weak field coupling terms in $\mathbf{C}$, meaning light generation requires larger PC features and PCSELs ($L \geq 1$ mm). Additionally, due to technological challenges, well separated features are preferred. Therefore, instead of dual lattice configurations like in Figure 2(a), simpler large triangle PC features are favored, as shown in Figure 2(b) and (c).

PCs with isosceles triangular features. Using diagonally-symmetric features, as shown in Figure 2(a)–(c), simplifies the matrix $\mathbf{C}$ and leads to analytic expressions for its eigenvalues $\Omega_{\mathbf{C}}$. In particular, all $\Im\Omega_{\mathbf{C}}$ are defined by combinations of only a few entries of the coupling matrices, specifically $\Im\mathbf{C}^{(\mathrm{RD})}_{1,1}$ and $[\mathbf{C}_{1,2} \pm \mathbf{C}^{(2\mathrm{D})}_{1,4}]e^{-i2\arg\xi_{(1,0)}}$. $\Omega_{\mathbf{C}}$ serve as accumulation points for the eigenfrequencies Ω in large cold-cavity PCSELs, providing an approximation for the gain of the fundamental mode. Thus, when designing PC features, we should aim for large $|\xi_{(1,0)}|^2$ (a prefactor of $\mathbf{C}^{(\mathrm{RD})}$) and adjust $\arg\xi_{(1,0)}$. Additionally, to prevent the dominance of $\mathbf{C}^{(1\mathrm{D})}_{1,2}$ in the overall one-dimensional coupling factor $\mathbf{C}_{1,2}$, $\xi_{(2,0)}$ (a prefactor of $\mathbf{C}^{(1\mathrm{D})}$) should be kept small. Isosceles triangles, characterized by the length b and the height h along the diagonal of the unit cell, are the simplest nontrivial diagonally-symmetric features. The factors $\xi_{(1,0)}$ and $\xi_{(2,0)}$ for these features can be expressed as analytic functions of b and h, as shown in Figure 4, where $|\xi_{(2,0)}(b,h)|$ is plotted. The dashed line represents right isosceles triangles (RIT), considered in early works on small PCSELs with air-void-based PCs. Regions above and below this line correspond to acute and obtuse triangles, while the empty region in the upper right corner indicates large triangles that overlap with neighboring PC features. The white box in the diagram represents an RIT with a side length of $0.8a$, as shown in Figure 2(b). Among other RITs, it exhibited the most desirable $L = 0.8$ mm-PCSEL characteristics at the lasing threshold [1]. The white triangle in Figure 4 marks a special stretched isosceles triangle (SIT) from Figure 2(c), where $\xi_{(2,0)}$ vanishes. This makes PCs with this SIT comparable to dual-lattice PCs, as seen in the lower panels of Figure 2(a) and (c).

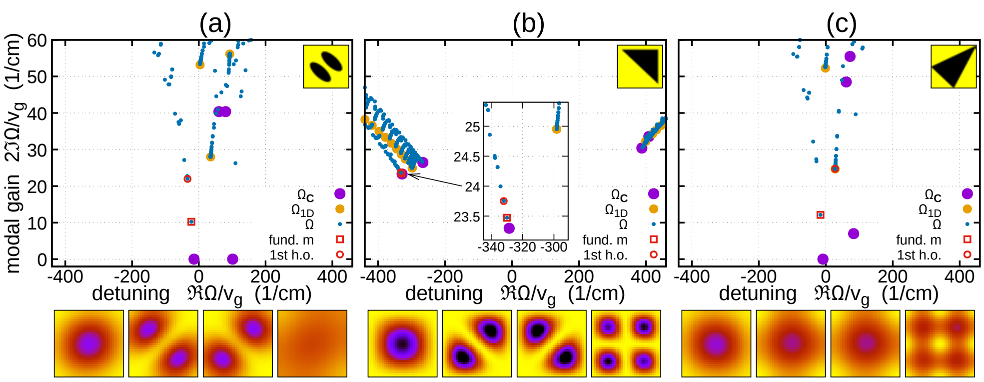


Fig. 5: *Mode calculations for three $L = 1$ mm PCSELs defined in Figure 2. Top: Eigenfrequencies Ω (blue), 1D modes in the decoupled system (orange), and $\Omega_{\mathbf{C}}$ (violet). Red box and circle: The fundamental and 1st higher-order modes. Bottom: Intensity distributions $|\Theta(x,y)|^2$ for four main modes in each case.*

Cold-cavity PCSELs. In Figure 5, mode calculations are shown for three cold-cavity $L = 1$mm-PCSELs from Figure 2. For the optimized RIT-PC-based PCSEL (panel b), four violet bullets Ω_C and orange bullets Ω_{1D} (one-dimensional modes of (2) with neglected cross-propagating field coupling [3, 5]) act as accumulation points for eigenfrequencies Ω (blue dots). Similar modal gain values suggest multimode operation of the well-biased PCSELs. In contrast, dual-lattice-PC-based (a) and special SIT-PC-based (c) PCSELs exhibit large threshold gain separation between two main modes (red circle and box), predicting single-mode operation with strong side-mode suppression in hot-cavity PCSELs. Both of these configurations have their drawbacks. First, the imaginary part of the leading Ω_{C0} is almost zero in both cases, leading to weak vertically outcoupled and emitted field intensity. The desired increase of $\Im\Omega_{C0}$ can be achieved by introducing deviations from the ideal dual-lattice or special SIT [2, 6] configurations. Second, the large separation between the fundamental Ω_0 and the leading Ω_C results in significant field leakage through the lateral borders, weakening the fields in the central part of the PC domain. This flattening of mode intensity is evident in the lower panels of Figure 5(a) and (c), compared to (b). Field leakage can be mitigated (at the cost of reduced modal gain gap) by increasing the lateral size L of the device.

Dynamic simulations. In all examples above, we considered modes in cold-cavity PCSELs. This means that discussions on single-mode lasing and side-mode suppression apply mainly near the lasing threshold, where the propagation factor $\Delta\beta$ in (1) and (2) remains spatially uniform. However, at high-power regimes, spatial hole burning of carriers, inhomogeneous pumping, and self-heating cause $\Delta\beta(x, y)$ to become non-uniform. This leads to significant changes in the calculated eigenfrequency landscape. To determine if single-mode lasing is achievable, we performed transient simulations using the full dynamic model for PCSELs.

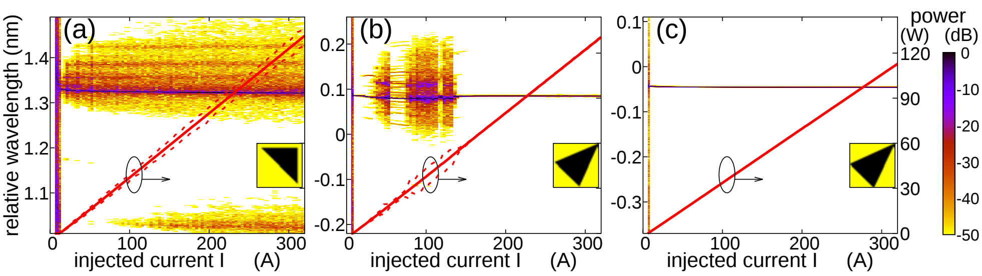


***Fig. 6:** Optical spectra (color maps) and emitted power (red lines) for $L = 2$mm PCSELs as functions of up-tuned bias current. Panels (a), (b), and (c) depict PCSELs with RIT- and two different SIT-based PCs.*

In Figure 6, we present simulations of three $L = 2$mm-PCSELs with an optimal RIT-based and slightly differing SIT-based PC layers. The vertical laser structure is defined in Figure 2(d) and [1]. Due to the small threshold gain separation in the cold-cavity device, the RIT-based laser (panel a) demonstrates multimode emission for all bias currents. In contrast, both SIT-based lasers exhibit the desired single-mode lasing. In case (b), where multimode lasing occurs within a limited bias current range, the SIT choice was made to increase emitted power (i.e., increase $\Im\Omega_0$) while maintaining a decent mode threshold gap in the cold-cavity laser. The emission power from this device is comparable to that of the optimized RIT-based laser. On the other hand, SIT features in case (c), also discussed in [6], were selected to improve side-mode suppression, but resulted in a reduced $\Im\Omega_0$. Consequently, our dynamic simulations show perfect single mode emission across the entire bias current range, with a slight decrease in emission power. These results give us confidence that achieving single-mode lasing in large-area all-semiconductor PCSELs with SIT-based PCs is possible.

Conclusions and outlook

In conclusion, we developed a numerical tool capable of efficiently constructing and solving the spectral problem for PCSELs [3, 4, 5]. Simulations and analysis of the field coupling matrix and calculated spectra led us to identify a special large SIT PC feature [6]. This configuration shares properties with conventional dual-lattice features used in modern air-void-based PCSELs and may be advantageous when designing all-semiconductor devices. A patent application for the use of SIT features in PCSELs has been submitted to the German Patent Office. Further improvements in PCSELs can be achieved by integrating the Bragg grating layers, tuning their separation from the active layer [6], modifying the vertical structure, or using alternative, more complex features with properties similar to those of the above considered SITs. Our first dynamic simulations [2] predict that large ($L \geq 2$mm) PCSELs with SIT-based all-semiconductor PCs should maintain good side-mode suppression. In contrast to our earlier work with RIT-based PCSELs [1], these should demonstrate the desired single-mode emission. Further simulations, using advanced models accounting for self-heating in PCSELs, will be conducted later within the PCSELence project. It remains to be seen whether the all-semiconductor PCSELs being built at the FBH will demonstrate the expected single-mode emission.

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1.2 Gelation (Phase) Transition in Coagulating Systems

Heide Langhammer and Dirk Peschka

Soft gels and gelation: Macroscopic and microscopic perspective

Gels are versatile materials that combine physical properties of liquids and solids. Typical examples for gels include gelatin used in food applications, gels and emulsions for medical products, and hydrogels in contact lenses. Hydrogels also play a crucial role in biomedical applications, particularly in tissue engineering, for their biocompatibility and ability to mimic the extracellular matrix, which provides a scaffold and mechanical support for maintaining the structure and function of living tissues. Gels consist of random networks of crosslinked particles, often formed by polymers that connect through entanglements or chemical bonds. These bonds can be created or broken through dynamic processes, allowing the network to adapt and evolve over time. Here, particles are broadly defined to include polymers or clusters of crosslinked polymers.

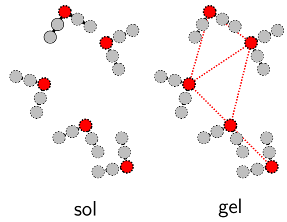

Fig. 1: *Sketch shows gelation transition from uncrosslinked polymers (sol phase) on the left to crosslinked polymers (gel phase) on the right due to the formation of bonds (dotted lines) creating an elastic polymer network*

The transition of a liquid-like suspension of particles, known as a *sol*, into a solid-like structure, called a *gel*, occurs through a process known as *gelation*, as sketched in Figure 1. This process involves the formation of crosslinks between particles, creating a stable and flexible network, i.e. a percolating, dynamic structure with distinctive macroscopic viscoelastic properties. Gels exist in a complex environment shaped by chemical composition, ions and charges, temperature, pH, pressure, and external forces such as mechanical stress or electric fields, all of which influence gelation.

These chemical and physical properties call for a complex mathematical framework for predicting their behavior. Understanding gels and the process of gelation requires a dual approach: examining the reversible and irreversible bonding processes that lead to the creation of polymer (particle) networks, and analyzing the macroscopic transition in viscoelastic properties due to these bonding processes.

Research in the WIAS Main Application Areas Materials Modeling and Flow and Transport focuses on gels as macroscopic systems with distinct mechano-chemical properties. In contrast, the research topic Coagulation emphasizes the microscopic properties of particle systems and the study of their gelation processes via the concept of coagulation. Research at WIAS aims to bridge these approaches by combining the microscopic stochastic particle interpretation with the macroscopic continuum representation of materials, working towards a unified understanding of gelation.

The nature of gelation, whether it constitutes a thermodynamic process driven by energy and entropy or a kinetic process governed by crosslinking rates, remains a subject of debate and connects thermodynamic continuum models with particle-based coagulation models. While thermodynamic approaches emphasize free energy landscapes and kinetic models focus on bond and cluster formation dynamics, combining these viewpoints promises deeper insights into the interplay between the microscopic and the macroscopic perspective.

Continuum approaches for soft visco- and poroelastic gels

Continuum models for soft gels typically involve systems of partial differential equations (PDEs) to describe strongly coupled viscoelastic and poroelastic phenomena. In particular, their softness and swelling, caused by solvents in polymer networks or water in hydrogels, are typically modeled using nonlinear PDEs. In the presence of mechano-chemical effects, such systems are characterized by a free energy

$$\mathcal{F} = \int_\Omega W(F_\mathrm{e}, \varphi, \nabla\varphi)\,\mathrm{d}x,$$

depending on the elastic deformation $F_\mathrm{e} = F F_\mathrm{p}^{-1}$ in a multiplicative decomposition, where F_p describes inelastic effects, $F = \mathbb{I} + \nabla\mathbf{u}$ is the deformation gradient expressed with the displacement $\mathbf{u}$. The dependence on an internal order parameter φ, e.g., representing chemical concentration of solvents or charges, accounts for the influence of a complex environment.

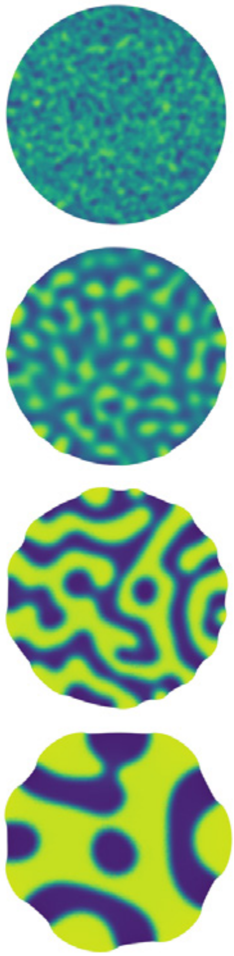

Fig. 2: Visualization of phase separation in a viscoelastic gel progressing over time from top to bottom. The gel exhibits volume changes (swelling), showing distinct swollen (yellow) and contracted (blue) phases. Image adapted from [2].

Minimizers of the free energy can give rise to phase separation and phase transitions, particularly in cases where W is non-convex, leading to highly non-unique minimizers. Consider the energy

$$W(F, \varphi, \nabla\varphi) = \tfrac{G}{2}\big(\mathrm{tr}(\mathbb{C} - \mathbb{I}) - 2\ln(\det F)\big) + \tfrac{\sigma}{2}|\nabla\varphi|^2 + \varphi\ln\varphi + (1-\varphi)\ln(1-\varphi) + \chi\varphi(1-\varphi),$$

where $\mathbb{C} = F^\mathrm{T}F$, G encodes the shear modulus, σ represents an interface term, and the remaining terms describe a Flory–Huggins-type mixing entropy used for polymer mixtures. The parameter χ controls the phase behavior: $\chi < 0$ promotes mixing, while $\chi > 0$ favors phase separation. The irreversible gradient flow dynamics of such a system is governed by a dissipation potential $\Psi^*(q;\eta)$ that describes irreversible effects and leads to an evolution $\partial_t q = \mathrm{D}_\eta\Psi^*(q; -\mathrm{D}_q\mathcal{F}(q))$ where the state $q = (\mathbf{u}, F_\mathrm{p}, \varphi)$ represents elastic displacements and inelastic deformations as well as scalar variables φ, describing an abstract but thermodynamically consistent dissipative dynamic, including phenomena such as viscous friction, viscoelastic relaxation, and phase separation or phase transition of sol and gel phase; see Figure 2. In particular, the bond reformation in the macroscopic gel leads to a relaxation of elastic stresses via the evolution of the inelastic variable F_p.

At WIAS, we have been investigating the energy-driven evolution of gels, proving the well-posedness of the resulting PDEs, modeling gel dynamics such as poroelasticity, phase transitions, and phase separation, as well as developing structure-preserving discretizations—and we continue to advance these research topics. These include finite element methods to approximate functionals in finite-dimensional subspaces, as well as time discretizations that respect the energy dissipation structure [1, 2]. These efforts in RG 1 *Partial Differential Equations* and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions* are aimed at biological applications in biomechanics and biomedicine in collaboration with researchers from Berlin Charité [3]. A key focus is on extending classical Kelvin–Voigt rheology of purely viscous solids to include viscoelastic relaxation of Maxwell type using gradient flows and GENERIC (General equation of non-equilibrium reversible irreversible coupling), to include the reformation of elastic crosslinks, which is joint work with Freie Universität Berlin (Andreas Zafferi) and Charles University Prague (Tomáš Roubíček) in the context of geophysical applications. Furthermore, currently extensions to charged polymers and conductive gels are explored as a natural extension of existing WIAS expertise [4, 5] on analysis, modeling, and simulation of charge transport and gelation on the particle level. The study of the gelation transition, in particular, represents a major milestone in this research with the University of Oxford (Andreas Münch, Sarah Waters), where insights from discrete particle systems are expected to play a critical role.

Particle systems with coagulation

A complementary perspective on the phenomenon of gelation is developed within the research topic Coagulation. In contrast to the continuum approach, the research of RG 5 *Interacting Random Systems* is dedicated to stochastic models that contain individual descriptions of a large number of particles interacting via pairwise coagulations that take place over time. Coagulation refers to the merging of particles into a new particle and is modelled as an irreversible change of the particle system, distinguishing it from the bonding processes we described earlier. Through successive coagulations, increasingly larger structures emerge, which may lead to a gelation transition depending on whether the larger structures are visible on the macroscopic scale: a phenomenon interpretable as either a phase transition influenced by thermodynamic potentials or a kinematic transition governed by the rates of dynamic processes. This duality reflects the interplay between statistical mechanics and particle-level dynamics in gelation processes.

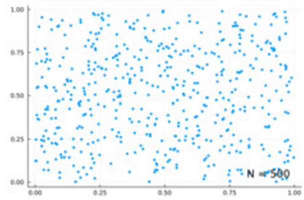

Fig. 3: *Initial configuration of the coagulation process*

When aiming for rigorous results about the *gelation transition*, a tractable model has to be found. A probabilistic approach was chosen, following the idea of Particle-based Modeling, and a stochastic process for coagulation is defined. We neglect the movement of the particles, as well as their spatial extension or viscoelastic properties of the network, focusing instead on two properties: their *mass* and *location* in an abstract state space. The interacting forces that lead to coagulations are captured via a so-called *coagulation kernel*, which is a function determining the rate at which a particle pair merges or forms a bond based on the particle properties. A precise introduction to this model, the so-called *Marcus–Lushnikov process*, is given below.

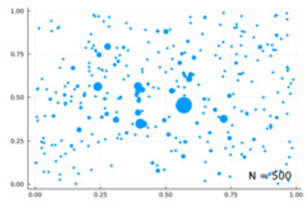

Fig. 4: *Configuration of the coagulation process after several coagulations took place*

Stochastic models for coagulation

The inhomogeneous random graph. A stochastic model for coagulation is given by a random graph, where edges are formed between its vertices over time, such that the clusters (i.e., connected components) of the graph can coagulate due to the addition of an edge. One initializes the process with N unconnected vertices, where each vertex v carries some spatial data $x_v \in \mathcal{S}$. Then, an edge between a vertex pair with data $x, x' \in \mathcal{S}$ appears at rate $\frac{1}{N}\kappa(x, x')$. In Figure 5, we illustrate how the cluster configuration of the graph can change through the addition of an edge. The goal is then to study the evolution of the clusters of the graph for a large number N. We extensively studied this model in [6], where we provide a detailed analysis of the gelation transition that marks the emergence of a *giant* cluster whose number of vertices is proportional to N.

The Marcus–Lushnikov process. The Marcus–Lushnikov process is a stochastic process that models the evolution of particles that undergo successive coagulation events. The particle data is given by a location in an abstract space $\mathcal{S}$ and an integer mass. At time $t \geq 0$, the random configuration of the process is described by the collection $(X_i(t), M_i(t))_{i=1}^{n(t)}$, where $(X_i(t), M_i(t))$ is the data of the i-th particle and the total number of particles at any time t is given by $n(t)$. Initially, the expected number of particles is given by N and each particle carries a mass that is equal to 1. Then, one samples random times for each particle pair that are independent and exponentially distributed. Their parameters depend on the data of the particle pair. More precisely, for a particle pair with data $(x, m), (x', m') \in \mathcal{S} \times \mathbb{N}$ the parameter is given by $N^{-1} K\big((x, m), (x', m')\big)$, where

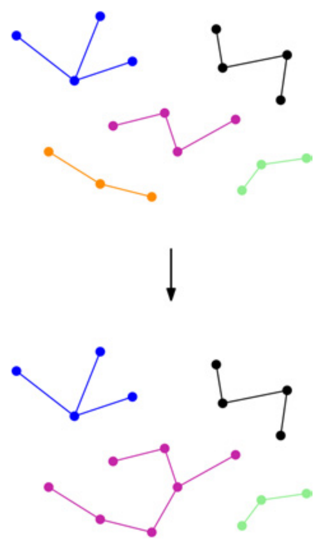

Fig. 5: *Transition of the cluster configuration in the inhomogeneous random graph*

K is the coagulation kernel. The smallest exponential time defines the first coagulation time and triggers a coagulation event. The corresponding particle pair is removed from the configuration and replaced by a new particle. For a coagulating particle pair with data $(x,m),(x',m')$ the new particle is defined to have a mass $m+m'$ and its new location z is sampled according to a distribution $\Upsilon((x,m),(x',m'),\mathrm{d}z)$ depending on the particle data. The transition of the configuration in a coagulation event is illustrated in Figure 6. We call Υ the *placement kernel*. After the transition, the parameters of the exponential times are updated according to the new particle configuration and the procedure is iterated. As mentioned above this model focuses solely on the coagulation mechanism that can be observed in different physical or chemical systems. An obvious choice for the space $\mathcal{S}$ would be $\mathbb{R}^d$, however, various choices are possible. For example, if one wants to model coagulation of molecules, then one can include geometric data or electrical charges into the particle description.

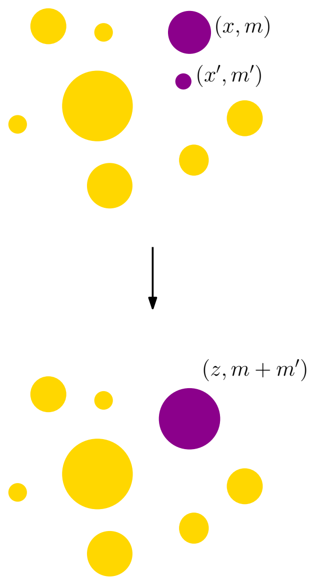

Fig. 6: *Transition of the particle configuration in one coagulation step*

The main example that we have in mind is a coagulation kernel that has the form

$$K\big((x,m),(x',m')\big)=\varphi(x,x')mm',\quad \text{for } (x,m),(x',m')\in\mathcal{S}\times\mathbb{N},$$

where φ is a non-negative continuous function. More precisely, one can think of a function that only depends on the distance of the two particle locations x,x' and is bounded from above. The fact that the kernel grows bilinearly in the masses ensures that the interaction rate with particles of large masses grows sufficiently fast, as their mass grows. From easier, i.e. non-spatial, versions of the model it is known that this is the regime where gelation can be observed.

The *Marcus–Lushnikov process* is the empirical process $\Xi^{(N)}=(\Xi_t^{(N)})_{t\geq 0}$, where, for $t\geq 0$,

$$\Xi_t^{(N)}=\sum_{i=1}^{n(t)}\delta_{(X_i(t),M_i(t))}\quad\in\mathcal{M}(\mathcal{S}\times\mathbb{N}) \tag{1}$$

is the empirical measure registering the particle data at time t. For a large number of initial particles, i.e. for the limit, as $N\to\infty$, one is interested in understanding the limit of $\frac{1}{N}\Xi^{(N)}$.

Large deviations approach to gelation

The usual approach to study the Marcus–Lushnikov process builds on its construction as a continuous-time Markov chain and aims to show that its limit, as $N\to\infty$, follows a certain dynamics, which can be described via a system of differential equations, called the *Smoluchowski equation*. However, it is known that this equation does not always have a solution, which is related to the possibility that after a finite time large particles are formed whose mass diverges as $N\to\infty$. If their masses make up a non-trivial portion of the entire mass in the system, we call the collection of those particles the *gel*. Unfortunately, the gel's influence on the system's dynamics is not captured in the Smoluchowski equation, and an extension of the equation is only possible in certain cases, giving the *Flory equation* or *modified Smoluchowski equation*.

We resort to an approach that describes all possible evolutions of the particle system by carefully studying the limit of the distribution of the process with the help of Large Deviations. A main challenge consists in finding a suitable description of the distribution and was solved in our work

[7] via a statistical mechanics approach that has not been used in that way before.

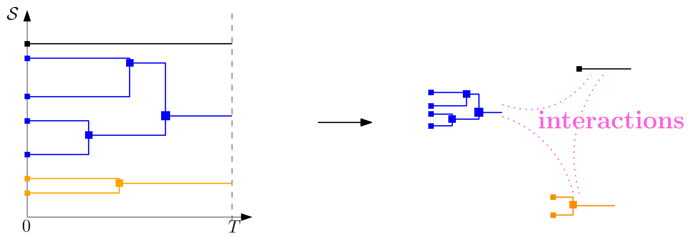

Fig. 7: *Illustration of the decomposition of the process into three interacting coagulation trees*

The key is to decompose the coagulation process into certain sub-processes, called *coagulation trees*, each of which tracks the evolution of particles that have coagulated by a fixed time T into one particle, see Figure 7. Thus, we reinterpret the outcome of the coagulation process on the time interval $[0, T]$ as interacting coagulation trees that are sampled according to a certain distribution. They *interact* with each other via an interaction cost that corresponds to the probability that none of the particles in distinct trees have coagulated during $[0, T]$. This approach is not only novel, but it is useful for deriving a large-deviations principle that describes the limit of the distribution of $(\frac{1}{N}\Xi_t^{(N)})_{t\in[0,T]}$, as $N \to \infty$, on an exponential level. Let us explain briefly how the theory of large deviations sheds light on gelation. Indeed, it can be used to identify the optimal state of the system that can be observed with high probability, as $N \to \infty$. If the optimal state only consists of particles of finite mass, as $N \to \infty$, then gelation did not occur, while otherwise gelation did occur.

Conclusions and outlook

In our work on PDEs for gels, we analyze and discretize models that incorporate poroelastic and viscoelastic properties grounded in thermodynamic principles [1, 2]. Moving forward, we aim to extend these models to account for more complex macroscopic aspects of gelation. In our work on the Marcus–Lushnikov process [7], we employ the large-deviations approach to derive criteria for gelation that depend on upper and lower bounds on the coagulation kernel. In our previous study on the inhomogeneous random graph [6], we were even able to determine a precise time of gelation and found a description of the spatial configuration of the macroscopic cluster. Several extensions of the model can be the subject of further investigations, e.g., allowing for fragmentation or movement of the particles.

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1.3 Stochastic Geometry in Homogenization

Martin Heida, Benedikt Jahnel, and Anh Duc Vu

The modern world has brought numerous technological advancements in a wide variety of fields, many of them dependent on the proper design of new materials, especially composites. First of all, the demand for specialized, high-performance materials is ever increasing as more and more use cases emerge; think of light-weight but sturdy wings for airplanes or degradation-resistant but efficiently functioning photovoltaic cells. The use of compound substances is almost ubiquitous here as many contrasting properties have to be combined. But also for less spectacular everyday life applications, we increasingly depend on a profound understanding of our materials across all ranges of size, since the scale at which we employ these materials is massive. The Hoover dam is a prominent and almost a century-old example, where the underlying geometric structure, like the steel beams inside the concrete or the microstructure of the concrete itself, has a tremendous impact on the stability of the entire object. Hence, a deeper understanding of not only the underlying materials but also the emerging macrostructures of these materials becomes necessary.

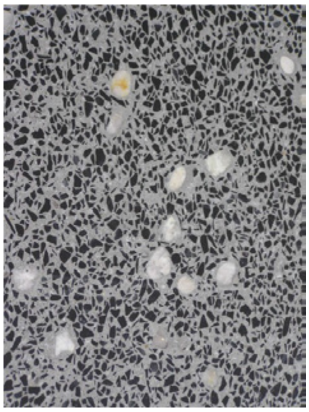

Fig. 1: *Polished concrete surface. Coarse black basalt is embedded in gray cement.*

A *concrete* example: Concrete is a mixture of cement, sand, and gravel, see Figure 1. At the same time, it is a perfect example of a porous medium: If not properly sealed, air and water, along with various aggressive chemicals, can penetrate deep into the material, slowly eroding it over time. This becomes problematic, for example, in bridges, sewage pipes, or dams, as the material eventually will erode even if sealed. To analyze the behavior of this mixture, one could try to track every single grain of sand and gravel and every pore in numerical simulations, but that would be way too complicated and time consuming. On the other hand, mathematical homogenization lets us simplify this problem by *averaging out* the tiny details of the material and look at it on a larger scale. Instead of focusing on each individual grain, we treat the concrete as if it were a single, uniform material with average properties. This method is extremely useful since

- it allows for simpler calculations as we only have to deal with one *averaged* substance now.
- In turn, this helps us to predict the macroscopic behavior of the compound material.

Such composite structures are common not only in engineered materials, but also in the natural world like volcanic rocks. Unfortunately, this *averaging out* proves to be far from simple. The effective physical properties of a composite material cannot be obtained by simple averaging over its constituents. Instead, we find that the underlying microscopic structure plays a vital role.

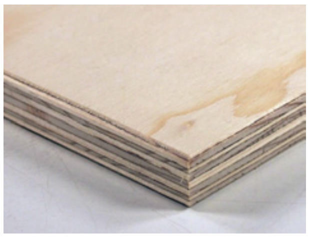

Fig. 2: *Plywood consisting of multiple horizontal wooden layers.* `https://commons.wikimedia.org/wiki/File:Spruce_plywood.JPG`

A brief introduction to homogenization

The goal of mathematical homogenization is to derive formulas that describe the macroscopic coefficients of the material in terms of their microstructure as well as the macroscopic equations that describe the material's effective behavior. It is important to emphasize that the macroscopic behavior may differ significantly from the microscopic behavior, particularly if certain effects dominate a complex system. A popular example for this is the dominance of friction between water and sand grains when water seeps into ground. This causes the microscopic Navier–Stokes equation to turn into the simple Darcy equation. The prime example that is typically presented to students first is the stationary diffusion equation

$$-\nabla \cdot \left(a(x/\varepsilon)\nabla u^{(\varepsilon)}\right) = f, \tag{1}$$

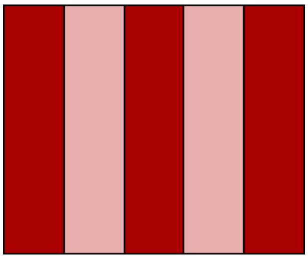

Fig. 3: *Composite with non-isotropic a_{hom}. Given conductance a_1, a_2 on dark/light regions, the effective vertical conductance is $(a_1 + a_2)/2$, but $2/(a_1^{-1} + a_2^{-1})$ in the horizontal direction.*

which—as the name suggests—can describe the diffusion of a substance in a carrier material. Also, it describes the flow of heat inside such a microstructure and other phenomena. Here, $a(x/\varepsilon) \geq 0$ denotes the conductivity of our heterogeneous medium in the point x, at scale ε of the microstructure, and f is some fixed function governing the heat source density. Given that a solution $u^{(\varepsilon)}$ exists for the partial differential equation (PDE), we study its behavior when ε tends to 0, i.e., when the scale of the microstructure becomes smaller and smaller. In this regard, we can formulate at least two goals, which are

1. examining the convergence of $u^{(\varepsilon)}$ (in a suitable sense) to some $u := u^{(0)}$ as $\varepsilon \to 0$ and
2. identifying the governing PDE that is solved by u.

In contrast to the above-mentioned example of the Navier–Stokes to Darcy transition, the governing equation for the evolution of u remains the diffusion equation

$$-\nabla \cdot (a_{\mathrm{hom}} \nabla u) = \tilde{f}, \tag{2}$$

where $\tilde{f}$ is proportional to f. The coefficient $a_{\mathrm{hom}} \in \mathbb{R}^{d\times d}$ is the macroscopic mobility, which is now independent from x. This opens an opportunity for numerical simulations since the discretization of a uniform medium is much easier than the one for the original heterogeneous structures.

Finally, we note in this context that even if a is chosen to be a non-negative scalar, a_{hom} might turn out to be a non-isotropic matrix. Intuitively speaking, the flow may very well be dependent on the direction considered due to the underlying microstructure. This is evident in the cases of Figure 2 and Figure 3.

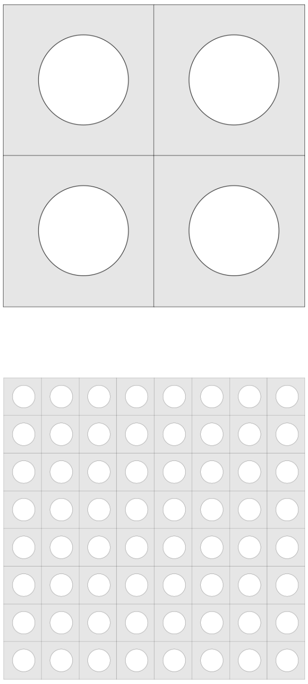

Fig. 4: *Foam at scale $\varepsilon = 1$ (left) and $\varepsilon = 1/4$ (right) with the solid depicted in gray and the air bubbles in white*

A small periodic example. We introduce a standard geometry model, which is used as an example for foams or concrete. We assume that inclusions into a carrying material are periodically repeating discs. Then, we can describe the conductivity of this material by choosing

$$a(x) := 1 - \chi_{B_{1/4}(\mathbb{Z}^d)}(x),$$

where $B_{1/4}(\mathbb{Z}^d)$ is the set of all points with a distance less than $1/4$ to the next point in $\mathbb{Z}^d$ and $\chi_{B_{1/4}(\mathbb{Z}^d)}$ is the characteristic function of this set, see Figure 4. In this simple case, a_{hom} is a $d \times d$ matrix given by

$$a_{\mathrm{hom}}(i,j) := \int_Y [e_i + \nabla w_i] \cdot [e_j + \nabla w_j] \mathrm{d}y, \tag{3}$$

where the $e_i \in \mathbb{R}^d$ are standard unit vectors and the $(w_i)_{i=1,\dots,d}$ are 1-periodic functions given as the solutions to the PDE $-\nabla \cdot [e_i + \nabla w_i] = 0$ in $Y = [-1/2, 1/2]^d \backslash B_{1/4}(0)$ with periodic boundary conditions. The latter are referred to as *cell solutions*. As can be seen from the formulas, a_{hom} is symmetric, but a calculation of the eigenvalues shows that it is typically not isotropic. With not too much effort, one can also prove that a_{hom} is positive semidefinite.

The realm of uncertainty: Stochastic homogenization

The above is a classical case of *periodic homogenization*. This makes sense for materials that have a predictable, often periodic structure, e.g., highly engineered materials or carefully planned out constructions. However, most real-world materials are far more erratic. Hence, the need to study *random microstructures* arises.

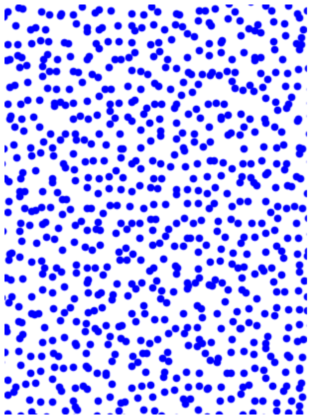

Fig. 5: *Random perforation based on a perturbed lattice*

The setup is mostly the same. Let $U \subset \mathbb{R}^d$ be a bounded, open domain. To model the randomness, we need a stationary ergodic dynamical system, that is, a tuple $(\Omega, \mathcal{F}, \mathbb{P}, \tau)$ consisting of a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and an underlying family of shift operators $\tau = (\tau_x)_{x \in \mathbb{R}^d}$, $\tau_x : \Omega \to \Omega$. These must satisfy stationarity and ergodicity; meaning that the space is *homogeneous* and *averaging* over shifts. We assume that all randomness is driven by such a dynamical system. Consider a random closed set $G \subset \mathbb{R}^d$ satisfying $G(\tau_x \omega) = G(\omega) + x$ for almost every $\omega \in \Omega$ and every $x \in \mathbb{R}^d$. G serves as our random perforation. Thus, our new, random PDE is of the form

$$-\nabla \cdot \left(a(\tau_{x/\varepsilon}\omega) \nabla u^{(\varepsilon)}(\omega) \right) = f \qquad \text{in } U^{(\varepsilon)} := U \setminus (\varepsilon G(\omega)) \tag{4}$$

for some fixed realization $\omega \in \Omega$. A classical example can be constructed via point processes $\mathbb{X} \subset \mathbb{R}^d$ like in Figure 5 and Figure 6: Consider a stationary ergodic point process $\mathbb{X}$ and denote its distribution by $\mathbb{P}$. Choosing τ_x as the shift operator in $\mathbb{R}^d$ by $x \in \mathbb{R}^d$, $\tau_x \mathbb{X} := \mathbb{X} + x$, yields a stationary ergodic dynamical system. Then, we can consider its Boolean model with radius $r > 0$ as a perforation, that is, $G(\mathbb{X}) := B_r(\mathbb{X})$. However, even this most natural perforation model highlights a plethora of problems.

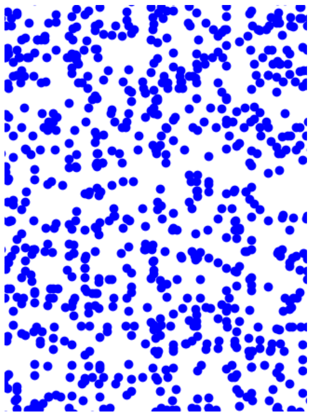

Fig. 6: *Boolean model of a Poisson point process*

Challenges. Stochastic homogenization presents several challenges, adding up to the already existing ones in periodic homogenization.

- Multiscale analysis: As before, capturing behavior at both microscopic and macroscopic scales necessitates careful asymptotic analysis.
- Convergence: Rigorously proving the convergence of the solutions $u^{(\varepsilon)}$ to the homogenized equation is often technically demanding. In the case of perforated domains, one often relies on extension operators.
- Randomness: Dealing with random coefficients requires probabilistic tools. However, completely new effects arise, which are unique to random geometries: arbitrarily large holes, sharp corners, thin tubes of material and, in general, a lacking control over geometric features.

It is, therefore, prudent to gather what is known and how the periodic setting can be translated to the stochastic one. One key aspect is dealing with the cell solutions. For that, we need some notion of partial derivatives on the probability space Ω. This can be defined as the dynamical system $\tau = (\tau_x)_{x \in \mathbb{R}^d}$, which introduces a strongly continuous group action on $L^2(\Omega) \to L^2(\Omega)$ by virtue of $T_x f(\omega) := f(\tau_x \omega)$. Periodicity is replaced by ergodicity, and so the form of a_{hom} and the (supposed) limiting equation can be easily guessed. a_{hom} has the same form as in (3) with $Y := \{\omega \in \Omega \,|\, 0_{\mathbb{R}^d} \notin G(\omega)\}$, while the limiting equation should be of the form

$$-\nabla \cdot (a_{\text{hom}} \nabla u) = \theta f \qquad \text{in } U, \tag{5}$$

where $\theta = \mathbb{P}(Y) = \lim_{\varepsilon \to 0} |U^{(\varepsilon)}|/|U|$ is the average density of our perforated domain. However, two key issues become apparent: showing convergence of the $u^{(\varepsilon)}$ and the exact shape of a_{hom}. In the following, we will give some insights into these.

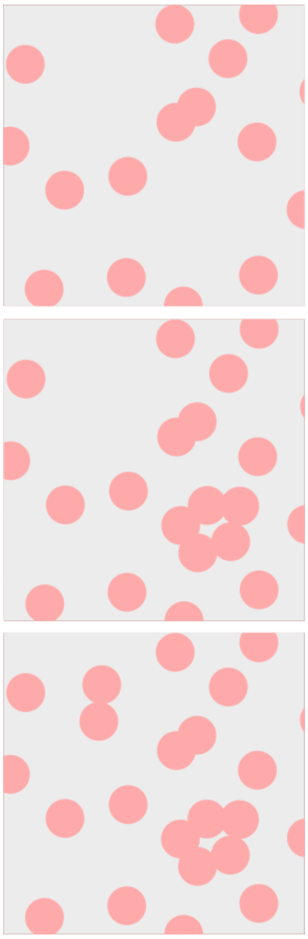

Fig. 7: *An approximation of an irregular perforation by regular ones*

Stochastic homogenization on irregularly perforated domains

While the homogenization of linear PDEs as introduced above is well understood, problems arise when the right-hand side f is replaced by a nonlinearity $f(u^{(\varepsilon)})$ or if nonlinear boundary conditions are supplemented on the interface between the union of all balls and their complements. In these cases, so-called *compactness results* as well as extension and trace operators become necessary. Unlike the periodic case, it is not possible to establish these statements for many random geometries, which is in part due to the already mentioned irregularities that may become arbitrarily bad locally (sharp corners, large holes, etc.).

In a joint project [1] between research group RG 1 *Partial Differential Equations* and Leibniz Group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks*, we were able to alleviate this issue. We established an indirect homogenization scheme justifying the limit solution in (5). This is driven by a regularization of the irregular perforation as depicted in Figure 7. For each of the regularized domains $G^{(n)}$, we are able to homogenize the corresponding equation (4), arriving at a homogenized limit $u_n^{(\varepsilon)} \to u_n$ with corresponding limit equation. Then, we were able to establish $u_n \to u$ as $n \to \infty$, where u solves (5). The situation is depicted in Figure 8.

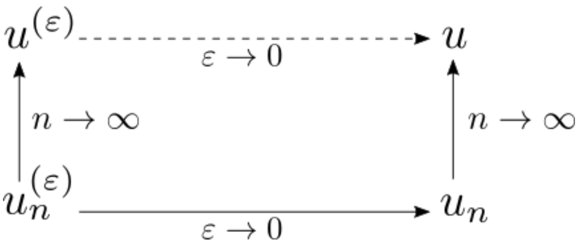

Fig. 8: *Convergences of the various solutions to (4) and (5) under regularization ($n \to \infty$) and microscale ($\varepsilon \to 0$). The dotted arrow is not known in general.*

Furthermore, this diagram is commutative in all cases where classical, direct homogenization results are available. Interestingly, our procedure requires $a_{\text{hom}} > 0$, i.e., a strictly positive definite a_{hom}—a requirement that is automatically fulfilled in the periodic case but may fail in the stochastic one.

Zero conductivity models

As previously mentioned, the shape of a_{hom} is highly dependent on the underlying stochastic model. It is difficult to calculate its exact shape even in the periodic case and regularity remains unclear in the stochastic one. This question marks the topic of our other collaborative project [2]. We study the pathological case of connected, albeit non-conductive random domains. As previously mentioned, this is a peculiarity of stochastic geometries. We move to a discrete lattice for simplicity, but the model and all equations easily translate to a continuous setting of a channel network. We constructed a stationary ergodic $\mathbb{Z}^d$-lattice model featuring $a_{\text{hom}} = 0$. Furthermore, for any fixed volume fraction, the model can be tweaked to exceed that density. In other words, even though the material looks arbitrarily close to a solid block on a microscopic scale, the random perforations are aligned in such a way that the resulting macroscopic structure is non-conducting. To that end, we essentially exploit the following idea: elongating edges retains connectivity but may decrease conductivity. Performing this modification on a suitable percolation model generates a lattice as in Figure 9. We briefly sketch the model for $d = 2$. It is based on the randomly stretched lattice, which is a two-stage random lattice. Given $p, q \in (0,1)$, we first generate independent, identically distributed geometric random variables $N_i^{(x)}, N_j^{(y)}$, $i, j \in \mathbb{Z}$, with $\mathbb{P}(N_0^{(x)} \geq l+1) = q^l$. Then, an edge $(i,j) \leftrightarrow (i+1,j)$ is open with probability $p^{N_i^{(x)}}$ (and analogously $(i,j) \leftrightarrow (i,j+1)$ with $p^{N_j^{(y)}}$). It was proved in [3] that this lattice model percolates for $p > 1/2$ and q sufficiently small, i.e., it contains an infinite cluster of open edges. To establish zero conductivity, we now elongate these edges. Instead of having length 1, we stretch edges of the form $(i,j) \leftrightarrow (i+1,j)$ to have length $\mathcal{S}(N_i^{(x)})$, where

$$\mathcal{S}(N) := \lceil q^{-N(1-\sigma)} \rceil, \quad N \in \mathbb{N},$$

and $\sigma \in (0,1)$ is chosen such that $q^\sigma > p$. Doing the same for vertical edges, we obtain an elongated lattice similar to Figure 10. Since $\mathbb{E}[S(N_0^{(x)})] < \infty$, we may stationarize the modified lattice to obtain a stationary ergodic model on $\mathbb{Z}^2$. To ensure that a given fraction of edges is open, we may *fill up* blocks where $N_i^{(x)}$ and $N_j^{(y)}$ are low. This results in Figure 9. To establish $a_{\text{hom}} = 0$, we rely on a variational formulation of (3), that is, almost surely

$$e_1^{\mathrm{t}} a_{\text{hom}} e_1 = \lim_{n \to \infty} \inf_{V \in \mathcal{D}_n} \frac{1}{2} \sum_{z, \tilde{z} \in [0,n]^2 \cap \mathbb{Z}^2 \,:\, z \sim \tilde{z}} |V(\tilde{z}) - V(z)|^2,$$

with $e_1 = (1,0)^{\mathrm{t}} \in \mathbb{R}^2$, is the first standard unit vector and test function space $\mathcal{D}_n$ consisting of functions $[0,n]^2 \to \mathbb{R}$ taking values 0 on the left and 1 on the right of the box. Here, $z \sim \tilde{z}$ denotes that the summation is only done over open edges $z \leftrightarrow \tilde{z}$ (in the elongated lattice). Control over the probabilistic behavior of the lattice allows us to minimize the expression above, yielding $a_{\text{hom}} = 0$.

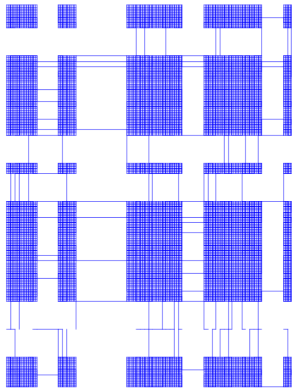

Fig. 9: *A connected lattice model featuring no conductance*

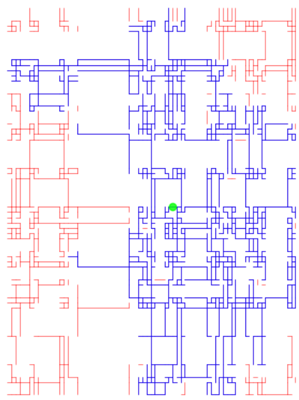

Fig. 10: *A connected lattice model featuring no conductance*

Conclusions and outlook

In our group collaboration between RG 1 and LG DYCOMNET, we were able to combine our expertise in homogenization and stochastic geometry to provide new models and methods for examining random materials via stochastic homogenization as a rigorous and versatile approach to understanding and modeling the behavior of systems in random media. By replacing detailed, computationally expensive microscopic models with effective macroscopic descriptions, this enables the analysis of complex systems with improved efficiency. As such, we strive to prove direct homogenization schemes for a wider class of models as well as to gain a better understanding of the effective conductivity in specific cases.

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1.4 Finite Element Methods Respecting Discrete Maximum Principles for Convection-Diffusion Equations

Volker John

Transferring important physical properties from a continuous model to a discrete version of this model is of utmost importance for many applications. Such properties might be conservation or balance laws that lead to constraints on solutions, like the conservation of mass for incompressible flow problems, or the guarantee of computing only physically admissible values with the discrete problem, like concentrations in the interval $[0, 1]$. There has been a long tradition in RG 3 *Numerical Mathematics and Scientific Computing* on developing, analyzing, and using such so-called *physically consistent* discretizations.

This highlight article considers discretizations of the elliptic linear second-order equation

$$-\varepsilon\Delta u + \mathbf{b}\cdot\nabla u + \sigma u = f \quad \text{in } \Omega \tag{1}$$

and its parabolic counterpart

$$\partial_t u - \varepsilon\Delta u + \mathbf{b}\cdot\nabla u + \sigma u = f \quad \text{in } (0, T]\times\Omega. \tag{2}$$

In (1) and (2), $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, is a bounded domain with Lipschitz boundary, T is a final time, $\varepsilon > 0$ is the diffusion coefficient, $\mathbf{b}$ the convection field, $\sigma \geq 0$ the reaction field, and f describes sinks and sources of the scalar quantity. Both problems have to be equipped with appropriate boundary conditions and the parabolic problem also with an initial condition. Problems (1) and (2) describe the transport of a scalar quantity, like temperature or concentration, by diffusion and convection. The reactive term arises in coupled problems that model, in addition to the transport, also chemical reactions, e.g., see [1, Chapt. 2.1.2]. The monograph [1] contains comprehensive explanations and extended references for all statements made in this highlight article.

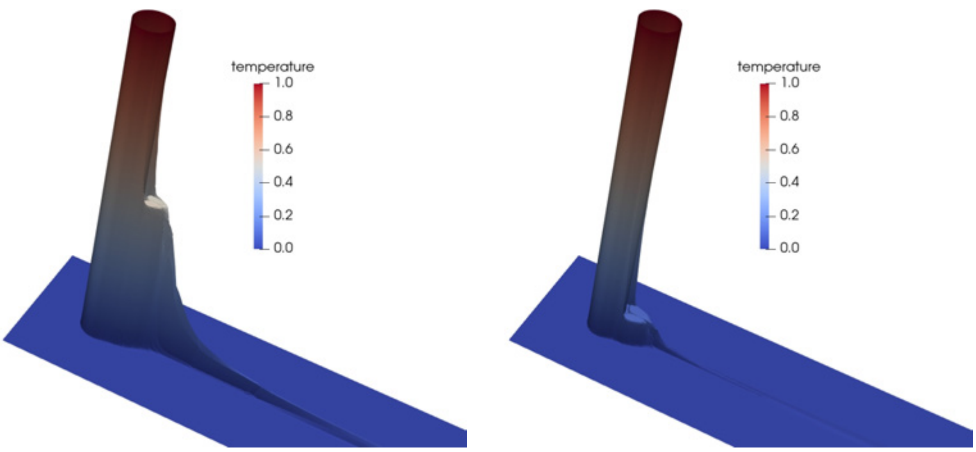


Fig. 1: *Stationary transport of temperature from a heated cylinder. The flow field is from left to right with $\|\mathbf{b}\|_{L^\infty(\Omega)} = \mathcal{O}(1)$. Left: Temperature distribution for $\varepsilon = 10^{-6}$. Right: Temperature distribution for $\varepsilon = 10^{-8}$. Pictures taken from [1]*

Although (1) and (2) are just linear problems, they pose challenges in their numerical solution, particularly in the convection-dominated regime. This regime is characterized by a large mesh Péclet number $\|\mathbf{b}\|_{L^\infty(\Omega)} h/\varepsilon$, where h is a characteristic scale of the mesh width. In the convection-dominated regime, solutions of (1) and (2) possess layers, compare Figure 1, which are very thin structures with steep gradients. From asymptotic analysis it is known that layers are of size $\mathcal{O}(\varepsilon)$ or $\mathcal{O}(\sqrt{\varepsilon})$, which is, in the convection-dominated regime, usually much smaller than the affordable mesh width. Consequently, these very important structures of the solution cannot be represented on given grids. This feature is typical for multiscale problems. Hence, from the numerical point of view, problems (1) and (2) are multiscale problems in the convection-dominated regime, where the layers are the unresolved (or subgrid) scales. It is well known that the physically consistent and accurate numerical solution of multiscale problems is challenging.

Solutions of (1) and (2) satisfy maximum principles for appropriate data. These principles are of high importance from the practical point of view, since they state, e.g., that concentrations take values in $[0,1]$ or that the temperature stays positive, and if, additionally, there are no sources of energy in Ω, the highest temperature is attained at the boundary of Ω for the steady-state problem. A discretization of (1) or (2) that is useful in practice should satisfy the discrete counterpart of the maximum principles, so-called *discrete maximum principles (DMPs)*. The satisfaction of DMPs is an important aspect of the physical consistency of a discretization. It should be noted, however, that the satisfaction of DMPs does not exclude that a numerical solution possesses small wiggles (with physically admissible values).

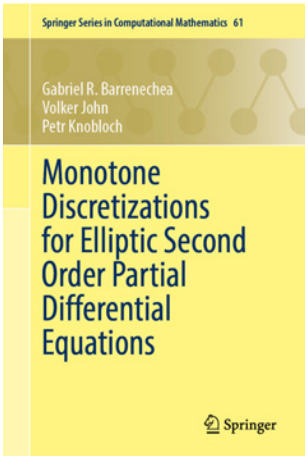


Fig. 2: *Reference [1]*

The difficulties to perform numerical simulations for convection-diffusion problems have been known for decades. Until about one decade ago, the main direction of research in Numerical Mathematics was the development of high-order methods, thus focussing on accuracy in certain norms of Sobolev and Lebesgue spaces, e.g., see the most cited monograph in this field [5]. Usually, these methods compute numerical solutions with spurious oscillations in a vicinity of layers. Early approaches for constructing DMP-preserving finite element methods, from around 1980, combine finite difference and finite volume upwind techniques with a finite element discretization of the diffusive term. Only in the first decade of this century, more sophisticated finite element methods, again adapting ideas from finite volume schemes, were proposed, e.g., in [4] for the steady-state problem (1). In the last decade, there has been an enormous development of new methods, among them the currently best performing DMP-preserving methods for (1). An overview of the state of the art of DMP-preserving finite element methods for (1) and (2) is provided in [2]. The monograph [1] contains a comprehensive presentation and numerical analysis of DMP-preserving methods for the steady-state problem (1).

This highlight article will concentrate on DMP-preserving methods for the steady-state problem (1). Since (1) is a linear boundary value problem, it seems to be natural to apply a linear discretization, i.e., a discretization that leads to a linear system of equations $A\underline{u} = \underline{g}$ with $A \in \mathbb{R}^{n\times n}, \underline{u}, \underline{g} \in \mathbb{R}^n$. If one uses Lagrange finite elements with the standard basis functions, then the vector $\underline{u}$ contains values of the finite element solution $u_h(\mathbf{x})$ at certain points in $\overline{\Omega}$, the so-called *nodes*. There is a classical theory for the satisfaction of global DMPs for the values of $\underline{u}$ from the 1970s. A widely used sufficient criterion states two conditions: The matrix A should have nonnegative row sums, and it should be a monotone matrix, i.e., A^{-1} has only nonnegative entries. A proper subset of monotone matrices is the class of M-matrices. An alternative theory is based on the concept of matrices of nonnegative type that are matrices with nonnegative row sums and with nonpositive off-diagonal entries. This concept allows also to investigate local DMPs.

The extension of a DMP property from the values in the nodes to the finite element solution is only possible for the lowest order conforming finite elements P_1 and Q_1. For all other finite element functions, values away from the nodes cannot be bounded by the values in the nodes.

Already for the simplest case of (1), the Poisson problem, i.e., $\varepsilon = 1, \mathbf{b} = \mathbf{0}, \sigma = 0$, it turns out that the standard Galerkin discretization leads to restrictions on the mesh if the satisfaction of DMPs is desired. For P_1 finite elements in two dimensions, this restriction is almost equivalent to the requirement that the triangulation is Delaunay. In three dimensions, the set of admissible meshes is neither a subset of the class of Delaunay triangulations nor vice versa. For Q_1 and P_2 finite elements, the latter in two dimensions, global DMPs (P_2 for the values in the nodes) can be proved only for very special grids. And for P_3 finite elements in two dimensions, it can be shown that DMPs are not satisfied even on special grids. This situation for the Poisson problem explains why the development of DMP-preserving methods for (1) and (2) has been concentrated on P_1 finite elements.

For convection-dominated problems, there are several linear discretizations that satisfy DMPs or are at least monotone (positivity-preserving). One class contains the already mentioned finite element upwind methods. In the late 1980s and 1990s, there were several proposals to formulate, in two dimensions, a counterpart of the Scharfetter–Gummel finite volume scheme in the framework of finite element methods. However, these proposals have not been used in practice.

Since in the convection-dominated regime one has to deal with a multiscale problem from the numerical point of view, an appropriate strategy for computing numerical solutions that are both accurate and DMP-preserving is to apply different techniques for the resolved scales and the subgrid scales. This strategy leads to nonlinear discretizations since the distribution of the scales in the domain depends on the solution. The first nonlinear discretization was proposed already in the 1980s, the Mizukami–Hughes upwind method. It defines the local upwind direction in such a way that the discretization locally behaves like a method with a matrix of nonnegative type. This upwind direction might depend on the numerical solution. However, numerical studies in [1] show that this method is usually not competitive with modern algebraically stabilized schemes. In the 1990s, many of so-called *spurious oscillations at layers diminishing (SOLD)* or shock-capturing methods, which augment a standard linear stabilized method with a nonlinear term, have been proposed. But none of them consistently succeeds in removing the spurious oscillations of the linear method, which were solely reduced to some extent. Only the development of algebraically stabilized discretizations, with the initial contribution [4] for steady-state problems, offered an approach for computing accurate and DMP-preserving solutions for convection-dominated problems.

Most of the known algebraically stabilized methods fit in the framework of algebraic flux correction (AFC) schemes. Consider P_1 or Q_1 finite element spaces with the standard nodal basis $\{\phi_i\}_{i=1}^n$. Let, without loss of generality, the nodes be ordered such that the $(n-m)$, $m < n$, Dirichlet values come last. Denote by

$$a(u, v) = (\varepsilon \nabla u, \nabla v) + (\mathbf{b} \cdot \nabla u + \sigma u, v)$$

the bilinear form of a variational formulation of (1). Then, the first step of the AFC schemes consists in assembling the matrix $A = (a_{ij})_{i,j=1}^n \in \mathbb{R}^{n \times n}$ of the Galerkin finite element method, i.e., $a_{ij} = a(\phi_j, \phi_i)$, $i, j = 1, \dots, n$. Let $\underline{u} \in \mathbb{R}^n$ be the solution vector, $\underline{g} \in \mathbb{R}^m$ the vector from assembling the source term, and $\underline{u}^{\mathrm{b}} \in \mathbb{R}^{n-m}$ the vector of the Dirichlet values. Then, the general form of an AFC scheme is given as follows:

$$\begin{aligned} \sum_{j=1}^{n} a_{ij} u_j + \sum_{j=1}^{n} b_{ij}(\underline{u}) \left(u_j - u_i\right) &= g_i, \quad i = 1, \ldots, m, \\ u_i &= u_i^{\mathrm{b}}, \quad i = m+1, \ldots, n, \end{aligned} \tag{3}$$

with a solution-dependent matrix $B(\underline{u}) = (b_{ij}(\underline{u}))_{i,j=1}^{n} \in \mathbb{R}^{n \times n}$ that should satisfy

$$b_{ij}(\underline{u}) = b_{ji}(\underline{u}), \quad i, j = 1, \ldots, n, \qquad b_{ii}(\underline{u}) = -\sum_{j \neq i} b_{ij}(\underline{u}) \quad i = 1, \ldots, n.$$

The symmetry of B guarantees that the AFC scheme is conservative, which is another important aspect of the physical consistency of the discretization. In AFC schemes, the term $B(\underline{u})$ is defined with the help of an artificial diffusion matrix $D \in \mathbb{R}^{n \times n}$, which can be easily computed from A by

$$d_{ij} = d_{ji} = -\max\left\{a_{ij}, 0, a_{ji}\right\} \quad \forall\, i \neq j, \quad d_{ii} = -\sum_{j \neq i} d_{ij} \quad i = 1, \ldots, n,$$

and a matrix consisting of limiters $(\alpha_{ij}(\underline{u}))_{i,j=1}^{n}$, $\alpha_{ij} \in [0,1]$, which is assumed to be symmetric, so that

$$b_{ij}(\underline{u}) = \left(1 - \alpha_{ij}(\underline{u})\right) d_{ij} \quad \forall\, i \neq j, \qquad b_{ii}(\underline{u}) = -\sum_{j \neq i} b_{ij}(\underline{u}) \quad i = 1, \ldots, n.$$

Inserting this expression in (3), defining the so-called *algebraic fluxes* $f_{ij} = d_{ij}(u_j - u_i)$, $i, j = 1, \ldots, n$, and rearranging terms leads to a problem of the form

$$\begin{aligned} \sum_{j=1}^{n} \left(a_{ij} + d_{ij}\right) u_j &= g_i + \sum_{j=1}^{n} \alpha_{ij}(\underline{u}) f_{ij} \quad && i = 1, \ldots, m, \\ u_i &= u_i^{\mathrm{b}}, && i = m+1, \ldots, n. \end{aligned} \tag{4}$$

By construction, the matrix on the left-hand side of (4) is an M-matrix with nonnegative row sums. With setting all limiters $\alpha_{ij}(\underline{u}) = 0$, one obtains a linear problem that corresponds to discretization with high artificial diffusion. AFC methods are designed such that limiters close to 1 are chosen in smooth subregions away from layers, to recover the high order of the Galerkin method, and limiters close to 0 are proposed in subregions including layers, so that the numerical diffusion becomes effective to suppress spurious oscillations. After the pioneering paper [4], whose proposal is nowadays called *Kuzmin limiter*, starting from 2016, a number of new and improved limiters have been designed. Most of these algebraic limiters can be computed directly from the given matrices and vectors. Thus, their implementation is independent of the dimension d of the problem.

The first comprehensive numerical analysis of AFC schemes was presented in [3]. The existence of a solution can be shown, using Brouwer's fixed-point theorem, if $\alpha_{ij}(\underline{u})(u_j - u_i)$ is a continuous function of $\underline{u}$. This property is satisfied for all known algebraic limiters. A uniqueness result is not available for any of the known limiters. As the primary goal, all limiters were designed in such a way that the discretization satisfies DMPs. For several of the more recently proposed limiters, this property holds without any restriction on an admissible mesh. The paper [3] contains also the first convergence analysis of AFC schemes. A consistency error is committed through the introduction of the algebraic stabilization. Using only that the limiters satisfy $\alpha_{ij} \in [0,1]$ gives an error bound for an energy norm that is augmented by a contribution from the algebraic stabilization that is of order 0.5 for the convection-dominated regime and that even does not tend to zero for the diffusion-dominated case. On the one hand, numerical studies in [3] demonstrate that both bounds are sharp within the assumptions for the analysis. But on the other hand, numerical experience shows that the order of convergence for smooth solutions is usually better. Whether or not the optimal (interpolation) order can be observed depends on the concrete limiter and on properties of the family of triangulations. The numerical analysis for providing a theoretical basis of these observations is open. Nevertheless, the numerical analysis of AFC schemes has been further developed and unified in recent years. For instance, the convergence analysis and the analysis for several algebraic limiters could be extended to general Lagrange finite elements, see [1].

From the practical point of view, it has been found that some AFC schemes cause high costs (many iterations) for solving the nonlinear discrete problems. In applications, however, convection-diffusion-reaction problems are usually a part of a coupled system, which is nonlinear anyway, so that the nonlinearity introduced by algebraically stabilized methods should not substantially increase the computational costs for solving the system.

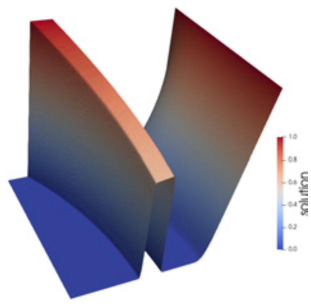
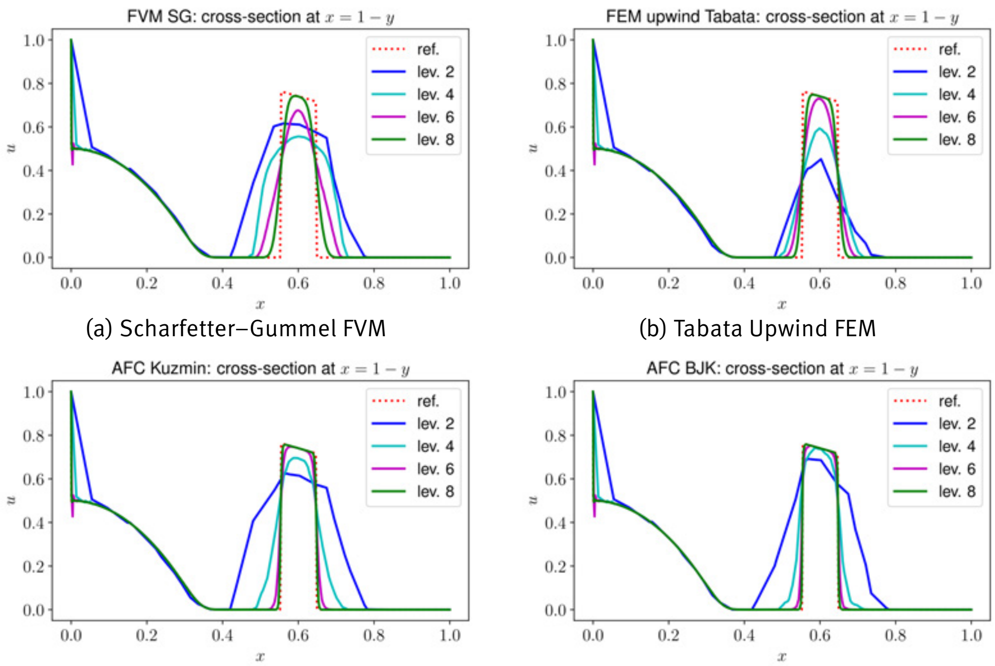


Fig. 3: *Solution of the problem that models the transport of a concentration through a domain; the inlet ($x = 0$) is on top and the outlet ($x = 1$) at the bottom*

In [1], many discretizations for (1) were studied numerically for an example that models the transport of (a concentration of) a species through $\Omega = (0, 1)^2$. The solution is depicted in Figure 3. In regions with high concentration, the problem is defined to be convection-dominated, in a small neighborhood of these regions it is reaction-dominated, and away from high concentrations, it is diffusion-dominated. Simulations were performed on a family of Delaunay triangulations that were generated with a mesh generator that is freely available for academic purposes. For assessing the accuracy, reference cross-sections were computed from a numerical solution on a very fine grid. Most methods that were studied are DMP-preserving, the others at least monotone.



(a) Scharfetter–Gummel FVM

(b) Tabata Upwind FEM

(c) AFC method with Kuzmin limiter [4]

(d) AFC method with BJK limiter

Fig. 4: *Problem that models the transport of a concentration through a domain; cross-sections at $x = 1 - y$ for two linear discretizations (top) and two AFC schemes (bottom) and for different levels of mesh refinement. Pictures taken from [1]*

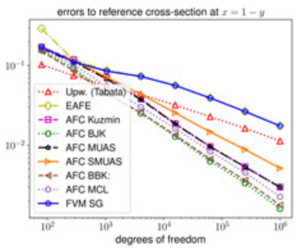


Fig. 5: *Problem that models the transport of a concentration through a domain; errors for cross-section at* $x = 1 - y$. *Picture taken from [1]*

None of the studied methods computed unphysical values, i.e., values not contained in $[0, 1]$. The evaluation with respect to accuracy was qualitatively the same for all cross-sections. Exemplarily, results for the cross-section $x = 1 - y$ are presented in Figures 4 and 5. As expected, the nonlinear discretizations gave more accurate solutions where the layers are usually much sharper than for the linear discretizations. It can be also observed that within both the class of linear discretizations and AFC schemes, there are noticeable differences in the accuracy for different methods. The most important conclusion from this numerical study is that the AFC schemes are well suited for the solution of convection-diffusion-reaction problems where different regimes are present in different parts of the domain.

Considering the following three aspects: order of convergence for smooth solutions, steepness of layers in numerical solutions, and efficiency for solving the nonlinear problems, there is currently no AFC method that performs best with respect to all of these aspects.

The concept of algebraic stabilizations can also be used within finite element methods for the time-dependent problem (2). These methods are called *FEM-FCT (flux-corrected transport) schemes*. There are even linear variants of FEM-FCT schemes that have been proved to be a good compromise of accuracy and efficiency in several application projects of RG 3.

Members of RG 3 have been working on different aspects of algebraically stabilized methods in recent years, often with collaborators. Two new limiters (BJK (Barrenechea, John, and Knobloch) and MUAS (Monotone Upwind-type Algebraically Stabilized) in Figures 4 and 5) were developed. Both of them satisfy DMPs for arbitrary elliptic second order problems on arbitrary simplicial triangulations. Approaches for solving the nonlinear problems were identified that are more efficient than previously used ones. An a posteriori error estimator for AFC methods was developed. It was clarified how AFC methods have to be applied on adaptively refined grids with hanging nodes. Comprehensive numerical studies provided a better insight in the advantages and shortcomings of several methods. And finally, for algebraic stabilizations of the parabolic problem (2), results concerning the existence and uniqueness of a discrete solution were obtained.

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1.5 Thematic Einstein Semester "Mathematics for Quantum Technologies"

Uwe Bandelow, Patricio Farrell, Anngeret Glitzky, Markus Kantner, Thomas Koprucki, Matthias Liero, and Michael O'Donovan

Quantum technologies have the potential to outperform a number of classical technologies by exploiting inherent properties of quantum systems such as superposition and entanglement. This includes quantum computers that employ quantum information processing to solve certain computational problems much more efficiently than their classical counterparts, tap-proof quantum communication networks for encryption and transmission of sensitive information, and highly sensitive quantum sensors that can exceed the accuracy of classical metrology systems by orders of magnitude. Developing these technologies requires precise preparation and control of quantum systems. This is achievable through advanced theoretical research, including high-dimensional simulations, quantum algorithm analysis, control optimization, and device design.

The Cluster of Excellence MATH+ operates a topical development lab in which current and emerging mathematical topics are explored in great detail. The main activity of the topical development lab is the organization of the *Thematic Einstein Semesters* (TES) with financial support by the Einstein Foundation Berlin. In the summer semester 2024, the TES "Mathematics for Quantum Technologies" was organized by researchers from the Freie Universität (FU) Berlin, the Technische Universität (TU) Berlin, WIAS, and Zuse Institute Berlin (ZIB) with a series of workshops, symposia, lecture series, seminars, and a summer school. In this article, we give a short report on the main events.

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Scientific events and workshops

"Quantum Computing in Academia and Industry." The kick-off symposium of the semester featured five talks by experts from both academia and industry, showcasing current topics in quantum information processing and computing. Jens Eisert (FU Berlin) explored the mathematics of near-term quantum computing, addressing quantum advantages, quantum machine learning applications, and challenges in error mitigation. Karl Jansen (Deutsches Elektronen-Synchrotron (DESY), Zeuthen) discussed scientific applications already feasible on current quantum hardware in combinatorial optimization and elementary particle physics. Presentations from industry representatives were given by Almudena Carrera Vazquez (IBM Zürich), André Carvalho (Q-CTRL, Berlin), and Cristina Cirstoiu (Quantinuum, Cambridge). The kick-off symposium received great interest and attracted more than 100 participants in total.

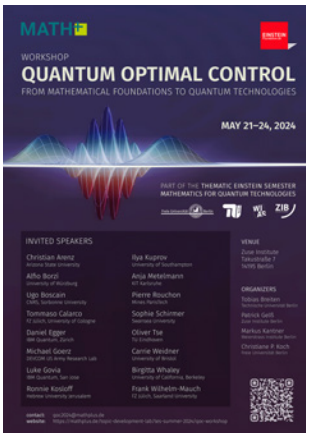
Fig. 1: *The kick-off symposium was held at the TU Berlin. Photo: Lukas Protz*

Annual Meeting Photonic Devices (AMPD 2024). The AMPD workshop, held at ZIB, centered on the mathematical simulation of novel photonic devices, with a special emphasis on applications in quantum technologies. The event fostered interdisciplinary collaboration between the mathematics and physics communities, aiming to advance the design and functionality of photonic devices critical to quantum systems.

Key discussions revolved around the numerical simulation of photonic devices that are relevant for quantum communication, quantum sensing, and quantum computation. Topics included the development of precise simulations to enhance device performance and the exploration of physical principles to optimize components like single-photon sources, integrated photonic circuits, and quantum detectors. By bridging theoretical frameworks and practical applications, the meeting highlighted the role of photonic devices in shaping the future of quantum technologies.

Fig. 2: *Group photo from the workshop on Quantum Networks and Quantum Cryptography*

"Quantum Cryptography and Quantum Networks." The workshop focused on current topics and developments in quantum communication and quantum networks, and included topics in both theory and experimental implementations. Key topics were quantum key distribution (QKD), large-scale quantum networks, security analysis for QKD, photonic implementations of quantum protocols, quantum repeaters, and device independence. The program featured a combination of advanced research presentations and several tutorials designed for students and early-career researchers.



"Quantum Optimal Control – From Mathematical Foundations to Quantum Technologies." The workshop on quantum optimal control attracted numerous pioneers and early career researchers from this field. The program comprised a total of 30 talks and 36 posters on a broad range of current topics at the interface between applied mathematics and theoretical physics, e.g., numerical methods and algorithms for quantum optimal control problems, controllability of quantum systems, quantum thermodynamics and control of open quantum systems, quantum computing algorithms, and quantum error correction as well as applications to specific model systems (cold atoms in optical lattices, Bose–Einstein condensates, superconductors). In addition, the participants were given the opportunity to learn about state-of-the-art software tools for quantum optimal control problems within the framework of an integrated software tutorial. The workshop received great interest and attracted about 100 registered on-site participants. In response to the considerable international interest, a hybrid option was set up at short notice, whereupon a further 50 participants registered for the online stream. The workshop was jointly organized by researchers from FU Berlin, TU Berlin, WIAS and ZIB.

"Tensor Methods in Quantum Simulation." Tensor-based methods are a key technique to tackle the simulation of high-dimensional quantum systems on classical computers. These methods were explored in great detail in a combination of summer school and research workshop held at ZIB, which brought together established and early-career researchers from physics and mathematics. The event began with a three-day summer school providing tutorials on tensor networks, quantum simulations, and their applications in machine learning. This was followed by a two-day research workshop featuring cutting-edge advancements.

Highlights included the exploration of tensor networks for hybrid quantum algorithms, insights on synergizing tensor networks with quantum circuits, and perspectives on quantum computing's future in scientific applications. A novel digital quantum approach for simulating fermionic scattering was demonstrated. The workshop underscored the growing integration of tensor methods and quantum computing.

"Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS)." The final event of the Thematic Einstein Semester was the international workshop "Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024)," organized by WIAS researchers together with Josef Weinbub (Silvaco Inc.). The interdisciplinary workshop brought together experts from mathematics, physics, engineering, and materials science to address challenges in modeling and simulation of semiconductor devices. Central topics were electronic structure theory, quantum and semiclassical transport theory, upscaling from atomistic to continuum scale models, and simulation studies for various semiconductor devices. A particular focus was on spin-qubit devices for applications in quantum information processing.

The workshop was complemented by a full day tutorial, which attracted numerous students and researchers at all career stages. The key topics of the tutorials were density functional theory and quantum transport theory for computational materials science and the combination of these approaches with machine learning techniques.

Fig. 3: *Participants of the AMaSiS 2024 workshop on the roof top of the Leibniz headquarters. Photo: Dirk Peschka*

Lecture series and special seminars

Quantum Thermodynamics and Quantum Control. Prof. Ronnie Kosloff (Hebrew University, Jerusalem) delivered an advanced course on open quantum systems, quantum thermodynamics, and coherent control of dissipative quantum systems. It covered foundational concepts and advanced methods, highlighting their relevance to emerging quantum technologies.

Forces of the Quantum Vacuum. The advanced lecture series by Prof. Ulf Leonhardt (Weizmann Institute of Science, Rehovot) focused on phenomena emerging from quantum vacuum fluctuations. The course provided a concise and self-contained introduction to the theoretical framework of quantum vacuum forces spanning from quantum electrodynamics to cosmology and aimed to develop both intuition and mathematical techniques for manipulating vacuum forces in technological applications.

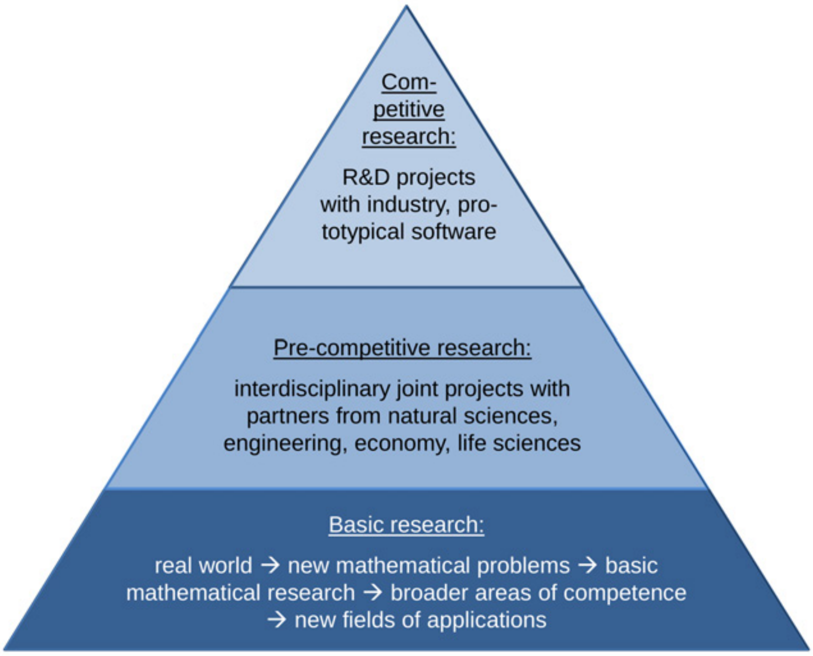
Quantum Wednesday. The workshops and lecture series were supplemented by this dedicated seminar series. Among others, following talks were given: “Quantum chaos and non-Hermitian physics in optical microcavities” (Jan Wiersig, Universität Magdeburg), “Kalman filtering for noise characterization in optical frequency combs” (Jasper Riebesehl, Technical University of Denmark), “Quantum sensing with ultra cold gases” (Naceur Gaaloul, Leibniz Universität Hannover), and “Variational Gaussian approximation for quantum dynamics” (Caroline Lasser, Technische Universität München).

2 WIAS in 2024

- Profile
- Structure and Scientific Organization
- Activities in Equal Opportunities and Work-Life Aspects
- Grants
- Participation in Structured Graduation Programs
- Scientific Software

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 multi-disciplinary 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.

2.1.1 Service to the Community

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, two 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 38 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 2024 took place from April 10 to 12 at the Leibniz-Institut für Verbundwerkstoffe GmbH (Leibniz Institute for Composite Materials, IVW) in Kaiserslautern. It was attended by 78 scientists from 25 institutions.

The **Mathematical Research Data Initiative (MaRDI)** (http://www.mardi4nfdi.de/) began operation on October 1, 2021. As the only mathematical consortium within the German *Nationale Forschungs-dateninfrastruktur* (NFDI), its goal 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 reusable. In this way, data will be better documented, the potential for reinventing the wheel will be avoided, and the reproducibility of research results will be improved. However, FAIR data does not automatically imply open data; rather, accessibility can be regulated by suitable licenses. This is especially important in interdisciplinary mathematical research, where data access might be restricted due to legal requirements or cooperation agreements. WIAS's role within MaRDI is to coordinate the consortium and contribute to the overall work program in the areas of statistics, machine learning, and interdisciplinary mathematics.

Currently in its fourth year, MaRDI continues to actively develop services for the community. It is active in two NFDI base services: The first base service is Data Management Planning (DMP4NFDI), where a mathematical-specific plugin will be implemented within the central RDMO instance at Technische Universität Darmstadt making it readily available to researchers. The metadata from this workflow will be incorporated into the MaRDI knowledge graph. In the second base service, MaRDI contributes to building a central Knowledge Graph Infrastructure (KGI4NFDI), connecting graphs from different disciplines and providing a SPARQL query endpoint. Furthermore, MaRDI seeks to integrate with other base services such as Jupyter4NFDI.

As a part of its general outreach program, MaRDI organizes workshops on Research Data Management for potential DFG clusters (SFBs, SPPs) and offers courses for undergraduates. Additionally, it has a touring exhibit, The MaRDI Station, which was featured on the MS Wissenschaft 2024 covering the general topic of "Freedom." Workshops and mini-symposia in the areas of discrete mathematics, scientific computing, and computer algebra were also 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.

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 was from November 2022 to October 2024 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.

Berlin's non-university research institutions launched a joint initiative in 2020 to strengthen the capital's role as an international science hub. They 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 2024, 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 one Focus Platform[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 54), 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:

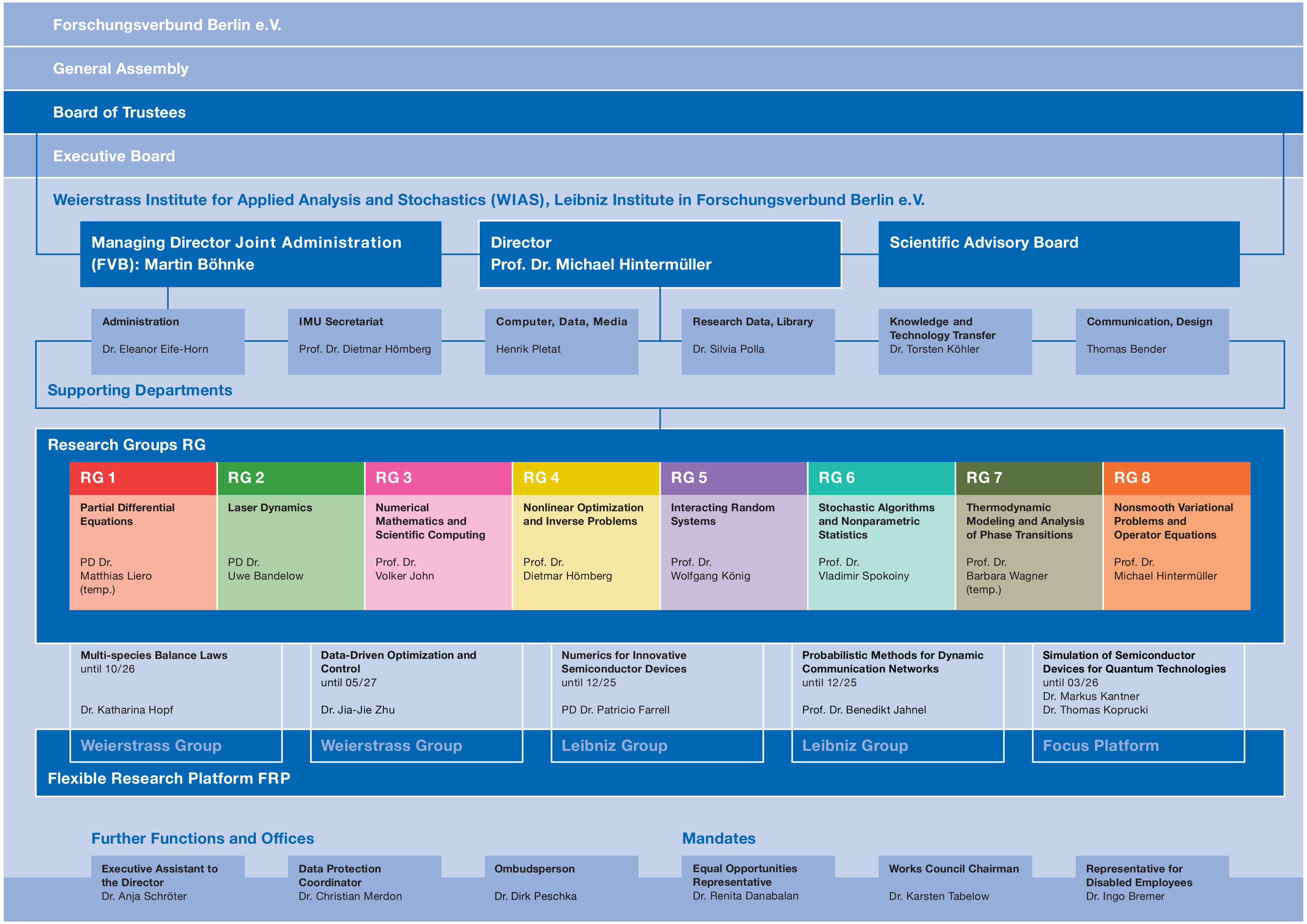
RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing
RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase 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 DOC. Data-driven Optimization and Control
WG MBaL. Multi-species Balance Laws (from November 1, 2023)
FP 2. Simulation of Semiconductor Devices for Quantum Technologies

The organization chart on page 42 gives an overview of the organizational structure of WIAS in 2024 (as of Dec. 31, 2024).

[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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Communication, Design Thomas Bender
Supporting Departments
Research Groups RG
RG 1 Partial Differential Equations PD Dr. Matthias Liero (temp.)
RG 2 Laser Dynamics PD Dr. Uwe Bandelow
RG 3 Numerical Mathematics and Scientific Computing Prof. Dr. Volker John
RG 4 Nonlinear Optimization and Inverse Problems Prof. Dr. Dietmar Hömberg
RG 5 Interacting Random Systems Prof. Dr. Wolfgang König
RG 6 Stochastic Algorithms and Nonparametric Statistics Prof. Dr. Vladimir Spokoiny
RG 7 Thermodynamic Modeling and Analysis of Phase Transitions Prof. Dr. Barbara Wagner (temp.)
RG 8 Nonsmooth Variational Problems and Operator Equations Prof. Dr. Michael Hintermüller
Multi-species Balance Laws until 10/26 Dr. Katharina Hopf
Data-Driven Optimization and Control until 05/27 Dr. Jia-Jie Zhu
Numerics for Innovative Semiconductor Devices until 12/25 PD Dr. Patricio Farrell
Probabilistic Methods for Dynamic Communication Networks until 12/25 Prof. Dr. Benedikt Jahnel
Simulation of Semiconductor Devices for Quantum Technologies until 03/26 Dr. Markus Kantner Dr. Thomas Koprucki
Weierstrass Group
Weierstrass Group
Leibniz Group
Leibniz Group
Focus Platform
Flexible Research Platform FRP
Further Functions and Offices
Mandates
Executive Assistant to the Director Dr. Anja Schröter
Data Protection Coordinator Dr. Christian Merdon
Ombudsperson Dr. Dirk Peschka
Equal Opportunities Representative Dr. Renita Danabalan
Works Council Chairman Dr. Karsten Tabelow
Representative for Disabled Employees Dr. Ingo Bremer

2.2.2 Main Application Areas

The research at WIAS focused in 2024 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

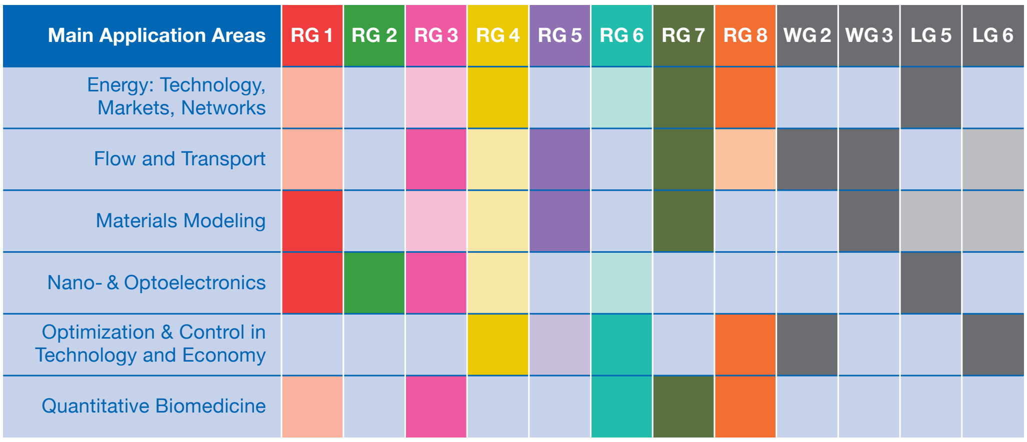
- **Energy: Technology, Markets, Networks**
- **Flow and Transport**
- **Materials Modeling**
- **Nano- and Optoelectronics**
- **Optimization and Control in Technology and Economy**
- **Quantitative Biomedicine**

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 2024 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 DOC is called WG 2, WG MBaL becomes WG 3, LG NUMSEMIC LG 5, and LG DYCOMNET LG 6 (the first ones are groups no. 2 and 3 supported by the Weierstrass Institute and the latter the groups no. 5 and 6 supported until now by the Leibniz Association at the WIAS).

In the following, special research topics are listed that were addressed in 2024 within the general framework of the main application areas.

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.

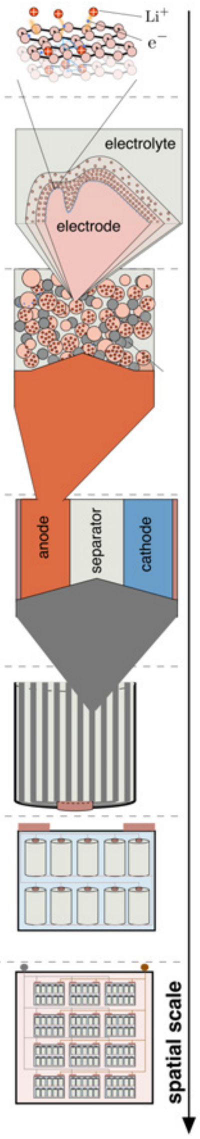


***Fig. 1:** Multiple scales in lithium-ion batteries*

Core areas:

- 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 RG 1 and 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 1, 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 and RG 7)
- Random diffusion dynamics for collisions of hard spheres (in RG 5)
- Biological particle flow with dormancy strategies (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)

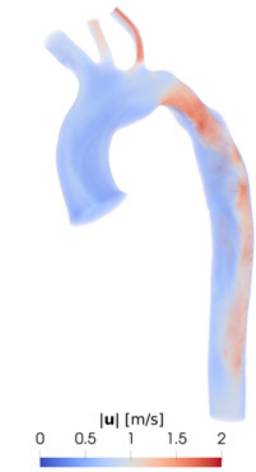


Fig. 2: *Simulation of pulsatile blood flow in an aortic coarctation, snapshot of the velocity field*

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.

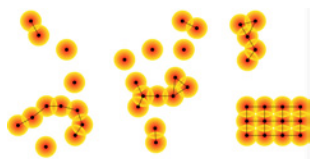


Fig. 3: *A realization of a many-body system showing a small crystal in the lower right corner*

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, RG 7, and LG DYCOMNET)
- Asymptotic analysis of nano- and micro-structured interfaces, including their interaction with volume effects (in RG 1 and RG 7)
- Dynamical processes in nonhomogeneous media (in 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 and RG 7)
- 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 and RG 7)
- Modeling of elastoplastic and phase-separating materials including damage and fracture processes (in RG 1 and RG 7)
- Derivation and analysis of local and nonlocal phase field models and their sharp-interface limits (in RG 1 and RG 7)
- Modeling and simulation of electronic properties of perovskites (in RG 1 and LG NUMSEMIC)
- Analysis of entropy-driven reaction-cross-diffusion systems (in RG 1 and WG MBaL)
- Variational modeling and asymptotic analysis of volume-preserving diffuse-interface models (in RG 7 and WG MBaL)

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.

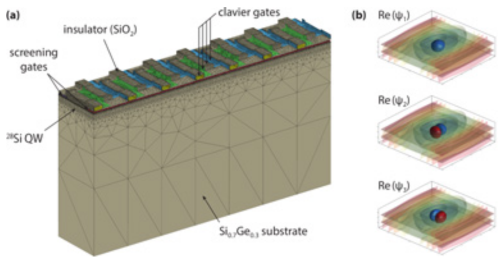


Fig. 4: *(a) Quantum bus for coherent transfer of quantum information in semiconductor quantum processors based on gate-defined quantum dots in Si/SiGe heterostructures. (b) Snapshots of low-energy electronic orbitals of the transported electron spin-qubit in the quantum bus; see also report of Research Group* Laser Dynamics *on page 74.*

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)
- Photovoltaic devices (in RG 1 and LG NUMSEMIC)
- 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.

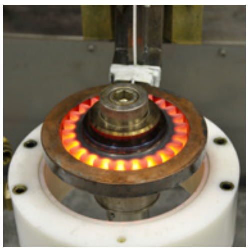


Fig. 5: *Induction heat treatment of a gear*

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 neurosciences are considered. They include classical tasks like registration, denoising, equalization, and segmentation. Moreover, (low-rank/sparse) data decomposition and functional correlations, e.g., in neurological processes, are also studied. These processes typically lead to complex, nonlinear, or nonsmooth inverse problems where often also statistical aspects play a central part for data modeling and analysis methods. The current focus of research is the consideration of (bio-)physics-based models for data and image analysis. Furthermore, mathematical 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.

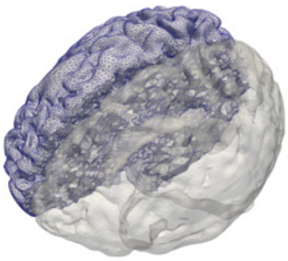


Fig. 6: *Computational model of brain tissue obtained from 3D MRI images*

Core areas:

- Numerical methods for biofluids and biological tissues (in RG 1, 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 ion channels in cells (in RG 7)
- (Bio-)physics-based quantitative imaging (in RG 6 and RG 8)

2.3 Activities in Equal Opportunities and Work-Life Aspects

In 2024, WIAS officially launched the **Iris Runge Program (IRP)**, introducing the first two postdoctoral researchers, Dr. Anieza Maltsi and Dr. Jin Yan. The Iris Runge Program is designed for early-stage female postdoctoral researchers to conduct their research at WIAS in a Research Group of their choice for a duration of 2 to 3 years. The inauguration event was held at WIAS on March 18, 2024, in conjunction with the touring photography exhibit Women of Mathematics from Around the World, which presents mathematics through the profiles of 34 female mathematicians. In the same year, two female master's degree candidates were accepted into the WIAS Female Master Students Program.

The Equal Opportunities office, represented by Renita Danabalan and Andrea Eismann, continues to be active in the recruitment process at WIAS for both scientific staff (postdoctoral researchers and Ph.D.s) and leadership positions. The representatives also supported the institute leading up to and during the evaluation process. In October 2024, the election of the Equal Opportunities office took place, where Renita Danabalan was re-elected. We thank Andrea Eismann for her service as Equal Opportunities Officer from 2020 to 2024.

WIAS is committed to diversity, equity, and inclusion. In particular, the active promotion of equal opportunities, including gender equality and opportunities for persons with disabilities, is an important management task at WIAS and is firmly anchored in the institute's mission. In this regard, WIAS scientific management ensures that one of its members takes charge of equal opportunities issues for a period of three years. This rotational appointment is currently held by Dietmar Hömberg, head of Research Group 4 *Nonlinear Optimization and Inverse Problems*, from 2023 to 2025.

audit berufundfamilie. WIAS is committed to fostering a sustainable family- and life-phase-conscious personnel policy that enables its employees to successfully combine their work, family, and private lives. Through measures such as flexible working hours and mobile work, the Institute supports its staff in achieving their professional and private goals.

Since 2013, WIAS has been certified and re-certified as a family-friendly employer by the "audit berufundfamilie." The quality seal of the audit, which is under the patronage of the Federal Ministry for Family Affairs, demonstrates the Institute's ongoing dedication to a sustainable personnel policy that adapts to the diverse needs of employees across various life phases and family circumstances. Following the successful completion of its fourth re-certification in 2023, WIAS was awarded the permanent audit certificate with distinction.

Zertifikat seit 2013
audit berufundfamilie

In 2024, the implementation and continuous enhancement of the family-friendly measures were overseen by project manager Pia Pfau, with the support from management representative Dietmar Hömberg. WIAS employees continued to have complimentary access to the benefit@work family service providing services like counseling on caregiving for relatives, support for parents, mediation of helpers, or confidential advice for personal or professional challenges. For psychological problems or to prevent stress and burnout, employees also had access to professional one-on-one coaching with a qualified therapist. Regular online lectures and workshops addressed topics such as parenting and education, caregiving, health, and fitness. Information about these services and support options was shared with the staff through regular email updates. Employees at WIAS also received circulars on leisure and holiday activities for children, as well as offers for learning support. On December 11, 2024, WIAS hosted a Christmas party for the younger children of its employees. The event featured the Saint Nicholas theme, with storytelling, handicraft activities, and a visit from Saint Nicholas himself. Eight children, accompanied by their parents, enjoyed the party very much.

To ensure accessibility and transparency, the bilingual "Work-Life Balance" section on the intranet provides comprehensive information about the Institute's benefits and services. This platform also documents the progress and future goals of WIAS's family- and life-phase-conscious personnel policy.

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 2024, having raised a total of 3.29 million euros, from which 41 additional researchers[2] (plus 15 outside WIAS; Dec. 31, 2024) were financed. In total in 2024, 24.7% of the total budget of WIAS and 38.7%[2] of its scientific staff originated from grants.

[2] Including scholarship holders.

For a detailed account of projects funded by third parties, the reader is referred to the appendix, Section A.2 Grants below on pages 123ff.

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.

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

Stochastic Analysis in Interaction

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. In Summer 2024, the DFG decided to support the second phase of the IRTG 2544 for another 4.5 years with over four million euros, such that the funding period has been extended until March 2029.
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, the WIAS participated in 2024 with one Ph.D. project running in RG 5 on "Large deviations for dense Erdős–Rényi 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

Research software at different levels of sophistication—from simple scripts to dedicated simulation codes—is indispensable for performing WIAS's knowledge and application-driven research and for transferring research results to industry and other fields of science. The need to implement complex models that are hard to realize with readily available software and to verify and transfer the research results within joint application projects requires the development of dedicated software as a part of the research portfolio of the institute. Several of these research codes and contributions to open source software ecosystems are made available to the scientific community and industrial users with the potential to trigger new scientific cooperations or generate financial revenues. Licensing models depend on the specifics of the corresponding projects. Codes are offered under open source and proprietary licenses as well as combinations thereof. See page 182ff. for a selection of software packages that WIAS made available in 2024.

3 IMU@WIAS

3.1 The Secretariat of the International Mathematical Union

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 (IMU EC), the Secretariat runs the 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 (IMU GA) 2018 passed a resolution to enter into a new and unlimited Cooperation Agreement, which was signed immediately after the 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 IMU Secretariat and IMU Treasurer since July 2020. In his function as the Head of the IMU 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 IMU Secretariat and actively participating in the implementation of the decisions and duties of the IMU EC and the IMU GA, which is done in support of the IMU Secretary General. He communicates with IMU member countries, drafts written materials, writes minutes and reports, and supervises the IMU website. His tasks include steering and overseeing the IMU Secretariat's business operations and IMU finances, as well as monitoring deadlines.

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 facilitating the working operations of both commissions, including provision of support to CDC and ICMI office holders, coordination of meetings, budgetary and policy oversight, reporting and general organization.

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, preparation and facilitation of annual audits, financial reporting, handling membership dues, supervision of third-party funds, all financial aspects of grants, and administering expense reimbursements.

Birgit Seeliger, *IMU Archivist*. B. Seeliger is responsible for the IMU Archive and for developing a strategy for preserving and making paper documents, photos, pictures, and IMU artifacts accessible, as well as supporting the decision process concerning electronic archiving of IMU digital documentation. She further provided administrative support to CWM in 2024.

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 both the hardware and software infrastructure, in particular, the IMU server and mailing lists, and planning the extension of the IMU's IT services for its members, commissions, and committees.

Vanessa Chung, *Community Manager and Grant Administrator*. V. Chung is responsible for coordinating and maintaining various communication activities of the IMU (including social media channels), administering the IMU's grant programs and application platform, and providing additional general support to the activities of the IMU Secretariat.

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 IMU Secretariat in 2024

Over the course of 2024, the IMU Secretariat continued to support the 2023–2026 IMU EC and other office holders. The IMU EC's second meeting of the term took place in March 2024, hosted at the Sydney Mathematics Research Institute (SMRI), University of Sydney, in Australia. The IMU Secretariat provided administrative and organizational support for the meeting. Among the various important topics discussed and decided at the meeting was the composition of the remaining 2026 prize selection committees, the 2026 Fields Medal Committee having already been formed at the 2023 IMU EC meeting. Preparations for the International Congress of Mathematicians (ICM) 2026 in

Philadelphia thus began to increase over the year, and will continue to shape the Secretariat's work over the coming period, as will the organization of the 20th IMU General Assembly, which takes place shortly before ICM 2026.

The IMU Secretariat continued the process of implementing the new grants application platform https://grants.mathunion.org/ for CDC in 2024. The platform has enabled the Secretariat to streamline and centralize the process for applicants, selection committees, and staff alike. All grant programs were successfully transitioned to the platform by summer 2024. To date, the feedback from CDC officers and reviewers, as well as applicants, has been extremely positive. The new program has additionally enabled the IMU Secretariat to take back administrative management of two grant programs, which had been outsourced to external partners. The handover process with the external partners has begun and will continue into 2025.

Fig. 1: *ICM 2026 Logo*

In early 2024, the IMU and CDC—with support from IMU Secretariat staff—successfully secured a three-year grant from the Simons Foundation for its new program, the *IMU-Simons Research Fellowship Program for Developing Countries*, which will run from April 2024 – April 2027. The grant provides USD 200,000 of funding per year to support mathematicians from developing countries with up to USD 15,000 to undertake a research visit of up to three months. As part of the application process, the IMU was certified as equivalent to a public charity in the USA.

The first half of 2024 saw intensive preparations for the ICMI General Assembly and International Congress on Mathematical Education (ICME), which took place in Sydney, Australia, in July 2024. The IMU Secretariat provided extensive administrative and organizational support to the organization of both events, including coordination of scheduling, organization of electronic voting, logistics, and publication of promotional materials around the event. Members of IMU Secretariat staff also provided support on site during the events.

In addition, other projects in 2024 included the ongoing development of an online archive repository and the organization and delivery of several webinars relating to CDC activities.

3.3 Office Committee Visit

The first visit of the 2023–2026 IMU Office Committee (IMU OC) took place at the IMU Secretariat in February 2024. The IMU OC is charged with monitoring the performance of the IMU Secretariat and assessing how it supports the IMU in fulfilling its mission. The IMU OC was newly composed in 2023, with former IMU EC Member-at-Large Luigi Ambrosio taking on the role of chair, and Andrea Solotar (CDC President 2023–2026) and Tamar Ziegler (IMU EC Member-at-Large 2023–2026) joining as new members.

The visit took place over two days. The IMU OC met with the IMU Secretariat leadership and staff over the course of the first day, with follow-up meetings with the IMU leadership on the second day. The IMU OC reported on its findings in April 2024. The report was highly commendatory, praising staff for their positive, purposeful, and engaged work. The IMU OC took note that all recommendations from the previous IMU OC visit in 2021 had been addressed. The 2024 report made an additional recommendation to upgrade the part-time position of IMU Assistant, which has since been realized.

The IMU OC noted with gratitude the invaluable support the IMU receives from WIAS, as well as the generous funding provided by the Federal Republic of Germany and the Land Berlin.

The next IMU OC visit will take place in early 2026, ahead of the IMU GA in New York City in July 2026.

3.4 Key Activities of ICMI in 2024

Frederick K. S. Leung, ICMI President (2021–2024), Jean-Luc Dorier, ICMI Secretary-General (2021–2024), and Lena Koch, ICMI and CDC Administrative Manager

Devoted to the development of mathematical education at all levels, the International Commission on Mathematical Instruction (ICMI) is a commission of the IMU.

ICMI has two constituent bodies: the Executive Committee (ICMI EC) and the ICMI Country Representatives (ICMI CRs) of the member states. Once every four years, the two bodies meet at the ICMI General Assembly (ICMI GA) for one day, prior to the beginning of the International Congress on Mathematical Education (ICME). ICME is the largest worldwide event in mathematics education, gathering around 2,000–3,500 participants involved in the broad enterprise of mathematics education: researchers, mathematicians, teachers, teacher educators, graduate students, curriculum developers, and policy makers.

In 2024, the ICMI GA was held in Sydney, Australia on July 7, 2024. In order to facilitate the participation of as many ICMI CRs as possible, the ICMI GA was held in hybrid mode. Forty-two Representatives were in Sydney and 16 participated online.

Fig. 2: *ICMI General Assembly Meeting, July 7, 2024 in Sydney*

Besides the ICMI CRs, the ICMI EC, the chair of the ICMI Nominating Committee Abraham Arcavi, officers of the ICMI Affiliate Organizations and members of the slate for the 2025–2028 ICMI EC, members of the IMU Secretariat, and a member of the US National Academy of Sciences participated in the ICMI GA. Voting was done electronically, and the 2025–2028 ICMI EC was elected. The support from the IMU Secretariat was crucial to the success of the ICMI GA and the election of the new ICMI EC.

Fig. 3: *ICME-15: "Come and be counted at ICME-15, 7–14 July 2024 at the ICC Sydney, Australia"*

The 15th Congress, ICME-15, was held from July 8 to 14, 2024. IMU President, Hiraku Nakajima, and IMU Secretary General, Christoph Sorger, as well as Paolo Piccione, ICMI liaison from the IMU EC, participated in both events. The Congress gathered 2,322 delegates from nearly 100 different countries, 193 delegates from developing countries being financed through the Solidarity Fund Grant. The program included 4 plenary lectures and 2 panels, 3 awardee lectures, 59 invited lectures, 56 Topic Study Groups divided in 2 streams, 50 Discussion Groups, 70 Workshops, 5 National Presentations, and several other events.

During ICME-15, specific ICMI activities were presented:

- ICMI Studies

ICMI presented its two recently completed Studies, ICMI Study 24 "Mathematics Curriculum Reforms Around the World" (published in 2023) and ICMI Study 25 "Teachers of Mathematics Working and Learning in Collaborative Groups" (published in 2024).

The 2021–2024 ICMI EC launched two new Studies during its term: ICMI Study 26 and ICMI Study 27. Study 26 focuses on the topic of Geometry, emphasizing "the role of geometry as a facilitator of advances in logical reasoning, strategic thinking, and exploring the role of Geometry as an arena or lever for developing children's and adolescents' mathematical creativity and flexible thinking." Study 27 on Mathematics Education and the Socio-Ecological reflects on "what is and might be the role of mathematics and mathematics education in multiple, intersecting, social, political, and ecological issues such as climate change, poverty, inequality, health crises, discrimination, and marginalization."

It is the hope of the ICMI EC that these two Studies will eventually impact classroom teaching, helping students to develop their capacity and habit of systematic, clear, precise, logical, and critical thinking, and become more aware of sociopolitical and ecological issues.

- Awardees Multimedia Online Resources Project (AMOR)

This project aims at building online resources reflecting highly significant and influential research in mathematics education at an international level, that can serve as a reference for researchers, educators, teachers, curriculum developers, policy makers, and other agents in the field. The resources can serve as a basis for a Ph.D. training program and induction into mathematics education research.

- The Capacity and Network Project (CANP)

CANP was created in 2011 and has been central in ICMI's endeavor towards equity and inclusion with an emphasis on initiating and building networks in and across under-represented countries, many of which are also low-income countries. To date, ICMI has supported five such projects; CANP1 (Francophone Sub-Saharan African Region), CANP2 (Central America and the Caribbean), CANP3 (Southeast Asia), CANP4 (East Africa), and CANP5 (Andean Region and Paraguay).

ICMI provides basic support to CANPs to enable systemic, sustainable, and locally grounded networks to promote mathematics education in areas of need identified at the grassroot level. Enhanced knowledge of mathematics is also important for teachers from a perspective of new developments in mathematics, for example, an understanding of the intersections between mathematics, data science, computing, statistics and, perhaps most significantly, technology (see Anjum Halai, Editorial). Four CANP's presented their activities and future plans at an ICME-15 session.

At ICME-15, participants experienced a truly global congress with diversity of participants, speakers and presenters. The congress showed that traditional questions about the learning and teaching of particular areas of mathematics, about teacher education and professional development, are increasingly linked to broader issues, such as inclusive mathematics education, educational inequalities, and the contribution of mathematics education to the development of informed, critical and engaged citizens. Meeting these challenges requires greater recognition of the contributions of the Global South to our community. The search for a better balance between the Global North and the Global South within ICMI has been a major objective of ICMI over the last few decades, even if much remains to be done (see Michèle Artigue's report on her experience at ICME-15).

In the ICMI December 2024 Newsletter Editorial, as outgoing ICMI President, Frederick Leung wrote: "As mathematics educators, we are not just teaching mathematics; we are teaching human beings mathematics. Our students have lives to live, and mathematics is just one of the many things they should learn, albeit a very important one. ... We should help them understand the world and its problems through the lens of mathematics, both as preparation for their future professions and to help them appreciate the relevance of mathematics" (see Frederick K. S. Leung, Editorial).

As the term of this ICMI EC comes to an end on December 31, 2024, we are confident that the next ICMI EC will work with the ICMI worldwide mathematics education community to better prepare our students to face this ever more complicated world.

ICMI wishes to express deep gratitude to the ongoing and vital support provided by WIAS and, in particular, by the IMU Secretariat in the organization of this year's activities.

3.5 Overview of 2024 Meetings and Events

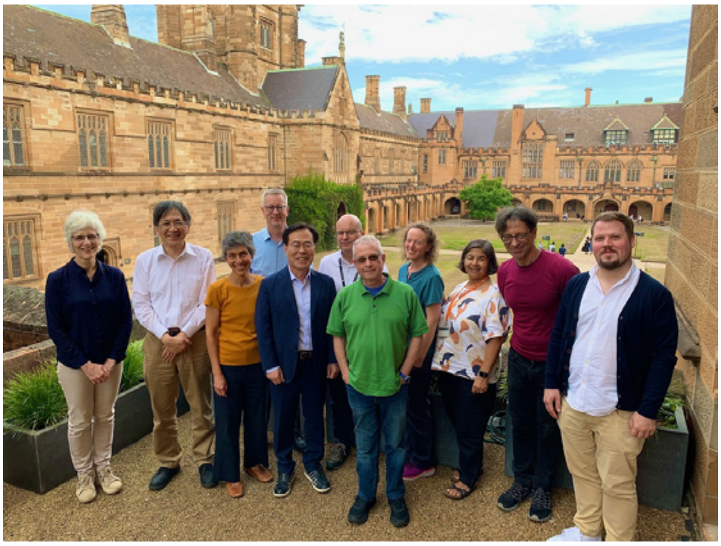


Fig. 4: *IMU Executive Committee Meeting, Sydney, March 2024*

IMU Office Committee Visit IMU Secretariat, Berlin, Germany, February 23–24, 2024. **Participants:** IMU Office Committee: Luigi Ambrosio (chair), Andrea Solotar, Tamar Ziegler; Christoph Sorger, Dietmar Hömberg, Michael Hintermüller, IMU Secretariat staff.

Meeting of the IMU EC, March 23–24, 2024. The second annual meeting of the 2023–2026 IMU EC was hosted by SMRI at the University of Sydney in Sydney, Australia. The meeting was followed by two days of mathematical discussions and talks at SMRI.

Participants: Hiraku Nakajima, Christoph Sorger, Ulrike Tillmann, Tatiana Toro, Nalini Joshi, JongHae Keum, Paolo Piccione, Günter M. Ziegler, Tamar Ziegler, Carlos E. Kenig, Scott Jung. Guests invited for particular agenda items: Dietmar Hömberg, Claire Voisin (ICM 2026 Program Committee, chair), and Jalal Shatah (ICM 2026 Local Organizing Committee, chair).

ICMI Executive Committee Meetings: July 5–6 and July 14, 2024. The final full meeting of the 2021–2024 ICMI EC took place in July 2024 in Sydney, Australia, prior to the ICMI GA. As is customary, there was a further short meeting held after the conclusion of ICME-15 on July 14.

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

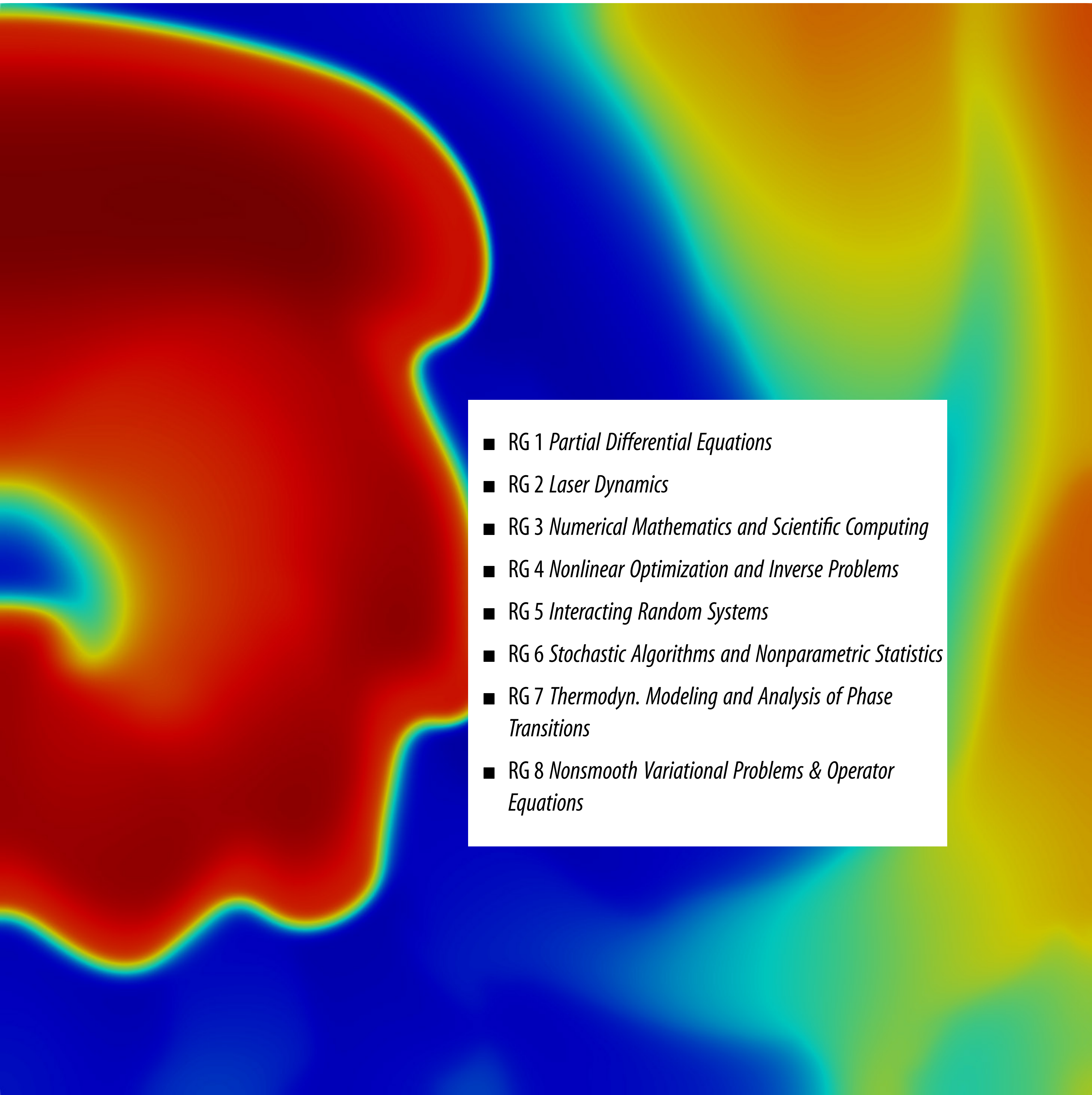
Meeting of the ICMI General Assembly, July 7, 2024. The quadrennial ICMI GA took place in July 2024 in Sydney, Australia. At the GA, the office holders for the ICMI EC for the 2025–2028 term were elected.

Participants: ICMI EC members, IMU EC liaison person, ICMI Administrative Manager, IMU Manager, and over 50 Country Representatives from around the world.

15th International Congress on Mathematical Education (ICME-15), July 7–14, 2024. ICME-15 took place in July 2024 in Sydney, Australia. There were close to 2,500 attendees during the congress.

Guests at the Secretariat. Bernard R. Hodgson, Curator of the ICMI Archive, visited the IMU Archive between May 21–25, 2024. Former IMU Secretary Helge Holden visited the IMU Secretariat on September 6, 2024, in his capacity as Chair of the 2026 Nominating Committee. Former IMU Secretary General Martin Grötschel visited the Secretariat in 2024 together with David Spergel, President of the Simons Foundation.

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 (acting):	Priv.-Doz. Dr. Matthias Liero
Team:	Dr. Thomas Eiter Dr. Janusz Ginster Priv.-Doz. Dr. Annegret Glitzky Dr. Martin Heida Dr. Georg Heinze Dr. Michael Kniely (long-term guest) Dr. Thomas Koprucki Dr. Anieza Maltsi (Iris Runge Postdoctoral Program of WIAS) Dr. Michael O'Donovan Willem van Oosterhout Dr. Dirk Peschka Anastasija Pešić Dr. Joachim Rehberg Stefanie Schindler Priv.-Doz. Dr. Burkhard Schmidt Dr. Artur Stephan Prof. Dr. Marita Thomas Michael Tsopanopoulos (long-term guest)
Team Assistant:	Andrea Eismann
Nonresident Members:	Prof. Dr. Alexander Mielke Prof. Dr. Jürgen Sprekels

The research group focuses on the analytical understanding of partial differential equations (PDEs) and their application to modeling in the natural sciences and engineering. Theoretical developments are closely linked to well-chosen problems in applications, primarily in the following areas:

- Nonlinear material models and multiscale problems in continuum
- Modeling of semiconductors, particularly for opto-electronic devices and quantum technologies
- Systems of evolution equations, including reaction-diffusion systems, Navier–Stokes equations

The methods employed include topics from pure functional analysis, mathematical physics, pure and applied analysis, the calculus of variations, and numerical analysis. Special emphasis is placed 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 with nonsmooth coefficients. Corresponding scientific software tools are developed in collaboration with other research groups.

In 2024, the group was successfully involved in cross-disciplinary projects in the Berlin Mathematics Research Center MATH+, in the DFG Collaborative Research Centers CRC 1114 *Scaling Cascades in Complex Systems* and CRC 388 *Rough Analysis, Stochastic Dynamics and Related Fields*, the DFG Priority Programs SPP 2410 *Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness*, SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*, and SPP 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Surfaces*, and in the NFDI consortium "Mathematical Research Data Initiative" (MaRDI). Moreover, members of RG 1 coordinated the project “UV Lasers: From Modeling and Simulation to Technology” (UVSimTec) in the framework of the Leibniz competition. Together with RG 2 *Laser Dynamics*, RG 1 contributed to the WIAS Focus Platform “Simulation of Semiconductor Devices for Quantum Technologies” (SemQTech).

Highlights

Georg Heinze successfully defended his Ph.D. thesis entitled “Graph-based nonlocal gradient systems and their local limits” in March and was appointed as a member of the GAMM Juniors in October. Alexander Mielke, former head and nonresident member of RG 1, was awarded the ISIMM Senior Prize 2024 by the International Society for the Interaction of Mechanics and Mathematics at the bi-annual “Symposium on Trends of Applications of Mathematics to Mechanics” in April.

The proposal for the DFG Transregio Collaborative Research Center CRC/TRR 388 *Rough Analysis, Stochastic Dynamics and Related Fields* was successfully defended in January 2024. Together with RG 6 *Stochastic Algorithms and Nonparametric Statistics*, RG 1 contributes via the subproject A2 “Optimal transport meets rough analysis.” This project applies methods and ideas from optimal transport theory to study probabilistic structures of equations amenable to a rough path type.

Optoelectronic and quantum technologies

The research group maintains strong collaborative ties with RG 2 *Laser Dynamics*, RG 3 *Numerical Mathematics and Scientific Computing*, and LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*. The Focus Platform SemQTec continues to advance semiconductor quantum computer development through joint efforts. The UVSimTec project, funded by the Leibniz competition, involves partnerships with key institutions like the Ferdinand-Braun-Institut (FBH), Leibniz-Institut für Kristallzüchtung (IKZ), Technische Universität Berlin, and the Friedrich-Alexander Universität Erlangen-Nürnberg.

In the Berlin Mathematics Research Center MATH+, RG 1 is involved in the subprojects AA2-17 “Coherent transport of semiconductor spin-qubits: Modeling, simulation and optimal control” (with RG 2 and Technische Universität Berlin) and AA2-21 “Strain engineering for functional heterostructures: Aspects of elasticity” (with Humboldt-Universität zu Berlin).

Multiscale models for UV-C light emitters. Aluminum gallium nitride alloys, (Al,Ga)N, are attractive for devices operating in the UV-C spectrum ($\lambda < 280$nm) due to their tunable direct band structure and wide band gap. To guide experimental design, simulations should capture the key physics—including alloy-disorder-induced carrier localization effects and composition- and microstructure-dependent optical polarization. Together with RG 3, LG NUMSEMIC, and Tyndall National Institute (Cork, Ireland), a multiscale framework connecting atomistic tight binding to drift diffusion was constructed. To account for band mixing, which leads to changes in the optical polarization of the emission, a hybrid effective mass (EM) model was built which takes input from atomistic simulations of (Al,Ga)N quantum wells.

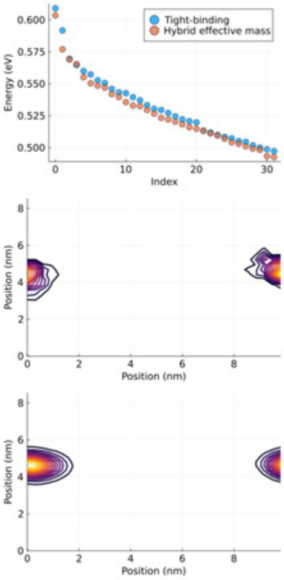


Fig. 1: *Energy of first 30 hole states from TB and hybrid EM (top); hole ground state in TB (middle) and hybrid EM (bottom)*

The hybrid EM model was benchmarked against atomistic tight-binding (TB) calculations. A direct comparison can be made as the simulations operate on the same energy landscape. The energy separation between states is in good agreement between the hybrid EM and TB models (top of Figure 1). This difference depends on the mass, indicating that the derived effective mass is close to the correct value. The band edge offset within the quantum well was adjusted to provide good agreement between the energy scales. The hole ground state charge density was also compared between tight-binding and hybrid EM models (middle and bottom of Figure 1). The position expectation value is similar between the TB and EM models, however, the localization is weaker in the EM model.

Vacancy-assisted charge transport models for perovskite solar cells. Perovskite solar cells are a groundbreaking technology in photovoltaics, expecting a significant impact on the field of renewable energies. Its progress is based on perovskite materials' outstanding optical and electronic properties. Modeling the transport of charge carriers is typically based on a drift-diffusion system consisting of the Poisson equation for the electrostatic potential and continuity equations for all mobile charge carriers: electrons and holes as well as ionic vacancies in the perovskite subdomain. Exemplary simulations with varying mobility of the ionic vacancies demonstrate the necessity to include the migration of ionic vacancies in the modeling, see Figure 2.

In cooperation with LG NUMSEMIC, analytical investigations for the instationary drift-diffusion model for perovskite solar cells including Fermi–Dirac statistics for electrons and holes and Blakemore statistics for the mobile ionic vacancies in the perovskite layer were carried out. The free energy functional is related to this choice of the statistical relations. The existence of weak solutions follows from introducing a regularized version of the system, a time discretization argument, and Moser iteration techniques, see [4]. In WIAS Preprint no. 3142, the uniqueness of weak solutions to the instationary drift-diffusion model was established. Improved integrability of the gradients of charge-carrier densities was derived, and regularized continuity equations with partially frozen arguments were analyzed. Regularity results for scalar quasilinear elliptic equations, as presented by Meinlschmidt & Rehberg (2016), were applied. This work provides a rigorous mathematical framework for understanding charge transport in perovskite solar cells, contributing to the reliability of these models for further research and development.

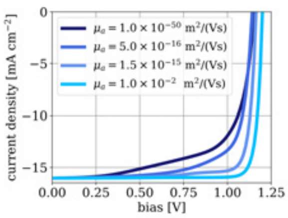


Fig. 2: *Current-voltage relations simulated for different mobilities of the ionic vacancies*

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. RG 1 cooperates with RG 4 *Nonlinear Optimization and Inverse Problems* in the subproject "Analysis of energy-variational solutions for hyperbolic conservation laws" within the Priority Program SPP 2410.

In the newly approved DFG Transregio Collaborative Research Center CRC/TRR 388 *Rough Analysis, Stochastic Dynamics and Related Fields*, RG 1 and RG 6 are running the subproject A2 “Optimal transport meets rough analysis.”

Self-similar patterns in coupled parabolic systems. Self-similar behavior is a well-studied phenomenon in (spatially) extended systems. However, most research has focused on scalar problems with exact self-similar solutions, such as the porous medium equation. Moreover, solutions are usually considered with trivial behavior at infinity, particularly in the case of finite mass or energy.

In the paper [3], a coupled nonlinear reaction-diffusion system on the real line was studied, where the reactions of the species are given by one reversible reaction pair $\alpha X_1 \rightleftharpoons \beta X_2$ satisfying the mass action law. Additionally, it is required that the solutions are prescribed at infinity by states that are in reactive equilibrium. These nontrivial limits at infinity can be interpreted as reservoirs with an infinite supply of mass on both sides of infinity, and it is explained how the mass flows from one mass reservoir to the other. By rescaling time and space according to the parabolic scaling, that is $\tau = \log(1+t)$ and $y = x/\sqrt{1+t}$, it is shown that solutions converge exponentially to a self-similar profile when the scaled time τ goes to infinity. In the original variables, these profiles correspond to asymptotically self-similar behavior describing how the solutions mix the steady states in the sense of diffusive mixing.

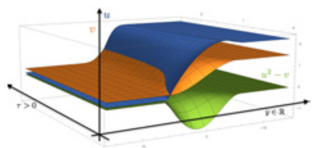


Fig. 3: *Behavior of solutions in scaled coordinates for $\alpha = 1$ and $\beta = 2$. Slow diffusive equilibration of concentrations u (blue) and v (orange) for two species X_1 and X_2, respectively, while net reaction $u^2 - v$ (green) decreases fast.*

Far-field structure of oscillatory flows. Oscillatory behavior of fluid flows can be observed in many situations in nature, for instance, around an oscillating body like a swimming fish or as cloud patterns behind mountain peaks, resembling a Kármán vortex street. To better understand the behavior of such time-periodic flows, their principal structure far away from the obstacle is investigated analytically. These insights can also be useful for the numerical implementation of such fluid-flow problems in unbounded domains.

In the joint article [1] with Ana Leonor Silvestre (University of Lisbon), time-periodic solutions to the Navier–Stokes equations were investigated that describe the flow of a viscous incompressible fluid past an obstacle. Implicit representation formulas for the velocity and pressure field of the fluid were derived, relying on the time-periodic fundamental solutions of a suitable linearization, the *Oseen equations*. From these formulas, far-field expansions of time-periodic solutions are obtained, which lead to sharp pointwise estimates as well as necessary and sufficient conditions for specific decay rates. In particular, the analysis revealed new terms showing that, in comparison with a steady flow, the decay rates of the velocity coincide, while the pressure of a general time-periodic flow decays at a slower rate.

Materials modeling and multiscale problems

The research in this topic was done in cooperation with RG 5 *Interacting Random Systems*, RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, and the Freie Universität Berlin. RG 1 participates in the Collaborative Research Center CRC *1114 Scaling Cascades in Complex Systems* via subproject B09 "Materials with discontinuities on many scales," and in the Priority Program SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*. RG 1 is also involved in the project AA4-8 "Recovery of battery aging dynamics with multiple timescales" within the Berlin Mathematics Research Center MATH+ with RG 4 and RG 7 and in the project PaA-2 "Modeling battery electrodes with mechanical interactions and multiple phase transitions upon ion insertion," jointly with RG 7, that was successfully acquired within MATH+.

Gradient systems on metric graphs. Transport of quantities on graphs is a relevant problem that arises in many areas of science, e.g., traffic on road networks, the distribution of gas in pipeline networks, or in population dynamics. In the joint work [2] with Jan-Frederik Pietschmann (Universität Augsburg) and André Schlichting (Universität Ulm), evolution equations on metric graphs with reservoirs were studied. Metric graphs are graphs where a one-dimensional interval is associated to each edge and, in addition, the vertices are able to store and exchange mass with these intervals.

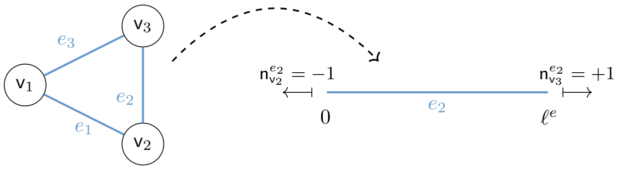


Fig. 4: *Example of a complete three-state metric graph defined in terms of the nodes* $\mathsf{V} = \{\mathsf{v}_1, \mathsf{v}_2, \mathsf{v}_3\}$, *edges* $\mathsf{E} = \{e_1, e_2, e_3\}$ *with* $e_1 = \mathsf{v}_1\mathsf{v}_2$, $e_2 = \mathsf{v}_2\mathsf{v}_3$, $e_3 = \mathsf{v}_3\mathsf{v}_1$ *with assigned one-dimensional intervals of lengths* $\ell : \mathsf{E} \to (0, \infty)$

Focusing on the case where the evolution is driven by an entropy functional defined both on the metric edges and vertices, they provided a rigorous understanding of such systems of coupled ordinary and partial differential equations as (generalized) gradient flows in continuity equation format. Approximating the edges by a sequence of vertices, which yields a fully discrete system, existence of solutions was established in this formalism. Furthermore, several scaling limits were studied using the recently developed framework of Energy-Dissipation-Principle (EDP) convergence with embeddings to rigorously show convergence to gradient flows on reduced metric and combinatorial graphs. Finally, numerical studies confirmed the theoretical findings and provided additional insights into the dynamics under rescaling.

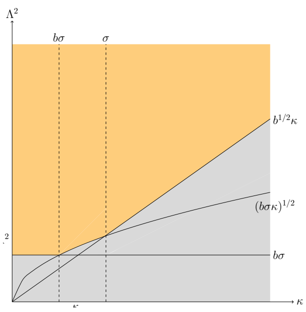


Fig. 5: *Sketch of the scaling law result. Parameter* $\Lambda > 0$ *is a coupling coefficient.*

Pattern formation in biomembranes. Biological membranes are lipid bi-layers surrounding the interior of the cells. For most eukaryotic organisms, it is hypothesized that two types of lipids (saturated and unsaturated) form nanoscale microdomains within the membrane, commonly referred to as *lipid rafts*. In [5], a variational model for this domain formation was investigated. The driving term in the proposed energy is a coupling between the approximation of the local curvature of the membrane and the order parameter, related to the local chemical composition. A scaling law for the infimal energy with respect to critical parameters of the model was derived. The scaling law is sketched in Figure 5 with the two colors representing two distinct scaling regimes. The gray area corresponds to the regimes where uniform structures are preferred, while the orange area corresponds to the regimes for which pattern formation is energetically favorable. As a main tool, new nonlinear interpolation inequalities that bound fractional Sobolev seminorms in terms of a Cahn–Hillard/Modica–Mortola energy were established.

Mathematical Research Data

The Mathematical Research Data Initiative (MaRDI), funded since October 2021, is the mathematical consortium within the *German Nationale Forschungsdateninfrastruktur (NFDI)*. The goal of MaRDI is building 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. MaRDI is currently working in its fourth year and is actively developing services for the community, such as a knowledge graph on mathematical models (mardi4nfdi.github.io/MathModDB/), that are developed within RG 1. These and other services are about to be integrated into the MaRDI Portal making it a central one-stop point of access. To foster this interdisciplinary cooperation, the *NFDI_BB* network was established, comprising all NFDI consortia in the Berlin-Brandenburg area. In July 2024, an *NFDI_BB* workshop on ontologies and knowledge graphs was organized jointly with RG 6 at the WIAS. Further workshops are planned on a bi-annual basis.

Workshops

The workshop "Optimal Transport from Theory to Applications: Interfacing Dynamical Systems, Optimization, and Machine Learning" (OT-DOM) took place at the Humboldt-Universität zu Berlin from March 11 to 15. It was organized jointly with RG 6, WG DOC, and Gabriele Steidl (Technische Universität Berlin). The emphasis was on the interaction between optimal transport and statistics, machine learning, imaging, optimization, and dynamical systems.

Fig. 6: *Prof. Olga Mula (Eindhoven UT) gives a talk at the OT-DOM workshop*

The international workshop "AMaSiS 2024: Applied Mathematics and Simulation for Semiconductor Devices" was organized jointly with RG 2, LG NUMSEMIC and Josef Weinbub (Silvaco Vienna) as part of the event series "Thematic Einstein Semester: Mathematics for Quantum Technologies." It was held at the Humboldt-Universität zu Berlin and the Leibniz Headquarters from September 10 to 13. AMaSiS 2024 had its focus on the mathematical modeling and numerical simulation of semiconductor devices. It dealt with quantum and semiclassical transport, electronic structure theory, computational materials science, and upscaling from quantum mechanics and particle systems to continuum scale modes.

Fig. 7: *Participants of AMaSiS 2024*

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4.2 Research Group 2 "Laser Dynamics"

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Team Assistant:	Veronica Bove

The research of this group is devoted to the study of mathematical problems that appear in nonlinear optics, optoelectronics, and quantum devices. These activities include mathematical modeling, theoretical investigation of fundamental physical effects, implementation of numerical methods, efficient modeling and simulation of complex devices, and development of related mathematical theory, mostly in the field of *dynamical systems*. The group mainly contributes to the WIAS main application area *Nano- and Optoelectronics*, and in particular to the application-oriented research topics *dynamics of semiconductor lasers*, *pulses in nonlinear optical media*, and *quantum models for semiconductors*.

In 2024, external funding was received within the Cluster of Excellence MATH+, 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 subproject AA2-17 "Coherent transport of semiconductor spin-qubits: Modeling, simulation and optimal control" together with the TU Berlin and RG 1 *Partial Differential Equations*. Collaboration partners in AA2-17 are the Rheinisch-Westfälische Technische Hochschule Aachen (RWTH), the JARA 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 *Numerical Mathematics and Scientific Computing*, LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*, 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 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). At the end of 2024, the group started the new project "Diode Laser Pump Sources for High-Energy Lasers in Fusion Power Plants" (DIOHELIOS) together with the FBH, funded by the Federal Ministry of

Berlin Mathematics Research Center MATH+

Leibniz Competition

DFG Deutsche Forschungsgemeinschaft

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Education and Research (BMBF). Moreover, since 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. A highlight in 2024 was the organization of the Thematic Einstein semester "Mathematics for Quantum Technologies" funded by MATH+ and the Einstein Foundation Berlin. It provided the opportunity to shed light on the mathematical aspects of the rapidly developing fields of quantum information processing, quantum cryptography, and quantum metrology by bringing together young researchers and experienced scholars from mathematics, theoretical physics, engineering, and related disciplines in a number of workshops, a summer school, and further activities.

Dynamics of semiconductor lasers

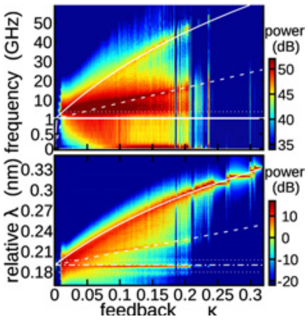

Fig. 1: *Radiofrequency and optical spectra mappings with increasing feedback. Lines mark spectral peaks predicted by mode analysis.*

Hierarchy of traveling wave models for study of semiconductor lasers. In collaboration with Prof. Deb Kane (Australian National University, Canberra), we continued the investigation of irregular dynamics in semiconductor lasers (SLs) with optical feedback from long external cavities (ECs) [1]. It is well known that significantly delayed optical feedback destabilizes steady-state emission, leading to chaotic lasing behavior commonly referred to as coherence collapse. This complex dynamic arises from the interaction of hundreds or even thousands of optical modes induced by the EC.

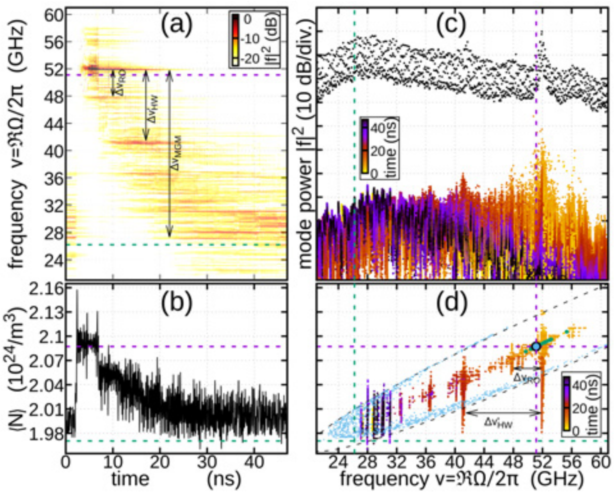

Fig. 2: *Mode analysis of the TW model for a semiconductor laser with delayed optical feedback. For more details, see [1].*

Our study employed the traveling-wave (TW) model (a 1+1-dimensional partial differential equation) and the LDSL-tool software kit to simulate and analyze the SL-EC system. The extensive set of optical modes were explored for comprehensive time-frequency domain representation of optical fields and carriers (Figure 2). Together with the calculated steady-state positions (shown as dashed loops in Figure 2(d)), our mode analysis allowed us to identify the origins of prominent resonance peaks observed in the computed radio frequency and optical spectra (highlighted by different white lines in Figure 1). Notably, we demonstrated the critical role of exceptional points (also known as *mode degeneracies*) in the emergence of low-frequency fluctuations within the system.

As a part of the Leibniz Collaborative Excellence project PCSELence, we developed simulation tools suited to support the design of all-semiconductor high-power photonic-crystal surface-emitting lasers (PCSELs) at the FBH. For more details, see the Scientific Highlights article on page 10.

Polarized frequency combs in a mode-locked VECSEL. We proposed a spin-flip-delay model for vertical external cavity lasers (VECSEL) with semiconductor saturable absorber mirrors, accounting for phase and amplitude anisotropies and their impact on polarization dynamics. The model shows that birefringence-induced refractive index anisotropy alters cavity round-trip times for orthogonal polarizations, leading to two linearly polarized pulse trains with different repetition rates. This results in the generation of two optical frequency combs with distinct line spacings, illustrating birefringence's effect on mode-locking dynamics. The model offers a framework for studying polarization-dependent behavior in mode-locked lasers.

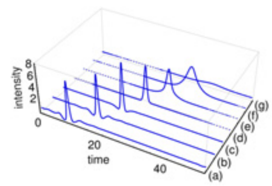

Fig. 3: *Soliton solutions of the NDDE model (a)*

Pulses in nonlinear optical media

Kerr cavity optical frequency combs. We developed a second-order neutral delay-differential equation (NDDE) model for a Kerr cavity with coherent optical injection [2], offering an approach beyond the mean-field limit of the Lugiato–Lefever equation (LLE). The NDDE model reveals dissipative solitons near, see Figure 3, and beyond the LLE limit, where they are destabilized by Cherenkov radiation. In contrast to the LLE, it captures overlapping resonances of different cavity modes. The flexibility of the model extends its use to various optical systems, including mode-locked lasers and coupled cavities. Desynchronization is mainly driven by an Andronov–Hopf bifurcation (see Figure 4), limiting synchronization when the injection pulse is wide. A criterion was proposed that links this bifurcation to the soliton's maximum displacement and the point where the injection pulse amplitude drops to a critical value, corresponding to a saddle-node bifurcation in the LLE with uniform injection. Numerical and analytical evidence validate this criterion. Synchronization of soliton frequency combs under pulsed laser injection was studied with the NDDE model. Solitons synchronize when injection pulses occur every M-th cavity round trip, with pulse amplitude scaled by M. This expands the synchronization range but increases energy costs, as pulse intensity scales with M^2.

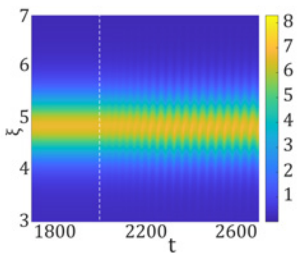

Fig. 4: *Transition from a stationary to an oscillating soliton via an Andronov–Hopf bifurcation*

Split-step methods for the pulse propagation equations. The numerical solution of the generalized nonlinear Schrödinger equation (GNLSE) by splitting methods, which are extremely fast and easy to implement, can be disturbed by so-called *spurious instabilities* looking like normal wave-mixing interactions (see Figure 5), but taking place at the edges of the numerical spectrum. A preliminary analysis of such instabilities for the simplest GNLSE splitting was performed in 2023.

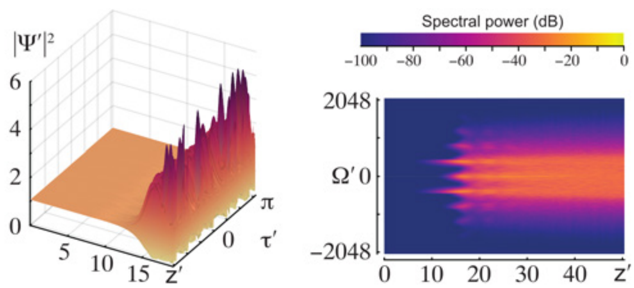

Fig. 5: *Development of a four-wave mixing instability in time (left panel) and frequency (right panel) domains. The numerical instabilities, which might appear at the edge of the spectrum, should be avoided.*

In collaboration with Prof. Raimondas Čiegis (Vilnius Gediminas Technical University, Lithuania), we extended the preliminary results in two aspects. First, we analyzed the numerical instabilities for an arbitrary multiplicative splitting and derived a general stability criterion [4]. Second, the

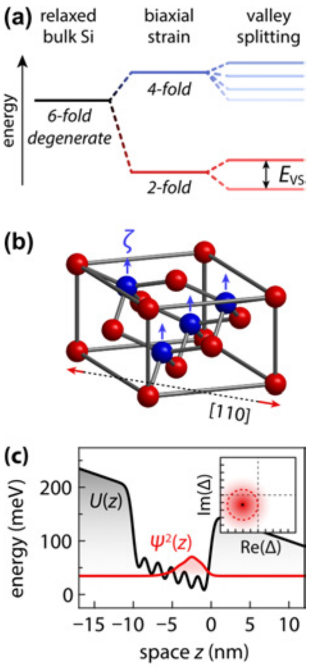

Fig. 6: *(a) Level scheme of strained silicon qubits. (b) Shear-strain induced deformation of the silicon crystal. (c) Electron density distribution and statistical distribution of the complex-valued intervalley coupling parameter (inset) for the long-period wiggle well.*

analysis was extended to three known additive splittings, one of which was found at WIAS in collaboration with Kurt Busch (Humboldt-Universität zu Berlin). In all cases, we were able to provide recommendations for practical applications of the split-step GNLSE solvers. All numerical schemes are implemented in a Julia package, which will be made publicly available at a later stage.

Simulation of semiconductor devices for quantum technologies

Electron spin-qubits in silicon-germanium (SiGe) heterostructures are a major candidate for the realization of scalable quantum computers. A critical challenge in strained Si/SiGe quantum wells (QWs) is the existence of two nearly degenerate valley states at the conduction band minimum that can lead to leakage of quantum information. To address this issue, various strategies were explored to enhance the *valley splitting* (i.e., the energy gap between the two low-energy valley states), such as sharp interfaces, oscillating Ge concentrations in the QW (known as "wiggle wells"), and shear strain engineering. We developed a comprehensive envelope-function theory augmented by nonlocal empirical pseudopotentials to incorporate the effects of alloy disorder, strain, and resonances across multiple Brillouin zones [5]. The model was applied to compute the valley splitting in a number of different heterostructures. Particular focus is on the long-period wiggle well, where strong deterministic enhancements can be achieved in the presence of shear strain, which breaks a nonsymmorphic screw symmetry of the crystal that otherwise inhibits the corresponding resonance mechanism. Our framework provides an efficient tool for quantifying the interplay of multiple physical mechanisms governing the valley splitting and paves the way to advanced epitaxial profile optimization.

References

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

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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). The main focus is on finite element and finite volume space discretization methods. A recent achievement in this respect is the publication of a new monograph on monotone discretizations for elliptic problems by V. John and his coauthors [1], see the corresponding highlight article on page 27. Many of the research topics of the group have been inspired by problems from applications in the field of physics-based data assimilation for medical imaging (in cooperation with RG 6 *Stochastic Algorithms and Nonparametric Statistics*), 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). Below, we outline some topics which were in the focus of the group during 2024.

Handling shape variability for data-driven simulation of blood flows

Mathematical modeling and simulation provide valuable tools to support image-based diagnosis combining available data and physical models, and providing additional insights also in the case of scarce medical data. In computational hemodynamics, possible applications include the quantification of biomarkers, such as pressure gradients or pathological velocity profiles, for early stage diagnosis and for post-operative monitoring.

This research, supported by the Berlin Mathematics Research Center MATH+ and in collaboration with the Institute of Computer-assisted Cardiovascular Medicine of the Charité, Berlin, focuses on the assimilation of medical data for the estimation of selected quantities of interest in the case of aortic coarctation (narrowing of the aorta). Blood flow in large vessels can be modeled using the incompressible Navier–Stokes equations for velocity and pressure, accounting, if necessary, for the arising of turbulent flows. The physical and geometrical complexity of flow simulations yields high computational costs. This aspect is particularly relevant for inverse problems, such as parameter and model state estimation from data, where typically multiple solutions of the associated physical model are required. For the efficient solution of inverse problems, our goal is to develop, analyze, and validate suitable methods exploiting the knowledge and the information from previous CFD simulations of aortic blood flow on a large cohort of real and virtual patients for training linear reduced-order models or deep neural networks.

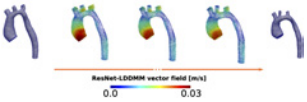

Fig. 1: *Sketch of the registration between two different geometries*

To develop robust surrogate models with predictive value, it is necessary to handle the geometrical variability across different patients, by *registering* the different patient geometries (i.e., finding suitable—smooth—maps between pair-wise computational domains) and mapping the physical solutions onto a common reference shape.

Our approach is based on the so-called *large deformation diffeomorphic metric mapping (LDDMM)*. Each aortic surface is described by a point cloud of arbitrary size, and the registration is sought in terms of the flow of an ordinary differential equation defined via a residual neural network, trained with a cost functional tailored to the case of aortic shapes, and taking into account the individual geometries (surface point cloud), on the vessel centerlines, and on the topology of surface meshes. The optimization is performed in a multigrid fashion, refining the surface mesh during the execution and allowing for the efficient handling of realistic meshes [2].

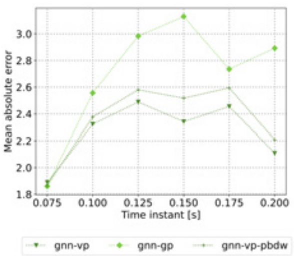

Fig. 2: *Pressure drop errors using the geometry (gnn-gp), the velocity solution (gnn-vp) and limited velocity observations (gnn-vp-pbdw)*

The considered dataset contains 776 (synthetic and real) patients, divided in 724 training and 52 test shapes. The computed registration maps yield a normalized Chamfer distance (standard distance between point clouds, rescaled by the vessel diameter) below 0.5% in average. The computed maps between a reference shape and the other patient geometries are used to map the individual solutions of the Navier–Stokes equations onto the reference domain and train different neural networks allowing to estimate the pressure field and pressure-related biomarkers from (i) the patient geometry, (ii) the velocity field, and (iii) partial velocity measurements.

Mass conservative reduced basis solver for multiscale heterogeneous catalysis with flow

The group has ongoing joint projects with the Fritz Haber Institut (FHI) and the Institute of Chemical and Process Engineering at the Technische Universität Berlin related to physically consistent simulation of heterogeneous catalysis with the aim to help interpreting and steer measurements, e.g., in in-situ surface characterization experiments. The endeavor involves several challenges, namely accurate modeling of the reaction processes at the catalytic surface, mass-conservative transport of the reactants through the possibly complicated experimental reaction chamber, e.g., an X-ray photoelectron spectroscopy (XPS) chamber as depicted in Figure 3, and a fast solving strategy.

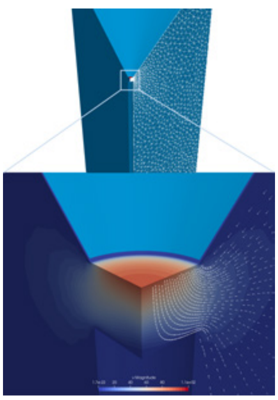

Fig. 3: *Axisymmetric velocity field in an XPS chamber*

The surface reactions are described by a *turnover frequency function* (TOF) that determines the reactivity of the present/modeled reactions under the current reaction conditions, e.g., species concentrations, temperature, and pressure. The ongoing DFG project "Atomistic-continuum coupling for heterogeneous catalysis by a reduced basis approach and multilevel on-the-fly sparse grid interpolation" aims at an accurate yet efficient evaluation of the TOF via on-the-fly first-principle kinetic Monte–Carlo methods (kMC) and a mass conservative reduced basis approach. The reduced basis consists of a set of basis functions that solve a suitably linearized reaction-diffusion-advection operator for one segment of the catalytic boundary. Therein, a divergence-free flow field is utilized that stems from a pressure-robust Navier–Stokes solver. The divergence constraint ensures physical bounds for the species concentrations obtained via a conservative finite volume method. Without the preservation of the exact divergence constraint, violations of the maximum principle are possible, see Figure 4. The discretization also works in axisymmetric problems via a reformulation in cylindrical coordinates.

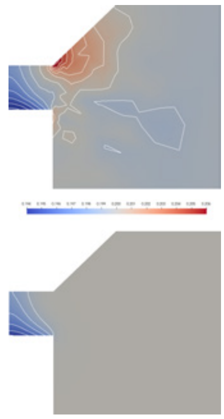

Fig. 4: *Species concentrations without (top) and with (bottom) mass conservative reduced basis*

The reduced basis solver is developed in Julia, based on the finite element and finite volume methods developed in the group and implemented in the context of the `WIAS-PDELib` framework described below. It is currently coupled to the kMC models with an on-the-fly sparse grid interpolation developed at FHI. The idea here is to use an interpolant of the kMC model that is locally refined upon request by the query points in the parameter domain of the TOF that are communicated by the Newton solver. Here, the surrogate values at the initial guesses do not need to be as accurate as the evaluations at later query points. The adaptive refinement along such a solver path is illustrated in Figure 5. In that way, the sparse grid surrogate learns the relevant features of the TOF similar to a neural network.

Surprisingly, already a very coarse reduced basis approach with a single basis function, representing a constant reactivity across the whole (small) catalytic surface, works very well in actual applications. This was demonstrated in a recent publication [3]. Since the approach allows for very fast evaluations of the parameter-to-solution map, it is well suited for using it to solve inverse problems in future.

Currently, it is assumed that the mixture is dominated by a non-reactive buffer species such that an incompressible flow solver can be employed. However, also compressible flow solvers are studied further and incorporated in future. Recently, a hybrid discontinuous Galerkin method was suggested that ensures gradient-robustness and mass-conservation also in a compressible setting [4]. Gradient-robustness, like pressure-robustness in the incompressible setting, ensures that gradients in the momentum balance are correctly balanced by the pressure and do not cause discretization errors of the velocity field. This is an important structural property of a flow solver especially in situations with small viscosities and dominant pressure forces.

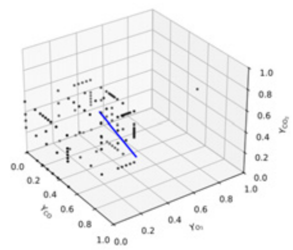

Fig. 5: *Sparse grid interpolation points (black) necessary to query the TOF surrogate along a solver path (blue line)*

Numerical methods and software for coupled PDEs

The group has a long tradition in conveying its research results in the field of design and numerical analysis of finite element and finite volume discretization methods for partial differential equations in the form of software, which can be used in various application projects. The previous generation of the software developed by the group included the PDE solver libraries `ParMOON` and `pdelib` implemented in C++/Python, and the mesh generator `TetGen`.

In recent years, these efforts shifted to new, more flexible and interoperable implementations in the Julia programming language, resulting in `WIAS-PDELib`, a collection of open-source Julia packages. They are registered in the Julia general registry and managed in a common GitHub organization in order to support flexible ways of interaction between the developers and the implementation of joint software quality standards regarding documentation, continuous integration, and code formatting.

Along with the finite volume solver `VoronoiFVM.jl` and the finite element solver `ExtendableFEM.jl`, packages for sparse matrix assembly, for creation, management, and partitioning of simulation grids, and for visualization are provided. On the other hand, differential equation system solvers, linear system solvers, automatic differentiation, core plotting tools, and other important components are taken from the Julia open-source package ecosystem.

Automatic differentiation is used in the assembly of Jacobi matrices of nonlinear systems of equations in `VoronoiFVM.jl` and `ExtendableFEM.jl`. These packages are used in an increasing number of WIAS projects like the one described above and projects on modeling and simulation of semiconductors, perovskites, and nanowires, lasers, quantum devices, ion channels in cooperation with RG 1, RG 2, RG 7, and LG NUMSEMIC.

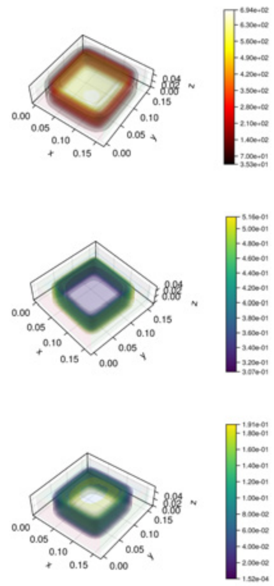

Fig. 6: *CO_2 reduction to CO in a photo-thermal catalytic reactor (Z dimension increased 10x). Top: temperature, center: CO_2 molar fraction, bottom: CO molar fraction.*

The visibility as open-source packages gives rise to new cooperations. For example, together with the Weierstrass Group *Multi-species Balance Laws* and the Institute of Solar Research of the German Aerospace Center (DLR), we developed a simulation code for photo-thermal reactors based on improved models for reactive flows of non-isothermal gas mixtures in porous media. It was implemented with the help of `VoronoiFVM.jl`. Figure 6 shows three-dimensional simulation results for such a photo-thermal reactor heated via insolation from the top, where the gas mixture flows from top to bottom, and one observes conversion of CO_2 to CO.

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4.4 Research Group 4 “Nonlinear Optimization and Inverse Problems”

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Dr. Holger Heitsch
Nina Kliche
Dr. Robert Lasarzik
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Dr. Sophie Luisa Plato
Dr. Andreas Rathsfeld
Janina Schütte
Dr. David Sommer

Team Assistant: 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 Conversion, Storage and Distribution of Energy, 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.

In the following, selected scientific achievements of the research group’s work in 2024 are detailed.

Stochastic and nonsmooth optimization

One of the basic research directions of RG 4 is stochastic and nonsmooth optimization. It is closely tied with participations in the research 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 (gas network optimization) was continued within the third and last funding period. Within MATH+, one project is devoted to weakly coupled mini-grids and another one to SARS-CoV-2 risk assessment and vaccine design (with Max von Kleist and Claudia Schillings, Berlin). The funding of the running PGMO project on "Optimal control problems with probabilistic constraints" (with Hasna Zidani, Rouen, and Wim van Ackooij, Paris) was terminated in 2024 and replaced by two new projects, one on probabilistic least squares and another one on chance-constrained linear complementarity problems (with Martin Schmidt, Trier), each of them funded for one year.

The major research in TRR 154 and PGMO was revolving around optimality conditions of risk averse control problems with uniform state chance constraints. These efforts led to the publications [1, 4]. For instance, in cooperation with RG 8, we were able to derive in [4] necessary and sufficient optimality conditions for such a problem governed by an elliptical partial differential equation (PDE). Here, one had to consider the potentially nonsmooth character of the arising probability function. On the applied side, optimal gas transport and the optimal control of weakly coupled mini-grids continued being the main objects of our investigations. In the latter topic, significant progress was made with respect to some more realistic battery modeling than in common operations research approaches. More precisely, energy demand, solar energy, and ambient temperature are considered as uncertain inputs, and the battery storage of the mini-grid is controlled in order to keep its state of charge and its temperature in desired ranges with high probability. Figure 1 illustrates the cooling energy employed for the battery as a part of the control variables in the problem. The ensemble of the achievements of RG 4 in the area of stochastic and nonsmooth optimization was presented in a plenary talk at the IFIP TC7 Conference on System Modeling and Optimization.

New internal cooperation was initiated on the topics of sweeping processes under uncertainty (with Olaf Klein, RG 7) and of distributionally robust chance constraints (with Jia-Jie Zhu, WG DOC *Data-driven Optimization and Control*). External cooperation was started with Georg Stadler (New York), with Martin Gugat (Erlangen), and with Hassan Farshbaf Shaker (Berlin), all of them on various aspects of optimal control with chance constraints.

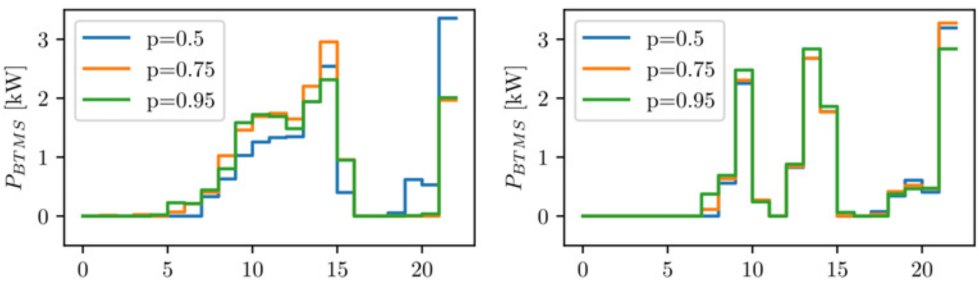

Fig. 1: *Energy for battery thermal management system employed to keep the battery temperature in a desired range with probability p. Solutions for a sunny (left) and a partially cloudy day (right).*

High-dimensional parametrized inverse problems

Sampling unnormalized densities with neural and tensor networks. Sampling from arbitrary probability measures has become ubiquitous in machine learning and is also a highly relevant task when considering inverse problems. Typically, the target density (which we assume to exist) is not known explicitly and, in particular, the normalization factor cannot be determined. For this problem, different approaches were developed and analyzed.

In a first approach, a neural network (NN) architecture was derived, which is shown to be able to resemble a Langevin Monte Carlo (LMC) process. Here, one step of the process consists of adding the gradient of the logarithm of the target density to the current state and distorting it by adding relatively small random noise. The NN architecture represents a surrogate model for the gradient, leveraging the popular ResNet (Residual NN) structure. Moreover, convergence bounds for the approximate flow to the target distribution in Wasserstein distance were shown. Measured in the number of gradient calls needed in the LMC and the NN architecture, the NN architecture outperforms a standard LMC sampler, which was examined with somewhat different goals in the previous year.

A second novel approach for sampling from unnormalized Boltzmann densities using low-rank tensor train (TT) representations was introduced in [5]. It inherently solves an underlying continuity equation and is based on the annealing path commonly used in Markov chain Monte Carlo (MCMC) methods, given by linear interpolation in the space of energies. Leveraging Fourier basis functions orthonormalized with respect to an H^2 –Sobolev norm for numerical stability, the approach dynamically adapts TT ranks via an exponential moving average. Inspired by Sequential Monte Carlo, deterministic time steps from the TT representation of the flow field are alternated with stochastic steps, which include Langevin and resampling steps. Numerical experiments, including numerically challenging Gaussian mixtures and high-dimensional settings, highlight its favorable performance when compared to stochastic and standard TT-based methods, resulting in an efficient computation of multimodal distributions and challenging sampling tasks. An application of this approach for sampling from a "many well density" is depicted in Figure 2.

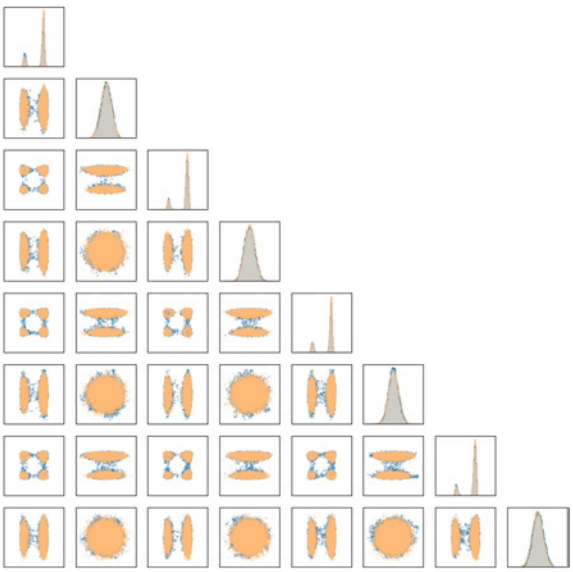

Fig. 2: *The figure shows samples of the first 8 marginals and two-dimensional joint distributions of the 16-dimensional many well problem in orange and samples generated by the tensor train approach in blue. It can be seen that the modes of the distribution were found and fitted accurately.*

Eulerian TT-based JKO for Bayesian inversion. An Eulerian discretization approach for approximating high-dimensional distributions in functional form was developed to enable efficient sample generation from an unnormalized posterior. By casting the task as a minimization problem over probability measures in Wasserstein space and solving it via an entropy-regularized Jordan–Kinderlehrer–Otto (JKO) scheme, the devised method is numerically efficient despite the inherently high computational complexity of the Eulerian approach. On the one hand, this is due to using an accelerated fixed-point method like the Anderson scheme. On the other hand, utilizing a low-rank tensor train format mitigates the curse of dimensionality of the lattice discretization. Moreover, a caching strategy turned out to also significantly reduce computational costs. The method was shown to achieve superior or comparable performance to Metropolis–Hastings MCMC numerically across synthetic data, see Figure 3, and in particular in the context of Bayesian inverse problems. The application of the method for the identification of geometry parameters in a parametric PDE setting is an ongoing project with the Physikalisch-Technische Bundesanstalt.

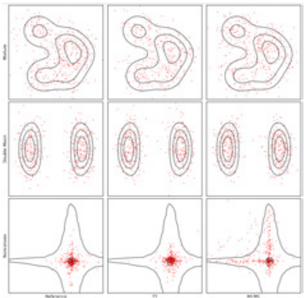

Fig. 3: *Posterior samples for different benchmark probability densities, generated with the exact (reference) density, the new TT-JKO method and a vanilla MCMC method*

Adaptive multilevel CNNs and wavelet Galerkin methods for parametric PDEs. A neural network architecture for the approximation of the parameter-to-solution operator of stationary random PDEs was developed and analyzed in [3]. It exploits the multilevel properties of the high-dimensional parameter-dependent solutions as illustrated in Figure 4, thereby allowing for an efficient surrogate learning that rivals best-in-class methods such as low-rank tensor regression in terms of accuracy and complexity. The neural network was trained with data on adaptively refined finite element meshes, thus reducing data complexity significantly. Error control was achieved by using a reliable finite element a posteriori error estimator, which was also provided as input to the neural network. The proposed U-Net architecture with convolutional neural network (CNN) layers mimics a classical finite element multigrid algorithm. It was shown that the CNN efficiently approximates all operations required by the solver, including the evaluation of the residual-based error estimator. A complete convergence and complexity analysis was carried out for the adaptive multilevel scheme, which differs in several aspects from previous non-adaptive multilevel CNN. Moreover, numerical experiments with common benchmark problems from Uncertainty Quantification were used to illustrate the practical performance of the architecture.

In the framework of deterministic explicit discretizations, an adaptive stochastic Galerkin finite element method for parametric or random elliptic partial differential equations was developed in [2], which generates sparse product polynomial expansions with respect to the parametric variables of solutions. For the corresponding spatial approximations, an independently refined finite element mesh is used for each polynomial coefficient. The method relies on multilevel expansions of input random fields and achieves error reduction with uniform rate. In particular, the saturation property for the refinement process is ensured by the algorithm. The results are illustrated by numerical experiments, including cases with random fields of low regularity.

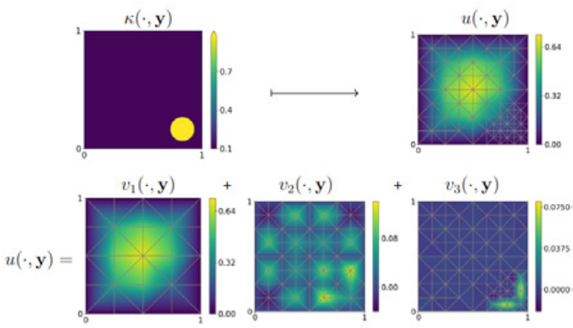

Fig. 4: *Multilevel decomposition of the solution of a parametric PDE as used in the multigrid algorithm that is reproduced in a CNN architecture. The parameter-to-solution map gets as input a realization of the conductivity field, which in this illustration contains a circular inclusion of a constant random conductivity.*

Optimal control of multifield and multiscale problems

A key focus of last year's research was the study of nematic electrolytes in anisotropic microfluids, which has significant implications for controlling fluid behavior on small scales, such as enhancing mixing efficiency in lab-on-a-chip devices. This research was carried out as part of the MATH+ project AA2-12"Nonlinear electrokinetics in anisotropic microfluids – Analysis, simulation, and optimal control," which aimed to develop a suitable partial differential equation (PDE) model to describe the behavior of these fluids and perform a rigorous mathematical analysis of the model's existence and uniqueness properties. Additionally, numerical algorithms were designed for solving the forward problem and compared to experimental data Figure 5. Moreover, a gradient-free optimization algorithm was implemented.

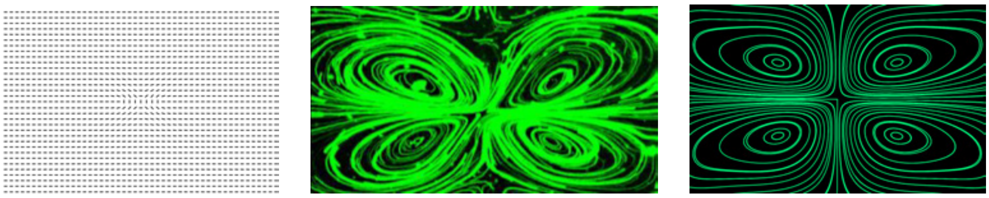

Fig. 5: *Physical vs. numerical experiments; left: the director field, middle: observed velocity field, right: simulated velocity field*

The analysis in the recently accepted paper [6] focused on establishing the existence of suitable weak solutions to the PDE model. These are weak solutions additionally fulfilling an energy-dissipation inequality. Deriving new *a priori* estimates, a novel existence result of weak solutions to such a general anisotropic electrolyte model was proven [6]. Additionally, weak-strong uniqueness was shown, verifying that under the assumption that a strong solution exists, all suitable weak solutions coincide with this strong solution, thereby validating the robustness of the solution concept. The proof of the relative energy inequality was based on the energy inequality for suitable weak solutions. This work successfully concluded the MATH+ project and also marked the completion of Luisa Plato's dissertation.

Building on the recent focus on generalized solution concepts based on inequalities for nonsmooth problems, we consider a PDE system describing damage propagation in viscoelastic materials. The model is highly nonsmooth, as the damage is represented by a phase-field variable that is constrained to the range $[0, 1]$ and unidirectional, reflecting the physical irreversibility of material damage (i.e., once damaged, the material cannot be restored during evolution). We establish the existence of generalized solutions and prove their global-in-time existence. Due to the system's high nonlinearity, the existence result can only be stated in a weak form, which precludes a proof of uniqueness. Nevertheless, we demonstrate the existence of a local-in-time strong solution and show that it coincides with the generalized solutions as long as the strong solution exists. This *weak-strong uniqueness* result is obtained via a suitable relative energy inequality [7].

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4.5 Research Group 5 “Interacting Random Systems”

Head:	Prof. Dr. Wolfgang König
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Team Assistant:	Christina van de Sand

The focus of the RG 5 *Interacting Random Systems* is the analysis of systems of objects subject to 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. Often, the group is also interested in dramatic changes of behavior as a result of parameter changes. These phase transitions can have profound implications in applications, representing, for example, changes in physical properties of a material (condensation or gelation), the rapid spread of disease in epidemiological models, or survival in biological models. The group is increasingly focusing on problems where spatial and geometric aspects of interactions are crucial for the large-scale behavior.

The group is sad to mention the leave of Robert Patterson, who worked at our institute for 14 years. Robert Patterson held the role of the Deputy Head of Group for many years. Willem van Zuijlen took over this role. The group continued the main organization of the German Science Foundation Priority Program *Random Geometric Systems (SPP 2265)*. Furthermore, intensive work continued in the German Science Foundation Collaborative Research Center *Scaling Cascades in Complex Systems (CRC 1114)* in cooperation with RG 1 *Partial Differential Equations* and Freie Universität Berlin.

The group is proud to report that Heide Langhammer successfully defended her Ph.D. thesis with *magna cum laude* and wishes her all the best as she moves on. Doctoral training is a major activity in the group, and Heide Langhammer was one of four doctoral students who were members of the group during the year.

The RG 5 *Interacting Random Systems* was involved in the organization of the following conferences:

- Workshop Junior Female Researchers in Probability, July 3 – July 5.
- 3rd Annual Conference of SPP 2265 Random Geometric Systems 2024, October 28 – 30.
- Probability meets Biology: Berlin Edition, November 27 – 29.

As usual, the head of RG 5 *Interacting Random Systems*, supported by group members, supervised many bachelor’s and master’s theses at Technische Universität Berlin. Additionally, Alexander Zass held a students’ seminar on Gibbs measures at Technische Universität (TU) Berlin. The group invested also quite some efforts in activities that bring pupils closer to mathematics, like the organization of the *Tag der Mathematik* (Day of Mathematics) at TU Berlin and the pupils' conference *MATh.en.JEANS* at the WIAS.

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. We describe the progressions in our highlight article on page 21. Furthermore, as we describe below, in this year we made progress within understanding the Bose–Einstein condensation, we started a new field of considering dormancy in spatial interacting random systems and made progress within the study of dynamical random graphs. On the last topic, we share many interests with the Leibniz Group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks*. For multiple topics, we explored an innovative general idea using Poisson processes on the random structures under interest; this idea is expected to prove useful for the analysis of many situations with phase transitions.

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

Probabilistic proofs for Bose–Einstein condensation

Since the detection of a mysterious condensation effect at ultra-low temperatures by Einstein and Bose in 1924, the Bose gas attracts a lot of research activity in mathematical physics and analysis. However, even though Feynman in 1953 vaguely suggested to adopt the length of the Brownian loops in the probabilistic description of the gas as an important order parameter, relatively little research has been done to rigorously examine the deeper content of this idea. For example, to our surprise, we detected that there was no probabilistic proof for the occurrence of the condensation effect in the literature yet in terms of the phenomenon of off-diagonal long-range order (ODLRO) of the corresponding Hamilton operator, the commonly agreed criterion for Bose–Einstein condensation. Proving this is technically cumbersome, since one needs to go substantially deeper than on the exponential scale. The object of study here (deriving from the Feynman–Kac formula) is the Brownian loop soup, a configuration of many Brownian loops of various lengths in a large box; for diverging total length of the loops, one investigates the occurrence or non-occurrence of particularly long loops if the density of paths exceeds some threshold.

In [2], we provided one proof for the validity of ODLRO in the Bose gas by combining a careful analysis of Brownian loops and combinatorial probabilities for the number of partitions with particular properties. Unfortunately, we were so far only able to handle a non-interacting system, but on the other hand, we considered various relevant boundary conditions, while the literature almost exclusively is restricted to periodic boundary conditions. Additionally to proving ODLRO, we also described the joint distribution of the lengths of the longest loops in terms of the Poisson–Dirichlet distribution.

In [1], we translated the techniques from [2] to a mean-field variant of the Bose gas, the so-called *semi-classical limit*, which is restricted to a fixed box (not growing with the number of particles), but having a decaying diffusivity. We proved ODLRO also in this model. A number of further research projects in this area were pursued in 2024 in the group and will continue in 2025 and beyond.

Dormancy in random environment

Dormancy is an evolutionary trait that has developed independently across various life forms and is particularly common in microbial communities. Dormancy is defined as the ability of individuals to enter a reversible state of minimal metabolic activity. Maintaining a dormant part beside the active part of the population leads to a decline in the reproduction rate, but it also reduces the need for resources, making dormancy a viable strategy during unfavorable periods. This maintainance requires energy and sophisticated mechanisms for switching between active and dormant states. Moreover, the increased survival rate of dormant individuals must be weighted against their lower reproductive activity. Despite its costs, dormancy still seems to provide advantages in variable environments.

In [3], we investigate the stochastic switching strategy and quantitatively compare the long-term behavior of populations with and without this dormancy mechanism. The model considered is a spatial model in continuous time where the population moves on a discrete lattice and branches, respectively is killed, according to a random time-dependent field of branching/killing rates. The novelty of this work lies in the fact that dormancy is considered in a spatial setting with a branching/killing mechanism, as so far in the literature either fixed population sizes or branching/killing without dormancy is considered.

The random environment of branching/killing rates is itself modeled as a field of randomly moving particles, which are interpreted as *catalysts* if they support branching and as *predators* if they support killing. Three types of these additional particles are considered:

- homogeneously distributed as an immobile Bernoulli field,
- just one single moving particle,
- a homogeneous Poisson field of moving particles.

For each of these types, both in the catalysts case and in the predators case, in [3] the large-time asymptotics of the expected total number (taken over both the random environment and the branching process) of particles in the branching random walk population is quantified in terms of mostly explicit formulas. These formulas quantify the effect of the dormancy, i.e., how much the population benefits in the predator case from dormancy and, in the catalyst case, how much the reproduction is slowed down.

Leadership and formation of “hubs” in processes with reinforcement

In a number of applications, it is of interest to model systems of agents with values subject to incremental growth over time, where the growth of various agents is reinforced over time. Thus, rich agents become richer. Here, we consider two different models:

1. One where the number of agents is fixed, and values are increasing independently over time,

2. Another, where the value represents the number of connections that an agent has and new agents arrive that connect to old agents.

In the first model, a natural question of interest is whether or not there exists an agent and a time after which that agent obtains the maximal value. In [4], we solve this problem in a rather general way, providing necessary and sufficient conditions for such an agent to appear. This extends existing literature on nonlinear urns, and has diverse motivations. For example, values might represent the market shares of companies, in which case the question of interest reflects whether there is a leading company that retains a dominant market share. It might also represent the formation of a dominant political belief, or the formation of a dominant neuron from competing neurites in the early stages of neuron development. See [4] for further discussion.

The latter model is a classical model of branching process, known as *Crump–Mode–Jagers branching processes*. The study of these models forms part of the longer term research plans of the group. In [5], we find criteria for the emergence of a hub in these models that obtains and retains the maximal number of connections over time, and criteria for the non-existence of such a hub. Moreover, in [6], a more general model is considered for which we obtain criteria for every agent to only obtain finitely many connections over time, so that the entire mass of connections is lost to newer and newer hubs. The motivation for the analysis of hubs in these models comes from the analysis of growing networks that represent structures such as social networks or genealogical trees associated with the mutations of a disease. In such applications, hubs correspond to influencers or super-spreaders. Thus, a better understanding of these hubs lends a better understanding of the potential evolution of such networks.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

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Team:	Simon Breneis Dr. Oleg Butkovsky Dr. Pavel Dvurechensky Dr. Davit Gogolashvili Wilfried Kenmoe Nzali Dr. Alexey Kroshnin Dr. Vaios Laschos Dr. László Németh Luca Pelizzari Aurela Shehu Dr. Alexandra Suvorikova Dr. Karsten Tabelow Dr. Nikolas Esteban Tapia Muñoz Sorelle Murielle Toukam Tchoumegne
Team Assistant:	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 Institute for Learning and Data*, the DFG International Research Training Group IRTG 2544 *Stochastic Analysis in Interaction*, 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, algorithms for stochastic and large-scale optimization problems. Research within this subarea covered both theoretical and applied statistical problems.

Highlights 2024:

- Collaboration with J.-J. Zhu (WG DOC *Data-driven Optimization and Control*) resulted in two publications at top-tier machine learning (ML) conferences: The International Conference on Artificial Intelligence and Statistics (AISTATS) and The Annual Conference on Neural Information Processing Systems (NeurIPS).
- The collaboration with Prof. Mathias Staudigl (University of Mannheim) resulted in publication of two papers on barrier algorithms for constrained non-convex optimization problems: one in the Mathematical Programming journal and one in the proceedings of the International Conference on Machine Learning (ICML).
- A new collaboration with the Leibniz-Zentrum Allgemeine Sprachwissenschaft (general linguistics, ZAS) and Universität Tübingen started with a project "Linguistic Meaning and Bayesian Modelling" (LMBayes) funded within the Leibniz competition.

In 2024, the members of the group made some significant contributions to statistical literature. The novel approach to statistical inference based on the theory of perturbed optimization was developed in [5]. The obtained results provide finite sample expansions and sharp non-asymptotic risk bounds a nonlinear regression problem in terms of the so called *effective dimension*. The approach was successfully applied to studying the estimation problem for Deep Neuronal Networks allowing to overcome the well known "curse of dimensionality" and "non-convexity" issues.

WIAS Preprint no. 3145 proposes a novel framework for generalized bootstrap for the barycenters in the Bures–Wasserstein space. We provide non-asymptotic statistical guarantees for the resulting bootstrap confidence sets. The proposed approach incorporates classical resampling methods, including the multiplier bootstrap highlighted as a specific example. Additionally, the paper compares bootstrap-based confidence sets with asymptotic confidence sets obtained in the work of Kroshnin et al. [2021], evaluating their statistical performance and computational complexities. The methodology is validated through experiments on synthetic datasets and real-world applications.

WIAS Preprint no. 3146 derives explicit Bernstein-type and Bennett-type concentration inequalities for matrix-valued supermartingale processes with unbounded observations. Specifically, we assume that the ψ_α -Orlicz (quasi-)norms of their difference process are bounded for some $\alpha > 0$. As corollaries, we prove an empirical version of Bernstein's inequality and an extension of the bounded differences inequality, also known as McDiarmid's inequality.

An important part of the group's research is devoted to optimization algorithms, including stochastic ones, motivated by machine learning (ML) applications. In 2024, a series of clipped stochastic algorithms for optimization problems, and, more generally, variational inequalities was proposed in the setting of heavy-tailed noise. The main idea was to clip stochastic gradients when their norm is too large. Carefully treating the emerging bias-variance trade-off, optimal (up to logarithmic factors) complexity guarantees for these algorithms were obtained in terms of the high probability of obtaining desired accuracy, a more reliable criterion than for the standard in-expectation guarantees. The results were published in the proceedings of International Conference of Machine

Learning (ICML) 2024 and in the Journal of Optimization Theory and Applications. Next, motivated, in particular, by training input-convex neural networks, we considered constrained nonconvex optimization problems where complicated structure of the constraints leads to infeasibility of standard projection-based methods. Instead, we used a barrier reformulation of the problem and proposed first- and second-order methods with optimal worst-case iteration complexity. The results were published in the proceedings of ICML 2024 and in Mathematical Programming.

Together with J.-J. Zhu (WG DOC), motivated by machine learning (ML) applications such as robust ML, sampling, and statistical inference, we continued the research on the interface of optimization, probability, and geometry. Particularly, motivated by the Wasserstein barycenter problem, training of implicit generative models, and distributionally robust optimization, we proposed and studied the Mixed Functional Nash Equilibrium problem, which is a joint optimization problem over the space of measures and a space of functions. For the setting of reproducing kernel Hilbert spaces, we proposed and theoretically analyzed an infinite-dimensional mirror prox algorithm for finding an equilibrium. The results were published at the Artificial Intelligence and Statistics Conference (AISTATS) 2024. Further, we proposed a new gradient flow dissipation geometry over nonnegative and probability measures, which is motivated by a combination of the unbalanced optimal transport and interaction forces modeled by reproducing kernels. We developed a particle-based optimization algorithm and provided both theoretical global exponential convergence guarantees and improved empirical simulation results for applying the new gradient flows to the sampling task of maximum mean discrepancy minimization. The results were published in the proceedings of the Annual Conference on Neural Information Processing Systems (NeurIPS) 2024 [4].

In 2024, jointly with RG 8 *Nonsmooth Variational Problems and Operator Equations*, we continued the work on the MATH+ project "Equilibria for distributed multi-modal energy systems under uncertainty" and developed a Cournot–Nash model for a coupled hydrogen and electricity market. The question of the existence of equilibrium was investigated in the corresponding preprint arXiv:2410.20534, and future research is devoted to distributed aspects of this model and numerical algorithms for finding an equilibrium.

The research group, in collaboration with the Leibniz-Zentrum Allgemeine Sprachwissenschaft (ZAS) and Universität Tübingen, started a new project "Linguistic Meaning and Bayesian Modelling" (LMBayes) funded within the Leibniz competition on statistical modeling of pragmatic meaning. The project is funded from July 2024 till June 2027.

The research group contributes to the WIAS main application area Quantitative Biomedicine, especially for (quantitative) imaging problems and in neuroscientific applications. In 2024, we started a new cooperation in this field with the Max Delbrück Center Berlin (MDC) to transfer the methods to application problems. Specifically, the methods and software for adaptive smoothing of functional magnetic resonance imaging developed in our research group were applied to very recent high-resolution, high-field data and demonstrated superiority over standard methods also in this application [6].

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

The research group is actively contributing to the Mathematical Research Data Initiative (MaRDI) (`http://www.mardi4nfdi.de/`) within the Nationale Forschungsdateninfrastruktu (NFDI). Within its task area "Cooperations with other disciplines" and in cooperation with RG 1 *Partial Differential Equations*, we build the knowledge graph on mathematical models and the respective ontology as underlying grammar for its description. This enables researchers from other fields like imaging applications to find, e.g., mathematical models for real-world problems together with the algorithms to solves 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. The MaRDI group at WIAS initiated the NFDI_BB network comprising all NFDI consortia in the Berlin-Brandenburg area to foster interdisciplinary cooperation on topics like knowledge graphs or artificial intelligence. Within the task area "Statistics and Machine Learning," we improve the knowledge base on statistical software and the representation of R packages that are hosted on CRAN within the MaRDI portal (http://portal.mardi4nfdi.de/). The research group also contributes to the management of MaRDI and the strategic development of the consortium.

Stochastic modeling, optimization, and algorithms

This project area focuses on the solution of challenging mathematical problems in the field of 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 2024:

- The DFG CRC/TRR 388 *Rough Analysis, Stochastic Dynamics, and Related Fields* was approved and started its operations; group member P.K. Friz is its Spokesperson. Members of the group are involved in projects A02, B01, B02, B03, and B08 of the CRC.
- The article "Multilevel Monte Carlo with numerical smoothing for robust and efficient computation of probabilities and densities" by Ch. Bayer, Ch. Ben Hammouda, and R. Tempone was published in the SIAM Journal on Scientific Computing.
- The article "Rough PDEs for local stochastic volatility models" by P. Bank, Ch. Bayer, P.K. Friz, and L. Pelizzari was accepted for publication in Mathematical Finance.
- The article "Polynomial Volterra processes" by E. Abi Jaber, Ch. Cuchiero, L. Pelizzari, S. Pulido, and S. Svaluto-Ferro was published in the Electronic Journal of Probability.

Fig. 2: *The CRC/TRR 388* Rough Analysis, Stochastic Dynamics, and Related Fields *started in 2024*

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. In addition to applications for deterministic integration methods (such as sparse grids or quasi-Monte Carlo (QMC), it can even dramatically improve the convergence of (multi-level) Monte Carlo solvers, as observed in [2]. 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.

In a collaboration with Research Group 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, we are developing new methods for the optimal control of batteries in the presence of stochastic electricity prices and aging of the battery. Due to the memory inherent both in the internal dynamic of the battery as well as many accurate electricity price models, the corresponding stochastic optimal control problems are naturally high-dimensional or even non-Markovian. This leads to challenging numerical problems that can be solved using techniques from rough analysis.

Research Focus *Quantitative Analysis of Rough and Stochastic Systems*

The investigation of rough volatility models continued. In [1], we exhibit a rough Markovian structure in general (non-necessarily Markovian) local stochastic volatility models.

The development of efficient Markovian approximations to rough volatility models was continued. 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, providing a fast and accurate simulation method for the rough Heston model. In addition, a first concrete characterization of the state space of Markovian lifts of stochastic Volterra equations was provided. This makes it possible to solve the corresponding pricing partial differential equation (PDE) numerically and to provide proper numerical analysis of the aforementioned simulation scheme for the rough Heston model.

Lipschitz functions in the sense of Stein are an important class of functions for many applications, including rough analysis and machine learning (in particular, neural differential equations). Given a high-dimensional, expensive-to-evaluate γ -Lipschitz function, we are looking at accurate and efficient methods for evaluating the function (together with its derivatives of order up to $\lceil \gamma - 1 \rceil$), e.g., for solving a (controlled) differential equation. The method suggested is based on local polynomial approximations together with refining estimates of the "local Lipschitz norm."

The research on signature transforms continued. In [3], we prove a fundamental structural theorem for log-signatures. Also, methods for optimal stopping and pricing of American options continued. In WIAS Preprint no. 3068 (accepted for publication in Finance & Stochastics), 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. In particular, these methods allow the pricing of American options in rough volatility models, see WIAS Preprint no. 3172.

In further developments, new model order reduction techniques were applied in the context of signature methods in finance, allowing to drastically reduce the dimension of the number of features, while retaining the signature's approximation quality up to machine precision, see WIAS Preprint no. 3163. Research on signature methods for optimal stopping problems and other classes of stochastic optimal control problems continues.

Another research focus of the group are applications of signature methods to machine learning. In an ongoing project, we show stability bounds for residual neural networks in the average regime with respect to the weight distribution. The notion of path signatures was extended to two-parameter objects, i.e., images, via Magnus expansion. This requires construction of the free differential crossed module over the free Lie algebra. In a related work, a two-parameter version of Hoffman's isomorphism is proven extending the link between iterated-sums and -integrals signatures to the corresponding two-parameter objects, see WIAS Preprint no. 3087.

Strong regularization by noise (that is, pathwise uniqueness) for stochastic equations is now well understood for a large class of random driving noises. On the other hand, very few results are available concerning weak regularization by noise (that is, uniqueness in law) when the driving noise is non-Markovian or infinite-dimensional.

In 2024, in joint work with Leonid Mytnik (Haifa), we introduced a new method for proving weak uniqueness of stochastic equations with singular drifts driven by non-Markovian or infinite-dimensional noise. We showed that a stochastic reaction-diffusion equation with a drift belonging to a negative Besov space has a unique weak solution in the same regime where weak existence is known. The same result holds for a stochastic differential equation driven by additive fractional Brownian motion. Moreover, in the one-dimensional case, we also established strong existence and uniqueness of solutions to this equation, improving upon the seminal results of Catellier and Gubinelli.

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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. Tom Dörffel Dr. André H. Erhardt Christine Keller Dr. Manuel Landstorfer Dr. Christoph Pohl Dr. Leonie Schmeller
Team Assistant:	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.

Multiphase flow problems in soft and living materials

In 2024, research studies of the RG 7 on multiphase problems in soft matter and biological systems were conducted 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*. In collaboration with RG 1 *Partial Differential Equations* (Dirk Peschka), the mathematical theory and numerical algorithms for hydrogels and their free boundary problems with liquid droplets and films were applied to the problem of liquid polymer film dewetting from the surface of a viscoelastic gel consisting of crosslinked and uncrosslinked polymer molecules. Our predictions were compared to experimental results obtained by our project partners at the Universität des Saarlandes.

Together with colleagues at the Julius Wolff Institute (Charité), we published our results on the evolution of patterns of cell populations on an extracellular matrix [2]. Our theoretical model combines agent-based models (ABM) with strain-stiffening hydrogels to predict long-time and large-scale organization of interacting cell populations. 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.

We further expanded our work on charge regulating polymer solutions and derived a fully dynamic thermodynamically consistent model that addresses longstanding open problems on arrested states after liquid-liquid phase separation.

Shape of liquid droplets on soft viscoelastic substrates. In collaboration with experimental physicists from the Universität des Saarlandes, we investigated the shapes of liquid polystyrene (PS) droplets on viscoelastic polydimethylsiloxane (PDMS) substrates. We derived axisymmetric sharp-interface models through energy minimization. Our theoretical predictions were compared to experimental results using atomic force microscopy for a range of droplet sizes and substrate elasticities. These shapes comprise the PS-air, PS-PDMS, and PDMS-air interfaces as well as the three-phase contact line, see sketch in Figure 1.

We found that the polystyrene droplets are cloaked by a thin layer of uncrosslinked PDMS molecules migrating from the PDMS network of the substrate. By incorporating the effects of cloaking into the surface energies in our theoretical model, we then showed that the global features of the experimental droplet shapes are in excellent quantitative agreement for all droplet sizes and substrate elasticities. However, our comparisons also revealed systematic discrepancies between the experimental results and the theoretical predictions in the vicinity of the three-phase contact line. Moreover, the relative importance of these discrepancies systematically increases for softer substrates and smaller droplets. We demonstrated that global variations in system parameters, such as surface tension and elastic shear moduli, cannot explain these differences, but instead point to a locally larger elastocapillary length whose possible origin is discussed in [3].

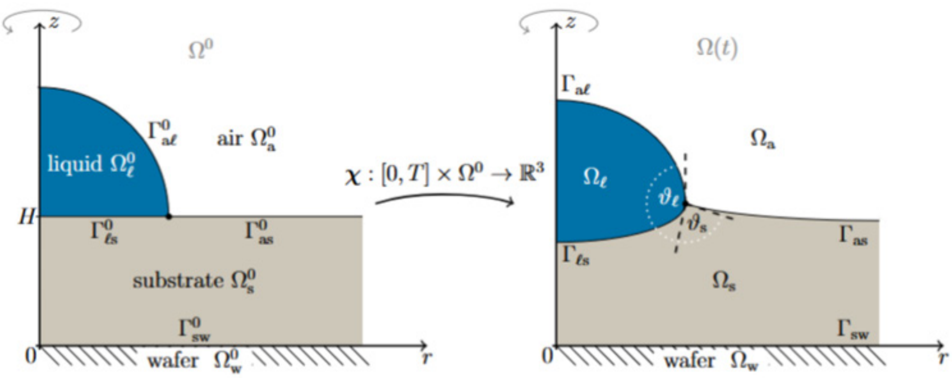

Fig. 1: *Sketch of axisymmetric liquid droplet (blue shading) on a viscoelastic substrate (gray shading) with contact line (black dot) and surrounding air phase (white) on a rigid wafer (stripe pattern) and capillary interfaces (black lines). The left side shows the reference domain (Lagrangian)* Ω^0 *, and the right side shows the deformed configuration (Eulerian)* Ω *and all referential and deformed interfaces* $\Gamma_{ij}(t)$ *. We denote the solid contact angle between* Γ_{as} *and* $\Gamma_{\ell s}$ *by* ϑ_s *and the liquid contact angle between* $\Gamma_{\ell s}$ *and* $\Gamma_{a\ell}$ *by* ϑ_ℓ *. The substrate is initially flat, and the liquid droplet is the half of an ellipsoid. The substrate is supported by a rigid wafer* Ω^0_w *surrounded by an ambient air domain* Ω^0_a *.*

Charge regulation leads to arrested states during phase separation of polyelectrolyte solutions. Jointly with collaborators from the Université de Lille, University College London, and University of Oxford, we showed in Celora et al. 2023 (https://doi.org/10.1063/5.0169610) the effects of charge regulation on liquid-liquid phase separation of polyelectrolyte solutions, where the solution consists of four different mobile species (water molecules, positive and negative ions from a dissociated monovalent salt, and polyelectrolytes with variable charge states).

The thermodynamics of the mixture can be given by the mean-field Helmholtz free energy density. Together with the definition of the specific charge regulation mechanism we then derive the form of the diffusive thermodynamic fluxes and pressure using the Maxwell–Stefan approach. Under the assumption that the friction coefficients between the different components are proportional to their molecular volumes and independent of their charge states, the Maxwell–Stefan conditions are used to give explicit definitions of the fluxes.

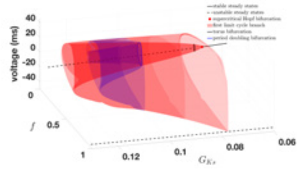

Fig. 2: *Bifurcation diagram for the reduced model*

One particular striking result of our stability analysis and numerical solutions of the new dynamics model is how charge regulation leads to the separation of highly and poorly charged polyelectrolyte chains accumulating on the dilute and coarcervated domains, respectively. This in turn naturally leads to a charge anisotropy across the phase separating interfaces, which in turn is responsible for the arrest of the coarsening process. Using such a minimal model for liquid-liquid phase separation, our work gives new insights and a possible explanation of the experimentally observed arrested states, in particularly in the context of cell biological applications.

Cardiac dynamics

Nowadays, interdisciplinary research is becoming increasingly important. One example is computational biology and physiology. In addition to the modeling of biological phenomena, their analysis also plays a decisive role. Our paper [1] focuses on the model reduction of a cardiac cell model. The presented approach enables an efficient analysis of a cardiac cell model while providing a near-perfect match of the dynamics of the original model with the reduced one.

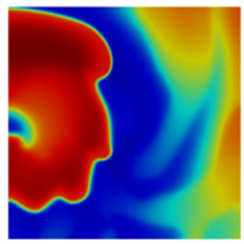

Fig. 3: *Spiral wave break-up followed by the sudden death*

Parameter ranges for the occurrence of cardiac arrhythmias are detected using bifurcation analysis, cf. Figure 2. Simulations on the macroscale are presented, and phenomena like normal beating, tachycardia and fibrillation are studied; cf. Figure 3.

Mathematical models and theory of electrochemical systems

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, we develop fundamental mathematical models for solid and liquid electrolytes, fuel cell and battery electrodes, and a variety of electrochemical reactions. These are employed in project-based research on electro-catalysis, bio-electrochemical systems, and various modern batteries. The development of models for lithium-ion batteries is a core competence of RG 7 that is continuously expanded by internal and external cooperations, third-party project funding, and new material developments. A further key feature of RG 7 is the numerical computation of the derived, in general, PDE-based mathematical models to carry out validation studies as well as simulations for the various applications. Mathematical techniques, such as asymptotic expansions, (periodic) homogenization theory, 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 2024, three MATH+ projects (PaA-2, AA4-9, AA1-14) as well as the Strategic Exploration Topic *Electrochemistry* were hosted by RG 7 in the area of electrochemical systems.

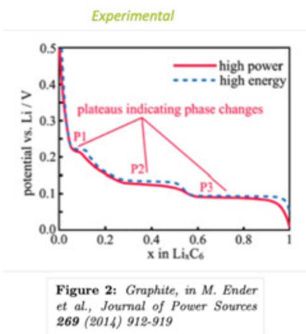

Fig. 4: *Open Circuit Voltage (OCV) of a graphite electrode as function of status of charge/amount of intercalated lithium*

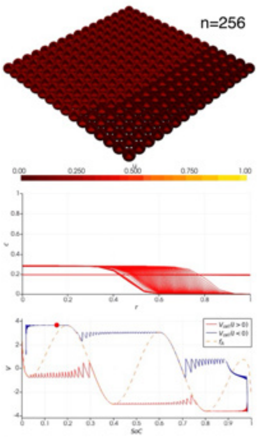

Fig. 5: *Top: computational domains and concentration profiles of the* $n = 256$ *particles. Middle: radial concentration profiles with phase separation. Bottom: computed cell voltage showing multiple plateaus and hysteresis.*

MATH+ project PaA-2 "Modeling battery electrodes with mechanical interactions and multiple phase transitions upon ion insertion" successfully started in 2024 with BMW as external cooperation partner. Lithium-ion batteries (LIBs) consist of porous intercalation electrodes that store lithium (Li) or sodium (Na) within their crystallographic structure. This storage process is governed by electrochemical reactions, represented as $Li^{+} + e^{-} \rightleftharpoons Li$, where the electro-neutral reaction product (Li) is embedded within the host electrode. During the intercalation process, two key phenomena can occur within the host material: (i) volume expansions and the resulting mechanical stresses, and (ii) phase separation between lithium-rich and lithium-poor phases, either within or among the electrode particles.

Both of these effects influence the cell voltage (see Figure 4), which is inherently dependent on the amount of lithium stored in the active material, i.e., the state of charge $y \in (0, 1)$. The objective of the project PaA-2 is to develop PDE-based models for battery electrodes that undergo mechanical deformation and phase separation during ion intercalation.

In 2024, we developed a mathematical model for an n-particle porous intercalation electrode, where the intercalation material is subject to m-phase transitions. The various particles are coupled through (nonlinear) Robin boundary conditions arising from the intercalation reaction in the limit of very slow charging rates. A roboust finite element method (FEM) scheme was developed and implemented in FEniCSx (current version of FEniCS, a software library for solving PDEs with finite elements, see https://fenicsproject.org/), which allowed us to reproduce the voltage plateaus in the Open Circuit Voltage (OCV) (see Figure 5). Further, we were able to predict voltage hysteresis between charging and discharging under OCV conditions.

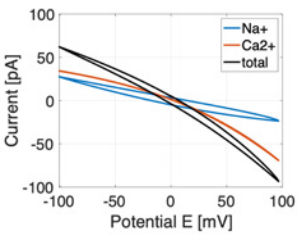

Fig. 6: *Computed current voltage relations under triangular shaped voltage signals (cyclic voltammetry)*

MATH+ project 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 (see Figure 6) of calcium ion channels (see Figure 7) 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 property of ion channels is their high specificity, i.e. they only allow certain ions to pass through and exclude others, see Keller et al. 2023 (WIAS Preprint no. 3072, 2023). There are three key mechanisms for this selectivity: size exclusion, electrical charges, and dehydration reactions. However, it is not fully understood which of the mechanisms plays the main role in selectivity or whether it is a balance between different mechanisms. We started a comprehensive parameter study with our model to identify the key parameters and find an experiment to distinguish whether the selectivity process is due to reaction rates or other aspects.

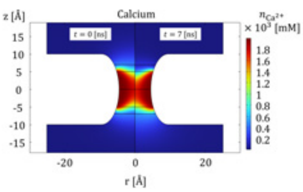

Fig. 7: *Simulation of the calcium distribution within an ion channel, left: initially, right: under current flow from top to bottom*

Dehydration usually requires a lot of energy that can act as a barrier for ions to enter the channel. The inclusion of dehydration and hydration reactions in our model therefore allows us to use the reaction rate as a gating variable. Exploiting this property, we derived a formalism that allows us to calculate the overall behavior of an ion channel network. Understanding how electrical signals are transmitted in cells (see Figure 8) and how different ion channels influence each other is the key to a better understanding of cellular communication and the response of cells to (external) stimuli.

The derivation of asymptotic models can help to significantly reduce computational costs. We derived a quasi-one-dimensional approximation for the Poisson–Nernst–Planck system coupled with the Stokes equations. The geometrical properties of often very narrow and comparatively long channels allow us to introduce a different scaling of pore radius and pore length. This introduces a small parameter, i.e. the ratio of radius to length, which can be used for the asymptotic ansatz. Our approach is not only valid for cylindrical channels, but also for other geometries, such as trumpet-shaped or conical pores.

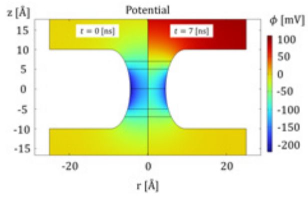

Fig. 8: *Simulation of the voltage distribution within an ion channel, left: initially, right: under current flow from top to bottom*

MATH+ project AA4-9 "Volatile electricity markets and battery storage: A model-based approach for optimal control" in collaboration with Christian Bayer (RG 6) and Dörte Kreher (Humboldt-Universität zu Berlin), models a volatile electricity market alongside a stationary battery storage device (SBSD) to minimize an electricity consumer's overall costs. This is formulated as a stochastic optimal control problem, coupled with a mathematical battery model, to determine optimal dynamic charging and discharging strategies. We assume that operating the SBSD does not impact the electricity market as a whole.

Initially, we focus on formulating a stochastic optimal control problem that captures the continuous, time-dependent charging and discharging of the virtual battery. These strategies are influenced by several factors, including: (i) fluctuations in electricity market prices, (ii) predictive indicators such as wind conditions and forward prices, and (iii) battery-specific conditions, such as degradation effects.

The inherent memory effects within the battery's internal dynamics, combined with the complexity of electricity price models, lead to high-dimensional or even non-Markovian stochastic optimal control problems. These challenges give rise to complex numerical problems that can be addressed using techniques from rough analysis. To solve these problems, we employed a discrete formulation that allowed the application of the dynamic programming principle, combined with the least squares Monte Carlo method, to approximate the value function and the optimal policy . We analyzed the properties of the value function and estimated a lower bound on consumption costs by simulating multiple price trajectories (see, e.g., Figure 9). Our results demonstrated that integrating a battery can significantly reduce costs, depending on its capacity. Finally, we estimated the amortization time, representing the period required for cost savings to offset the initial investment.

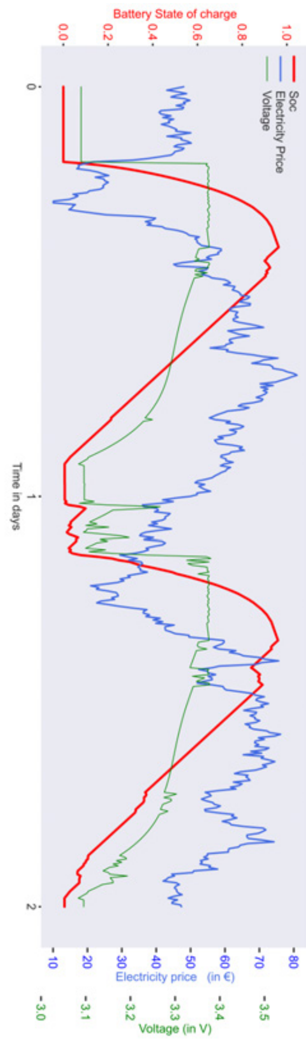

Fig. 9: *Optimal strategy for a sample path with a battery that can satisfy the power demand for 12 hours*

Strategic Exploration Topic *Electrochemistry* investigated two aspects in 2024, (i) the development of a growth model for the solid-electrolyte interphase (SEI) on insertion electrodes, and (ii) models for electrode microstructures capturing binder phases.

(i) The SEI is a key component for the functionality, safety, and long-term stability of lithium ion batteries. The SEI forms at the electrode surface by an electrochemical reaction where lithium ions and solvent molecules from the electrolyte react with electrons from the electrode phase. It is a crucial aspect of the LIB degradation causing capacity and power fade over time. Multiple reaction products can occur, and the investigation with experimental techniques remains difficult. The SEI growth mechanism as well as the SEI composition are subject to current research work, and we contribute to this research by the development of a thermodynamically consistent growth model.

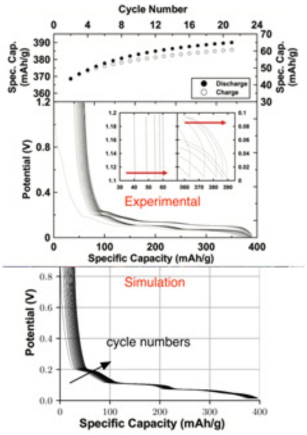

Fig. 10: *Top: experimental data for the SEI growth (Smith et al., J. Electrochem. Soc. 158 (2011)), bottom: numerical simulation. The trajectories capture the increasing number of cycles*

Our developed model accounts for solvents (S), anions (A^-), and cations (Li^+) in the electrolyte, intercalated lithium (Li) and electrons (e^-) in the electrode, as well as reaction products (B) in the SEI phase. At the electrode/electrolyte interface, two competing reactions are considered, the actual intercalation reaction $Li^+ + e^- \rightleftharpoons Li$ and the SEI growth reaction $Li^+ + e^- + S \rightleftharpoons B$. The result is a coupled system of PDEs that we solve using the finite element method and the FENiCSx implementation. This allows us to compute the growth of the SEI during cycling charging and discharging of the battery (see Figure 10), as well as the influence of the material parameters on battery performance.

(ii) A battery electrode is a porous medium consisting of active intercalation material, conductive additives, as well as binder that provides mechanical stability, surrounded by liquid electrolyte. As the binder and conductive additive only weakly absorb X-rays, their spatial distribution is difficult to distinguish in such imaging studies. However, for proper micro-scale simulations of such an electrode, information of the particular geometry of all the components is required. We started to develop a model for the binder distribution based on the wetting of the active material particles by the binder-solvent mixture. Based on Cahn–Hilliard-type equations, the drying of this mixture is modeled as a phase separation between binder and pore space (see Figure 11). Physical parameters such as the contact angle between binder and active particle will then be determined by simulation of the electrochemical performance of the resulting electrode. Meshing techniques allow us to deduce explicit micro-structures for full battery simulations or cell problems in homogenized battery models.

Hysteresis and uncertainties

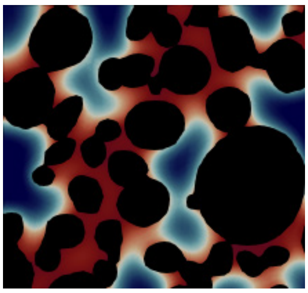

Fig. 11: *Simulation of the Binder phase (red) in a porous battery electrode (black: active phase, blue: electrolyte phase)*

The investigations on uncertainty quantification (UQ) for models for magnetorestrictive materials involving hysteresis operators were continued, and an error in the Forward-UQ computations was corrected.

With RG 4, a joint investigation on controlled polyhedral sweeping processes with polyhedrals being subject to uncertainties was started.

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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 Stefan Kater Dr. Denis Korolev Dr. Ioannis Papadopoulos Felix Sauer Clemens Sirotenko Luise Teigeler (WIAS Female Master Students Program) Qi Wang
Team Assistant:	Pia Pfau

The research group RG 8 *Nonsmooth Variational Problems and Operator Equations* continued its work in optimization and equilibrium problems involving the presence of nonsmooth structures. The focus of the group is on the mathematical modeling, analysis of the underlying variational problems and operator equations, and development and implementation of numerical solution methods. Research is typically motivated by applications from the physical sciences and often involves partial differential equations (PDEs) and variational inequalities (VIs), and in all cases contains 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 VIs, nonsmooth problems under uncertainty, and neural network-based and data-driven approaches in optimization.

Two Masters students, Luise Teigeler (from the WIAS Female Master Students Program) and Pierre Marie Ngougoue (from the Berlin Mathematical School (BMS)), were supervised by members of the group. Both have submitted their Masters theses on the topics of plug-and-play algorithms for magnetic resonance imaging and risk-averse optimal control of quasi-variational inequalities under uncertainty, respectively.

Felix Sauer joined the group as a Ph.D. student and is working on PDE-constrained generalized Nash equilibrium problems on networks inspired by gas markets. Caroline Geiersbach received a call to the Universität Hamburg and took up the position in October.

Members of the group also participated in conferences and workshop, including organizational activities. Michael Hintermüller was the co-meeting director at "VARANA 2024: Variational Analysis and Applications" in Erice. Amal Alphonse and Marcelo Bongarti organized a minisymposium at IFIP (International Federation of Information Processing) TC7 (Technical Committee 7) in Hamburg in August. Michael Hintermüller gave a number of talks, including in Linz, Changsha, Hong Kong, and Montreal.

The joint collaborative project HybridSolver brought together RG 8, the Leibniz Institute for Composite Materials IVW in Kaiserslautern, and the Universität Kaiserslautern-Landau (Scientific Computing team), supported by the industry partners Bosch and Comsol. It was started on October 1, 2024. WIAS is the leader institute for this project, with Michael Hintermüller being the head. The project focuses on multiscale simulation using hybridization of numerical solvers with physics-informed neural networks.

A special issue book collecting research achievements of the second phase of the DFG SPP 1962 *Nonsmooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* is at the final stages of hand-over to the publisher Birkhäuser and is expected to be published in 2025.

Michael Hintermüller handed over the reins of the MATH+ chairmanship to a new chairs' team.

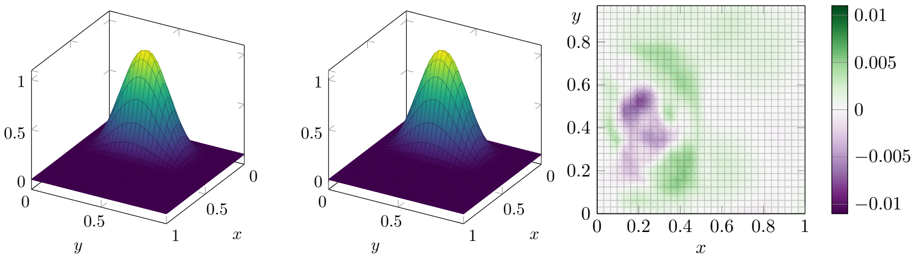
A neural network approach to solving variational inequalities

In [1], a learning approach utilizing neural networks was developed to solve elliptic variational inequalities of obstacle type. The technique involved writing the VI equivalently as a minmax problem, which is advantageous since it directly involves minimizing over the solution candidate and maximizing over the test function of the natural formulation of the VI, without requiring the existence of an associated energy functional (which is not available, e.g., when the elliptic operator is non-symmetric).

The minmax problem is solved by parametrizing the solution and test function by neural networks and the application of a gradient descent ascent algorithm. An error analysis bounding the statistical error (which comes from approximation of integrals via Monte Carlo) and the approximation error (which comes from the choice of the neural network spaces) was also provided, justifying our approach.

[1] was concluded with comprehensive numerical simulations demonstrating the theory to some examples in one and two space dimensions, including examples from optimal control and examples that feature biactivity that is a form of degeneracy that is typically difficult to handle by active set methods. Our approach handled these problems with ease, showing an advantage over the above-mentioned traditional means. Furthermore, we also demonstrated mesh independence in the sense that the size of the network does not greatly affect the quality of the solution. Other aspects, such as the choice of parameters and the effects of random seeds, were also quantitatively analyzed. The code is also available on GitHub.

This work is a collaboration with the Bundesanstalt für Materialforschung (BAM, Berlin) and Tripadvisor (UK). It further builds upon expertise in the group in numerical solvers for variational inequalities and quasi-variational inequalities [2].



(a) Learned solution (b) Exact solution (c) Difference

Fig. 1: *Results of our approach in learning a particular example from optimal control*

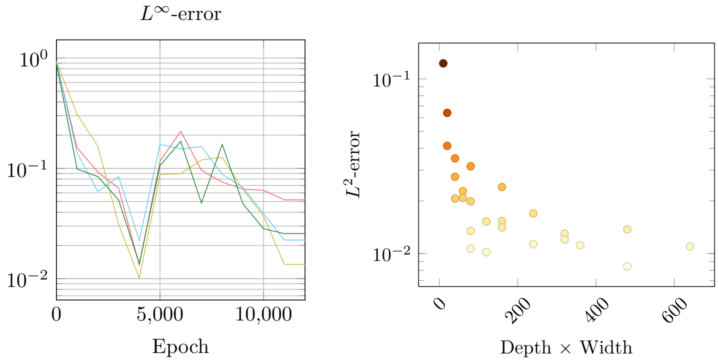


Fig. 2: *Training behavior for different initializations and mesh independence study (quality of solution vs. size of neural network)*

Nash equilibrium problems constrained by hyperbolic PDEs

The group continued its research activities in the third phase of the Collaborative Research Center CRC/TRR 154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks*, contributing to projects B02 "Multicriteria optimization using the example of gas markets" and C08 "Stochastic gradient methods for almost sure state constraints in optimal control of gas flow under uncertainty," under the leadership of co-PI Michael Hintermüller. These projects address various analytical and numerical aspects of generalized Nash games involving partial differential equations (PDEs), with a particular emphasis on models of gas markets governed by hyperbolic dynamics.

Given the limited exploration of generalized Nash equilibrium problems involving PDEs in the current literature, significant effort was dedicated to establishing a framework for modeling and analyzing gas market dynamics. Initial work focused on proving existence results for generalized Nash games under relaxed continuity conditions for constraint mappings. This line of research is particularly relevant because optimization under state constraints often leads to constraint mappings with limited regularity. Continuity of such mappings is frequently linked to the smoothness and compactness properties of solution mappings, which is often available for elliptic and parabolic PDEs, but not for hyperbolic PDEs. Thus, it is essential to develop existence results that do not rely heavily on these structural properties.

Beyond existence results, the characterization of Nash equilibria was a central focus. Under appropriate constraint qualification conditions, first-order optimality conditions for equilibria were derived. In certain cases, regularization techniques were employed to approximate these complex systems with more tractable problems, facilitating the design of numerical methods for equilibrium computation.

Data-driven methods for quantitative imaging

RG 8 focuses on advancing quantitative magnetic resonance imaging (qMRI) and, more broadly, on inverse problems, related optimization strategies, and learning-based approaches. Unlike classical MRI, which can be described mathematically as a linear inverse problem, qMRI integrates the image reconstruction process with an underlying parameter-dependent physical model. The goal of qMRI is to estimate these model parameters using only a limited number of measurements. Due to constraints on acquisition time, the undersampling factor is typically high, necessitating the use of sophisticated regularization methods to achieve meaningful solutions. The recent work of the group in this context, which is surveyed in the overview article [3], can be broadly categorized into two key areas:

Data-adaptive regularization strategies. This approach builds on the classical variational method, where the goal is to reconstruct an image or parameter map by solving a minimization problem. These problems are typically expressed as the sum of a **data-fidelity term**, which measures the discrepancy between the reconstruction and the measured data, and a **regularization term**, which incorporates prior knowledge into the reconstruction process.

Classical regularization terms often rely on simple *a priori* assumptions such as sparsity in a predefined dictionary or smoothness. However, recent advancements aim to select regularization terms in a data-adaptive manner while preserving the robustness and interpretability intrinsic to the variational framework. Specific examples explored by the group include:

- **Patch-based dictionary learning approaches**: Here, a data-adaptive representation is learned for small image patches, enabling a more flexible and tailored regularization mechanism; see [4].
- **Data-adaptive regularization parameter choice**: Here, a spatially dependent regularization parameter—which controls the strength of the regularization—is adaptively determined based on the data. This approach allows the model to locally balance fidelity to the measured data and regularization, leading to more accurate reconstructions.

Both approaches can be formulated as bilevel optimization problems, a longstanding focus of RG 8. However, due to their complexity, these problems must often be approximated to enable practical and efficient solution methods. The group explores different approximation methods, e.g., by alternating minimization or by unrolling strategies where the lower-level problem is approximated by a number of steps of a solution algorithm.

Learning (parts of) the physical model. The physical models underlying qMRI are macroscopic approximations of real-world phenomena. They are highly sensitive to measurement noise. To address these limitations, the group has explored methods for learning components of the physical model—or even the entire solution map—directly from data using neural networks. However, the inclusion of neural networks introduces additional complexity due to their nonsmooth components (e.g., activation functions). This results in optimization problems that are both nonsmooth and non-convex. In a series of papers, the group developed tailored numerical solvers specifically designed to address these challenges, demonstrating their convergence in the infinite-dimensional setting.

Additionally, various stationarity concepts were analyzed to better understand the properties of the solutions. These theoretical advancements are complemented by promising numerical results, showcasing the practical efficacy of the proposed methods. For details we refer to [5] and the references therein.

Multilevel methods for nonsmooth optimization

The group continued its research in multilevel optimization schemes. In this project, the analysis of a multilevel proximal trust-region method for nonsmooth optimization was studied. The problem (which originates from PDE-constrained optimization and data science) requires minimizing the sum of smooth and nonsmooth functions.

This multilevel proximal trust-region algorithm was developed to solve nonsmooth optimization problems. Exploiting ideas from the multilevel literature allowed us to reduce the cost of step computation, a major bottleneck in single-level procedures. This work unifies the theory behind proximal trust-region methods and certain multilevel recursive strategies. Global convergence was proved, and a nonsmooth subproblem solver was provided.

In view of the application, work began on training a fully connected neural network to solve PDEs. The ℓ^1 norm of the neural network parameters was considered as a regularization. By identifying suitable restriction and prolongation operators, a large-scale nonsmooth problem was solved via a sequence of approximate solutions on various levels of the original problem, plus a highly accurate solution on the coarsest level. Specifically, full-rank and row-orthonormal matrices are provided as the restriction operators, which coarsen the number of nodes in every hidden layer. The transposes of the restriction operators were used as the prolongation operators mapping the solution in the coarsest case back to the finest case.

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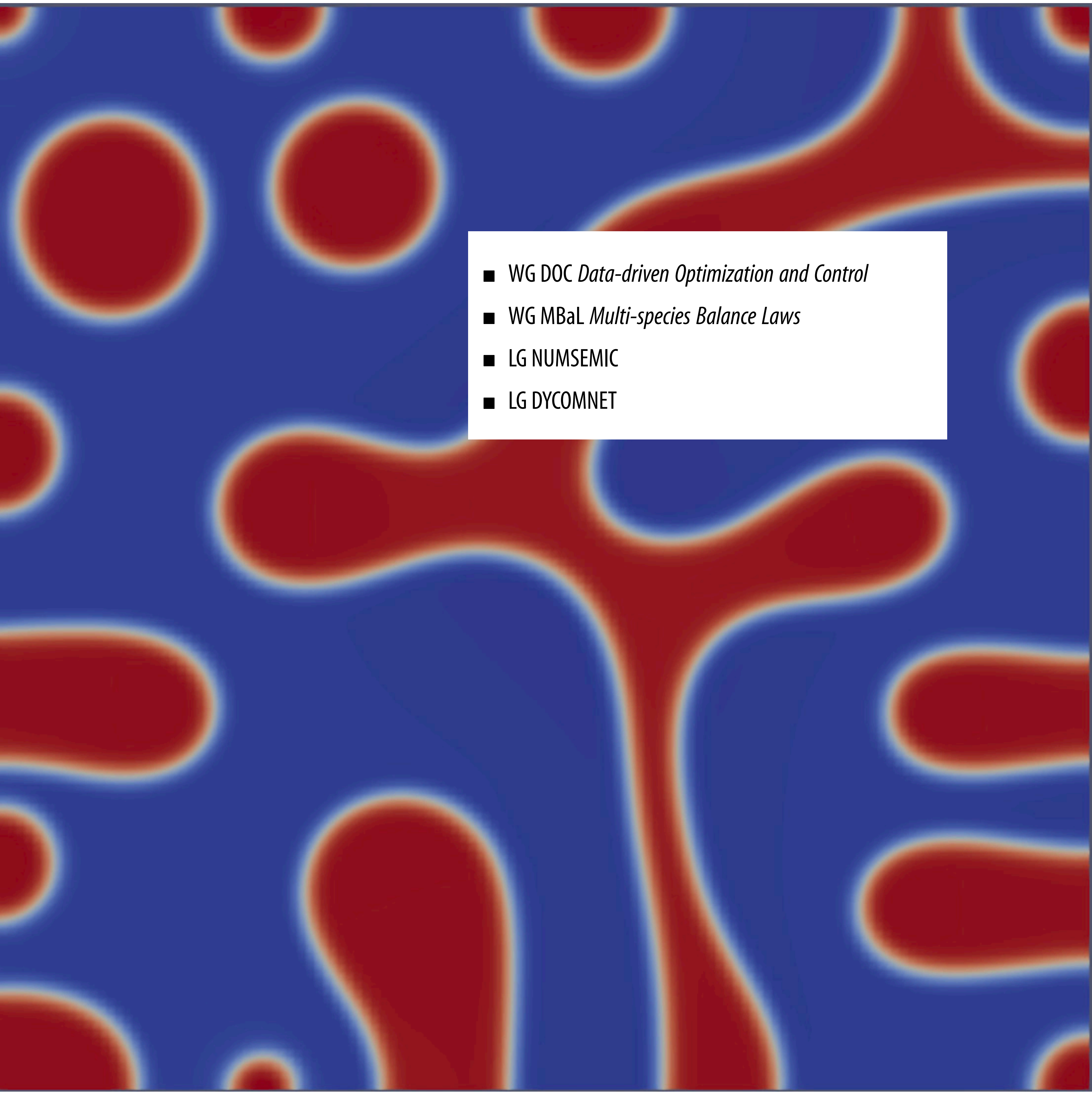
5 Flexible Research Platform



- WG DOC *Data-driven Optimization and Control*
- WG MBaL *Multi-species Balance Laws*
- LG NUMSEMIC
- LG DYCOMNET

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

Head: Dr. Jia Jie Zhu
Team: Zusen Xu
Team Assistant: 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 been prolonged to May, 2027. In 2024, doctoral researcher Zusen Xu has joined the group. Another Ph.D. student is scheduled to join the group in early 2025. The WG currently has a running MATH+ project (AA5-10, jointly funded by 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 project funds one postdoc position placed at RG 3. In addition, we were awarded a DFG Project on "Optimal transport and measure optimization foundation for robust and causal machine learning" within the Priority Program SPP 2298 *Theoretical Foundations of Deep Learning*. We are excited to be a part of this group and contribute our expertise in machine learning and optimal transport. During March 11–15, 2024, we organized a DFG workshop on "Optimal Transport from Theory to Applications – Interfacing Dynamical Systems, Optimization, and Machine Learning (OT-DOM)" in Berlin, with internationally renowned experts such as Gabriel Peyré (École Normale Supérieure, France) and Philippe Rigollet (Massachusetts Institute of Technology, USA). This was jointly organized with Pavel Dvurechensky (RG 6 *Stochastic Algorithms and Nonparametric Statistics*), Matthias Liero (RG 1 *Partial Differential Equations*), and Gabriele Steidl (Technische Universität Berlin). The workshop attracted significant interest from the machine learning and optimal transport communities. In Winter semester 2023/24, Jia-Jie Zhu was co-lecturing a master-level course on nonparametric statistics at Humboldt-Universität zu Berlin together with Vladimir Spokoinyi (RG 6). In 2024, WG DOC leader Jia-Jie Zhu gave numerous invited talks at prestigious institutions such as the École Polytechnique Fédérale de Lausanne (Switzerland), the University of British Columbia (Canada), and at the Workshop on "Optimal Transport and PDEs" at the Institute for Mathematical Sciences, National University of Singapore, which greatly boosted the visibility of the group in the international research community in machine learning and optimal transport.

WG DOC's overarching goal is to study mathematical foundations and applications of machine learning and computational optimization algorithms. The research focus of WG DOC includes the theory and application of robust machine learning algorithms and statistical inference. We are heavily invested in optimal transport/gradient flow theory for machine learning, such as applications to generative modeling and inference. On the other hand, we have acquired significant expertise in optimization and learning with probability measures. This also fits the research landscape of WIAS, such as in transport, gradient flows, mechanics, partial differential equations (PDE) and dynamical systems research.

In 2024, we completed multiple projects, which were submitted for publication. For example, we published a paper entitled "Interaction-force transport gradient flows" [1] at NeurIPS 2024, the Thirty-Eighth Annual Conference on Neural Information Processing Systems, in collaboration with Alexander Mielke (RG 1) and Pavel Dvurechensky (RG 6). In this work, we propose a novel gradient flow inspired sampling algorithm useful for inference and generative modeling, which combines the advantages of both Wasserstein gradient flows and interaction energy gradient flows. This work establishes new theoretical foundations for generative modeling previously heuristically developed in the literature, whereas our algorithm is provably convergent based on the principled PDE gradient flow theory.

Additionally, our paper "Analysis of kernel mirror prox for measure optimization" [2] was accepted at AISTATS 2024, the 27th International Conference on Artificial Intelligence and Statistics. This work provides a theoretical analysis of the kernel mirror prox algorithm for measure optimization problems, with applications in distributionally robust optimization and optimal transport. We establish convergence rates and complexity bounds for this algorithm, advancing the state-of-the-art in computational methods for measure optimization.

Furthermore, our paper "An inexact Halpern iteration with application to distributionally robust optimization" [3], in collaboration with researchers at National University of Singapore, is in the final round of revision for publication in the Journal of Optimization Theory and Applications. This work develops a novel inexact Halpern iteration method for solving distributionally robust optimization problems. The algorithm provides theoretical guarantees while being computationally efficient, making it particularly suitable for large-scale machine learning applications.

We also made significant progress in theoretical research on gradient flows and optimal transport, thanks to our successful collaboration with Alexander Mielke (RG 1). In our joint work "Kernel approximation of Fisher–Rao gradient flows" [4], we for the first time gave a rigorous theoretical view of various kernel-based inference methods from the perspective of the Helmholtz–Rayleigh principle and nonparametric regression. Our formulation further showed that score-matching generative models can be unified in the gradient flow.

Our paper "Inclusive KL minimization: A Wasserstein–Fisher–Rao gradient flow perspective" [5] provides fundamental insights into a large family of machine learning algorithms such as the Maximum Mean Discrepancy (MMD) flow, which is widely used in generative modeling. We show that those algorithms are actually performing forward Kullback-Leibler (KL) inference, which can be unified in the Bayesian inference perspective.

In the domain of financial mathematics, our collaboration with RG 6 researchers Christian Bayer and Luca Pelizzari on "Pricing American options under rough volatility using deep-signatures and signature-kernels" [6] combines modern machine learning techniques with signature methods. This work offers a comprehensive view of using kernel methods and deep learning in signature methods.

Most recently, the theoretical work with Alexander Mielke (RG 1) on "Hellinger–Kantorovich gradient flows: Global exponential decay of entropy functionals" [7] establishes important results on the exponential convergence of a large family of gradient flows in the space of measures. This research provides crucial theoretical foundations for understanding the behavior of certain optimization algorithms in the space of measures, such as those used in sampling, distributionally robust optimization, and information geometry. Importantly, we discover several new results in the analysis of the Hellinger-type gradient flows as well as the Hellinger–Kantorovich (also known as Wasserstein–Fisher–Rao) gradient flows.

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5.2 Weierstrass Group MBaL “Multi-species Balance Laws”

Head:	Dr. Katharina Hopf
Team:	Moritz Immanuel Gau
Team Assistant:	Andrea Eismann

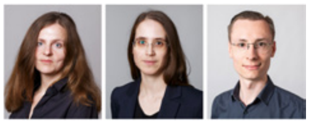

Fig. 1: *From left to right: Andrea Eismann, Katharina Hopf, Moritz Immanuel Gau*

The Weierstrass Group WG MBaL was established as a part of the Flexible Research Platform in November 2023 and is funded by WIAS budget resources. In mid March 2024, Moritz Immanuel Gau joined the group as a new Ph.D. candidate. The group is involved in the Topical Activity Group “Mixtures” by the European Mathematical Society. The group’s head was recently appointed chair of the section “Applied Analysis” of the GAMM Annual Meeting 2025. Within WIAS, WG MBaL has been engaging in collaborations with the Research Groups RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, see the WIAS Preprints [2]–[4].

Research topics. WG MBaL is concerned with the mathematical analysis of strongly coupled systems of partial differential equations (PDE) describing the evolution of interacting species with different mechanical properties. The group’s research is driven by applications in reaction-cross-diffusion systems and phase separation processes enjoying a formal gradient-flow structure, typically given in the dual Onsager form. A key interest lies in systems with a non-simple Onsager structure that reflects the multi-component character of the application and allows for dynamical asymmetry. Particular challenges in the analysis stem from degenerate or rank-deficient mobilities, leading to mixed-type systems of PDEs that may involve parabolic, elliptic, as well as hyperbolic features. To gain insights in such problems, the group takes advantage of the rich toolbox of nonlinear PDEs combining, e.g., asymptotic analysis with entropy techniques and variational methods.

In summary, important aspects of WG MBaL’s research concern:

- Dissipative processes on multiple time scales
- Onsager structures with a rank-deficient mobility
- Cross-diffusion and interface phenomena
- Entropy tools and variational methods
- Mixed-type systems of PDEs

In the subsequent two paragraphs, recent progress in two central themes will be described, which illustrate the research questions addressed by WG MBaL.

Asymptotic geometric effects in viscoelastic phase separation. Phase separation occurs widely in multi-component systems involving immiscible or partially miscible constituents. If a material’s constituents have different mechanical properties, like in the case of polymer solutions, the internal time scales dictating the unmixing process may differ between species, inducing a dynamic asymmetry in the system. Phase separation involving polymeric species is generally referred to as viscoelastic phase separation (VPS). In collaboration with partners from the UK and motivated by applications in cell biology studied by Barbara Wagner (RG 7), WG MBaL aims to gain insights in the qualitative aspects of VPS through model reduction and suitable singular limit analysis. The focus here is on a thermodynamically consistent degenerate Cahn–Hilliard model for VPS proposed by Zhou, Zhang, and E [5]. A particular interest lies in the cross-diffusive coupling of the order parameter to a bulk stress variable that allows for dynamic asymmetry and enables complex transient morphologies.

In [3], the formal sharp-interface asymptotics in a variant of the Zhou–Zhang–E model were shown to lead to nonlocal lower-order counterparts of the classical surface diffusion flow. For nonconstant cross-diffusive coupling, a (new) class of interface dynamical laws of "fractional surface-diffusion"-type was thereby obtained. These geometric laws are expected to describe the dynamics of phase boundaries in VPS during the latest stages of the evolution.

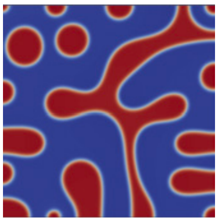

Fig. 2: *Late-stage VPS: Volume-preserving curvature flow induced by square-root of the minus Laplace–Beltrami*

Analysis of electro-energy-reaction-diffusion systems. Electro-energy-reaction-diffusion systems are thermodynamically consistent continuum models for reaction–diffusion processes that account for temperature and electrostatic effects in a way that total charge and energy are conserved. The modeling of such systems has a long tradition at WIAS and goes back to a work by Albinus, Gajewski, and Hünlich [1]. Yet, a rigorous long-time analysis under physically relevant model assumptions has remained open. The joint work [4] provides a comprehensive study of the equilibrium problem, thus addressing the first step of a systematic analysis. The results were presented in Prague, September 2024, in an invited talk at the Modelling, PDE Analysis and Computational Mathematics in Materials Science conference.

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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. Dilara Abdel Zeina Amer
Team Assistant:	Imke Weitkamp

Leibniz Group NUMSEMIC (left to right): Patricio Farrell, Dilara Abdel, Yiannis Hadjimichael, Zeina Amer, and Imke Weitkamp

The Leibniz Group NUMSEMIC was established on the WIAS Flexible Research Platform 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 LG NUMSEMIC is to develop partial differential equation (PDE) models as well as physics-preserving numerical techniques for new semiconductor materials and technologies.

In 2024, there were various highlights. In February, Dilara Abdel successfully defended her Ph.D. thesis on *Modeling and simulation of vacancy-assisted charge transport in innovative semiconductor devices* [5]. The MATH+ project "Electronics of nanotextured perovskite devices" started. Four international researchers visited our group. In September, the workshop "Applied Mathematics and Simulation for Semiconductor Devices" (AMaSiS 2024) was organized jointly with research groups RG 1 *Partial Differential Equations* and RG 2 *Laser Dynamics* as well as Josef Weinbub from Silvaco. Furthermore, Patricio Farrell was elected Vice Chair of the Committee for Mathematical Modeling, Simulation and Optimization (KoMSO).

The following topics drive our research:

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

In the following, we present these applications in greater detail.

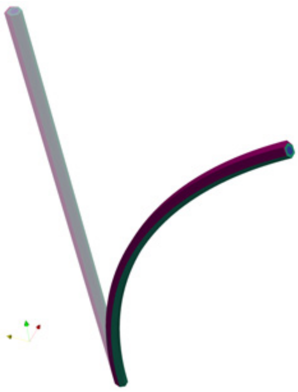

Fig. 1: *A bent nanowire*

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 describe 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 [1]. 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 significantly impacts the band structures and, consequently, the charge transport properties [2]. 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) and the Leibniz Institute for High Performance Microelectronics (IHP).

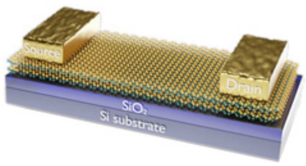

Fig. 2: *Two-dimensional memristor from [3]*

Two-dimensional memristive devices. The von Neumann architecture is far from ideal for AI applications due to its unacceptably high energy consumption. By contrast, 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 [3]. Apart from modeling and simulations, also the numerical analysis, including entropy dissipation relationships, of the model is currently analyzed with colleagues from the University of Lille/INRIA Lille, see the preprint "Numerical analysis and simulation of lateral memristive devices: Schottky, ohmic, and multi-dimensional electrode models" by Dilara Abdel, Maxime Herda, Martin Ziegler, Claire Chainais-Hillairet, Benjamin Spetzler, and Patricio Farrell (https://arxiv.org/abs/2412.15065).

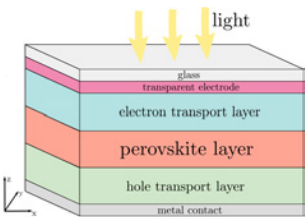

Fig. 3: *Perovskite solar cell*

Perovskite solar cells. Perovskite-silicon tandem solar cells have rapidly advanced in photovoltaics, achieving power conversion efficiencies of over 30%, surpassing silicon solar cells in lab settings. With lower production costs and high efficiency, they hold great potential for renewable energy. 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, facing challenges like stability, lifespan, and toxicity.

Together with Helmholtz Zentrum Berlin (HZB), Zuse Institute Berlin (ZIB), and Jürgen Fuhrmann (RG 3), Dilara Abdel and Patricio Farrell study electronic properties that lead to the superior performance of nanotextured perovskite devices such as perovskite–silicon tandem solar cells. We develop real-life two- and three-dimensional charge transport simulations based on drift-diffusion models, including correctly limited ion migration. Moreover, together with Annegret Glitzky and Matthias Liero (both RG 1), Dilara Abdel proved the existence of weak solutions to the underlying charge transport model.

Laser models. Together with Hans Wenzel (Ferdinand-Braun-Institut, FBH), Eduard Kuhn, and Markus Kantner (both RG 2), Zeina Amer and Patricio Farrell develop optoelectronic models and simulations within `ChargeTransport.jl`, coupling charge transport to a Helmholtz problem. Together with the Universities of Catania and Florence, LG NUMSEMIC also studies the existence of a solution to a laser model. This work extends recent results on existence and uniqueness for perturbed models of the lateral photovoltage scanning problem [6].

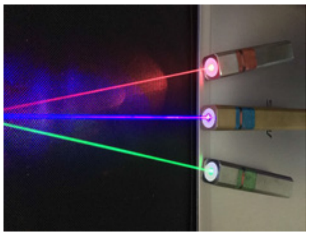

Fig. 4: *Lasers. Source: Pang Kakit CC BY-SA 3.0.*

Fluctuations and coupling with atomistic effects. LG NUMSEMIC investigates together with researchers from Tyndall National Institute, INRIA Lille, as well as Michael O'Donovan Thomas Koprucki (both RG 1) 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` [7]. Fluctuations, albeit on an entirely different scale, play also a role in [8], joint work with the Universities of Pisa and Florence. Here, a data-driven approach was developed to reconstruct fluctuations in the doping profile.

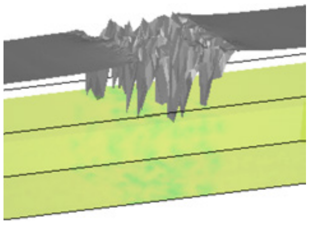

Fig. 5: *Random fluctuations in the band edge energy on atomic scale*

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5.4 Leibniz Group DYCOMNET “Probabilistic Methods for Dynamic Communication Networks”

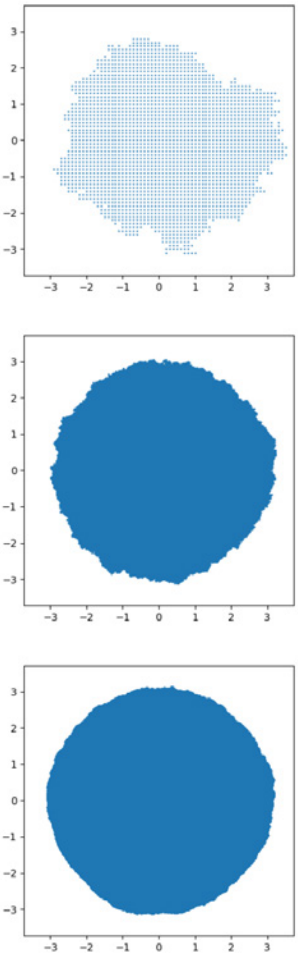

Fig. 1: *Realization of reached sites at times* $t = 10, 50, 190$ *in first contact percolation based on single periodic contacts*

Head:	Prof. Dr. Benedikt Jahnel
Team:	Dr. Julia Hörrmann Dr. Lukas Lüchtrath Dr. Anh Duc Vu Jonas Köppl
Team Assistant:	Christina van de Sand

The Leibniz Junior Research Group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks* is co-funded by the Weierstrass Institute and the Leibniz Association through the Leibniz Competition 2020. As of 2024, the group is in its fourth year of a planned five-year lifetime. The overarching objective of DYCOMNET is to conduct cutting-edge research on complex, spatially distributed communication networks, leveraging advanced tools from stochastic geometry, statistical mechanics, and stochastic dynamics. A key focus lies on the modeling and analysis of dynamic peer-to-peer networks with the help of random point processes, interacting particle systems, and large-deviations theory. The group aims to deliver rigorous results, particularly for the study of connectivity properties of these networks. This includes exploring phenomena such as percolation phase transitions, which highlight critical thresholds for long-range network connectivity.

In 2024, thanks to a successful application at the cluster of excellence MATH+, DYCOMNET could fill an additional postdoc position, with Julia Hörrmann between March and July and Anh Duc Vu from August 2024, working on the subproject EF 45-3 “Data transmission in dynamical random networks.” As a first result in that project, the team was able to derive *shape theorems*, see Figure 1, for the model of *first contact percolation* [4]. Here, similar to the classical model of *first passage percolation*, messages can be transmitted between neighboring vertices along contact times given as random closed sets. One of the key findings is that the set of reachable sites is larger if the contact-time distribution is more rigid.

In total, DYCOMNET produced 13 preprints in 2024, with three already published. One of the highlights is the article [1] in which, together with Martin Heida from RG 1 *Partial Differential Equations*, the team was able to exhibit a percolating ergodic and isotropic random lattice model, in all dimensions $d \geq 2$, which has zero effective conductivity in all spatial directions and for all non-trivial choices of the connectivity parameter. The model is based on the so-called *randomly stretched lattice*, where additional elongated layers contain few open edges, see Figure 2 for an illustration.

Another highlight is the preprint [5], which features precise asymptotic tails for the distribution of the size of the typical connected component in the subcritical percolation regime of a spatial random graph model called the *soft Boolean model*. In that model, a *Boolean model* (in which any pair of independent and identically distributed (i.i.d.)-marked vertices of a homogeneous Poisson point process are connected whenever their distance is smaller than the sum of their marks) is augmented by a *random connection model* (in which any pair of vertices is connected with a probability that decays as a power law with rate given by the distance of the vertices). In parameter regimes in which the model is subcritical, i.e., almost all clusters are finite, and for sufficiently small intensities, the team was able to derive precise decay rates of the probability of clusters to be large. In particular, the rates are given in terms of the system parameters and undergo a phase transition with respect to the influence of the Boolean part in the construction. On the other hand, in preprint [6], large and moderate deviation results are derived for the probabilities of atypically large displacements of a sample path of a Poisson navigation, see Figure 3 for an illustration and further explanation.

In the domain of statistical mechanics, in the preprint [3], together with Alexander Zass from RG 5 *Interacting Random Systems*, the team was able to establish a variational principle (i.e., an alternative description of the equilibrium states of a statistical mechanics system in terms of a minimization problem) for a large class of Gibbs point processes based on i.i.d.-marked Poisson point processes with unbounded range. Still in the domain of infinite-volume statistical mechanics, the preprint [2] provides a class of examples of interacting particle systems on one- and two-dimensional hypercubic lattices that admit a unique translation-invariant stationary measure, which is not the long-time limit of all translation-invariant starting measures, due to the existence of time-periodic orbits in the associated measure-valued dynamics. This is the first such example and shows that even in low dimensions, not every limit point of the measure-valued dynamics needs to be a time-stationary measure.

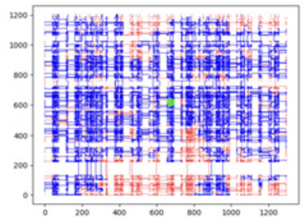

Fig. 2: *Realization of a non-conductive medium given by an elongated randomly stretched lattice. Blue edges belong to the centrally placed green dot's cluster (restricted to the observation window).*

Finally, the success of DYCOMNET in 2024 is underlined by a German Academic Exchange Service DAAD travel award, granted to our team member Jonas Köppl, which will allow him to further pursue his excellent research for four months at the prestigious University of California, Los Angeles. In September 2024, our team member Anh Duc Vu successfully defended his Ph.D. at the Technische Universität Berlin on the topic "Percolation in Random Environments and Stochastic Homogenisation." In 2024, members of DYCOMNET served as organizers for a contributed session on "Gibbs Measures – Continuum and Discrete" at the "Bernoulli-IMS 11th World Congress in Probability and Statistics" in Bochum, as well as for the week-long Eurandom workshop on "Interacting Particles in the Continuum" within the Eurandom Ambassador Program at the Technical University of Eindhoven. A special highlight in 2024 was the three-day DYCOMNET workshop at WIAS on "Dynamic Spatial Random Systems" featuring two minicourses plus eight international expert presentations and many guests from around Europe. Last but not least, members of the team gave about 16 presentations at national and international conferences, workshops and seminars, also including several outreach talks.

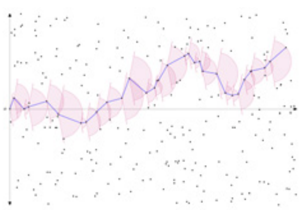

Fig. 3: *Realization of a random directed path started in the origin where each point chooses its closest neighbor towards the right in a Poisson point cloud*

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[6] P.P. Ghosh, B. Jahnel, S.K. Jhawar, *Large and moderate deviations in Poisson navigations*, WIAS Preprint no. 3096, 2024.

A Facts and Figures

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

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

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

A.1.1 Offers of Professorships

1. C. Geiersbach, W1 Professorship, March 22, Universität Hamburg, Fachbereich Mathematik.

A.1.2 Awards and Distinctions

1. A. Mielke, *ISIMM Senior Prize 2024*, April 4.
2. ———, *MATH+ Distinguished Fellowship*.
3. P. Farrell, *Vice Chair of the Committee for Mathematical Modeling, Simulation, and Optimization (KoMSO) since November 18, 2024*.
4. G. Heinze, *Member of the GAMM Junior Group, Gesellschaft für Angewandte Mathematik und Mechanik*, July 18.
5. M. Hintermüller, *Board Member of Berlin's non-university research institutions initiative BR50 (Berlin Research 50)*.
6. ———, *Chair of the Berlin Mathematics Research Center MATH+ until October 2024*.
7. ———, *Spokesperson of MaRDI – The Mathematical Research Data Initiative within the National Research Data Infrastructure*.
8. D. Hömberg, *Chair of the European Consortium for Mathematics in Industry (ECMI)'s Research and Innovation Committee*.
9. ———, *Head of the Secretariat of the International Mathematical Union (IMU)*.
10. ———, *Treasurer of IMU*.
11. M. Thomas, *Speaker of the Collaborative Research Center 1114 "Scaling Cascades in Complex Systems"*.

A.1.3 Defenses of Ph.D. Theses

1. E. Gladin, *Cutting plane methods and dual problems*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, Berlin Mathematical School, supervisor: Prof. Dr. V. Spokoiny, August 20.
2. J.M. Oeschger, *Microstructure imaging using MRI: Diffusion MRI and biophysical models under the influence of noise*, Universität Hamburg, Fachbereich Physik, supervisors: Dr. K. Tabelow, Dr. S. Mohammadi, June 21.
3. M. Theiss, *First order mean-field games and mean-field optimal control*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, December 20.
4. D. Abdel, *Modeling and simulation of vacancy-assisted charge transport in innovative semiconductor devices*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Dr. P. Farrell, February 15.
5. S. Breneis, *Rough paths and rough volatility*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Dr. Ch. Bayer, Prof. Dr. P. Friz, April 9.
6. G. Heinze, *Graph-based nonlocal gradient systems and their local limits*, Universität Augsburg, Mathematisch-Naturwissenschaftlich-Technische Fakultät, supervisor: Prof. Dr. J.-F. Pietschmann, March 15.
7. H. Langhammer, *Spatial particle processes with coagulation*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, November 7.

8. L. Plato, *Cross-diffusion in population dynamics and electrokinetics – Analysis and numerics*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. D. Hömberg, Dr. R. Lasarzik, September 26.
9. D. Sommer, *Kernel learning, optimal control and Bayesian posterior sampling with low rank tensor formats*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. M. Eigel, April 16.
10. A.D. Vu, *Percolation in randoms and stochastic homogenisation*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. B. Jahnel, September 30.

A.1.4 Supervision of Undergraduate Theses

1. N. Adriel, *Intermediate-scale order statistics* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, June 13.
2. M. Blagojevic, *The Nash equilibrium problem: Beyond convexity* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, September 20.
3. J. Breuer, *A numerical analysis of energy-variational solutions for electroosmotic flow in nematic liquid crystal* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. R. Lasarzik, August 22.
4. K. Chimezie Nwokebirinwa, *Dependence of hydrogen embrittlement on the time scales of crack propagation in the Paris law* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Dr. D. Peschka, November 6.
5. N. Corsi, *Existence of local time for the solution of stochastic heat equation* (master's thesis), Università di Trento, Dipartimento di Matematica, supervisor: Dr. O. Butkovsky, March 22.
6. C. Daubermann, *Interior point algorithms with inexact step computation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, September 24.
7. A.K. El-Rahhal, *Evaluierung verschiedener numerischer Optimierungsstrategien für reale Produktionssysteme* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, March 8.
8. J. Faust, *Große Abweichungen für die Lokalzeiten einer Irrfahrt mit zufälligen Leitfähigkeiten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 19.
9. M. Grützner, *On a variational model for microstructures in shape-memory alloys: Energy scaling behavior* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. J. Ginster, September 24.
10. M. Hain, *Invariance principle for the random conductance model — An alternative approach* (bachelor's thesis), Technische Universität Braunschweig, Carl-Friedrich-Gauß-Fakultät, supervisors: Prof. Dr. S. Andres, Prof. Dr. B. Jahnel, December 30.
11. L.E.Z. Hanke, *Große zufällige Partikelsysteme mit Koagulation und Fragmentation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 16.
12. Ch. Helms, *Neural networks and random matrices* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, April 23.
13. S.I.E. Jänchen, *Phasenübergang im Widom-Rowlinson-Modell* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, March 25.

14. X. Jiang, *Asymptoten für einen Multityp-Verzweigungsprozess in zufälliger Umgebung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 11.
15. F. Jur, *First-Passage Perkolation auf einem Poisson'schen Punktprozess* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 31.
16. D. Kamecke, *Central limit theorem for a many-body system* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. W. van Zuijlen, June 19.
17. A. Korzec, *Stochastic finite element methods and discretizations of random PDEs* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, December 2.
18. Z. Ma, *Prinzip Großer Abweichungen für einfache Irrfahrten auf Zd* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. P. Friz, August 9.
19. M. Matthaiou, *Solutions to elliptic boundary value problems based on machine learning techniques that satisfy the discrete maximum principle* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. V. John, August 27.
20. I. Meyer, *Condensation in a mean-field Bose gas* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, November 4.
21. T. Okunola, *Data-driven models for battery degradation* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, March 1.
22. H. Reichle, *Mathematical analysis of minimizing movement schemes for oscillatory energies* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. J. Ginster, September 18.
23. A. Ril, *Random walks in Weyl chambers of types C and D* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, August 22.
24. Th. Schmidt, *Witten-Laplacian mit binären Spinvariablen* (bachelor's thesis), Technische Universität Braunschweig, Carl-Friedrich-Gauß-Fakultät, supervisors: Prof. Dr. V. Bach, Prof. Dr. B. Jahnel, November 7.
25. H.V. Vu Tran, *Phasenübergang im dichten Erdös-Rényi Graphen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, February 22.
26. D. Xing, *Scharfe Phasenübergänge in gerichteter Perkolation* (master's thesis), Technische Universität Braunschweig, Carl-Friedrich-Gauß-Fakultät, supervisor: Prof. Dr. B. Jahnel, November 7.
27. J. Yuan, *Irrfahrten konditioniert auf kurzem Aufenthalt im Negativen* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 14.
28. M.I. Gau, *Dimension reduction of a thermo-visco-elastic problem at small strains* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. M. Liero, May 16.
29. A. Talasikar, *Asymptotic expansions and simulations of induced electrokinetic flows around polarizable particles* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. D. Peschka, July 22.

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 was 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 were examined. Moreover, a continuous differential equation perspective on neural networks was analyzed, which should allow for an efficient optimization procedure. The project was 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.

- **Approved project, starting in 2025:**

  dealii-X: An Exascale Framework for Digital Twins of the Human Body (in RG 3)

  The dealii-X CoE aims to elevate existing pre-exascale applications of digital twins for the brain, heart, lungs, liver, and mechanobiology to exascale readiness, providing an ideal computational platform for the integration of the developed software.

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

- **BMBF Funding Program on Flexible, Resilient, and Efficient Machine Learning Models**

  Joint project "Flexible, Resilient and Efficient Multi-scale Simulation using Hybridisation of Established Numerical Solvers with Physically-informed Neural Networks (HybridSolver)" in RG 8, Head: M. Hintermüller (October 1, 2024 – September 30, 2027)

  This collaboration project is headed by the Director of WIAS and head of RG 8, Michael Hintermüller. and brings together a consortium of academic and industry experts, with the WIAS, the Chair of Scientific Computing (SciComp) at the Universität Kaiserslautern-Landau (RPTU), and the Leibniz-Institut für Verbundmaterialien (IVW). The project also benefits from the industrial insight of BOSCH and COMSOL, who serve as advisory board members.

- **BMBF Funding Program "Fusion 2040 – Research on the Way to the Fusion Power Plant"**

  Joint Project "Diode Laser Pump Sources for High-Energy Lasers in Fusion Power Plants (DioHELIOS)" of the consortium partners ams-OSRAM, Ferdinand-Braun-Institut – Leibniz-Institut für Höchstfrequenztechnik (FBH), Fraunhofer-Institut für Lasertechnik ILT, Jenoptik, Laserline, and TRUMPF. WIAS participates as a subcontractor of the consortium partner Ferdinand-Braun-Institut (in RG 2).

Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Bonn

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

  ### The Berlin Mathematics Research Center MATH+

  The highlight of the collaboration with the mathematical institutions in Berlin since January 2019 has been 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,

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

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 2024, WIAS again dedicated considerable financial and personal resources to the Center: Its Director, Prof. M. Hintermüller (RG 8) is a member of the MATH+ Executive Board. Together with Prof. W. König (RG 5), Dr. U. Bandelow (RG 2), Prof. P. Friz (RG 6), Prof. V. Spokoiny (RG 6), Prof. M. Thomas (RG 1), Dr. Chr. Bayer (RG 6), and Dr. R. Henrion (RG 4), he is also a member of the MATH+ Council; Dr. U. Bandelow (RG 2) is a Scientist in Charge of the Application Area AA2 "Nano and Quantum Technologies," Prof. P. Friz (RG 6) and Dr. R. Henrion (RG 4) are 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," 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)

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

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)

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

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

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/Transregio (TRR) 388: "Rough Analysis, Stochastic Dynamics and Related Fields,"** Technische Universität Berlin

  In Summer 2024, the DFG decided to establish this new Collaborative Research Center at TU Berlin. This decision in particular acknowledges Berlin's worldwide outstanding role as a trendsetter in stochastic analysis with modern methods. The speaker is TU professor and external WIAS member Peter Friz. This CRC is run by the three Berlin universities, and the WIAS participates in various partial projects in research groups 1, 5, and 6. The first funding period started in October 2024 and extends until June 2028. WIAS is contributing in the subprojects "Optimal transport meets rough analysis (in RG 1 and RG 6 with TU Berlin), "Statistical learning from path observations" (in RG 6 with HU Berlin), "Microstructural foundations of rough volatility models" (in RG 6 with HU Berlin), "Signature methods for optimal control in finance" (in RG 6 with TU Berlin), and "Bayesian inference and mean field appoximation for nonlinear (S)PDE" (in RG 6 with HU Berlin).

- **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 with FU Berlin) and C02 "Interface dynamics: Bridging stochastic and hydrodynamic descriptions" (in RG 1 and RG 5, 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 2025.

WIAS participated in 2024 with the coordination funds and the subproject “A non-smooth phase-field approach to shape optimization with instationary fluid flow.” A book on the second phase of the SPP is in preparation with Springer.

- **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 RG 1, 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 contributed in 2024 to the priority program with the subproject “Analysis for thermo-mechanical models with internal variables” (in RG 1).

- **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 since 7/2024 with the subproject “Spatial coagulation and gelation” (in RG 5).

- **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.

  The subproject “Optimal transport and measure optimization foundation for robust and causal machine learning” (in WG DOC) started on October 2, 2024.

- **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.

- **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.

- **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)

  "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)

Leibniz-Gemeinschaft (Leibniz Association), Berlin

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

  "Leibniz-MMS: Mathematische Modellierung und Simulation" (Leibniz MMS: Mathematical Modeling and Simulation; June 2024 – May 2027, in Director's office)

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

  "Numerical Methods for Innovative Semiconductor Devices" (January 2020 – December 2025, 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-Institut für Techno- und Wirtschaftsmathematik, Deutsches Forschungszentrum für Künstliche Intelligenz Kaiserslautern, and Leibniz-Institut für Polymerforschung 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-Institut (FBH). Further partner: Center of Excellence for Photonic-Crystal Surface-Emitting Lasers at Kyoto University (April 2023 – April 2026)

"Linguistic Meaning and Bayesian Modelling," joint project with RG 6, coordinated by the Leibniz-Zentrum Allgemeine Sprachwissenschaft (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)
- Thematic Einstein Semester "Mathematics for Quantum Technologies" (April – September 2024, co-organized by RG 1 and RG 2)

National Research Data Infrastructure

- MaRDI (see page 39)

  "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): "Chance-constrained linear complementarity problem" and "Probabilistic least squares and applications" (both in RG 4)

Mission-oriented research (examples)

- Bosch, Stuttgart: "Deep-learning-based surrogate modeling for time-dependent physical systems "
- Ferdinand-Braun-Institut, Berlin: "Simulation of the spatio-temporal dynamics of high-power semiconductor lasers" (in RG 2)

A.3 Membership in Editorial Boards[2]

1. M. Brokate, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague, Czech Republic.
2. ———, Editorial Board, Mathematical Methods in the Applied Sciences, John Wiley & Sons, Ltd., Chichester, UK.
3. A. Mielke, Associate Editor, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
4. ———, Associate Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
5. ———, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
6. J. Sprekels, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest.
7. ———, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague, Czech Republic.
8. ———, Editorial Board, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
9. Ch. Bayer, Associate Editor, Quantitative Finance, Taylor & Francis Online, London, UK.
10. A.H. Erhardt, Editorial Board, Frontiers in Applied Mathematics & Statistics, Section Mathematical and Statistical Physics, Frontiers Media S.A., Lausanne, Switzerland.
11. ———, Editorial Board, Frontiers in Physics, Section Mathematical and Statistical Physics, Frontiers Media S.A., Lausanne, Switzerland.
12. P. Farrell, Editor, Open Mathematics, De Gruyter, Berlin.
13. C. Geiersbach, Editorial Board, Computational Optimization and Applications, Springer-Verlag, Heidelberg.
14. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Heidelberg.
15. R. Henrion, Associate Editor, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
16. ———, Editorial Board, Journal of Convex Analysis, Heldermann Verlag, Lemgo.
17. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
18. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
19. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
20. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
21. M. Hintermüller, Associate Editor, ESAIM: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
22. ———, Associate Editor, Advances in Continuous and Discrete Models: Theory and Modern Applications, Springer Nature, New York, USA.

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

23. ———, Associate Editor, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, USA.
24. ———, Associate Editor, Foundations of Data Science, American Institute of Mathematical Sciences, Springfield, USA.
25. ———, Editorial Board, Interfaces and Free Boundaries, European Mathematical Society Publishing House, Zurich, Switzerland.
26. ———, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
27. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
28. ———, Editorial Board, Optimization Methods and Software, Taylor & Francis, Oxford, UK.
29. ———, Series Editor, International Series of Numerical Mathematics, Springer-Verlag, Basel, Switzerland.
30. ———, Series Editor, Handbook of Numerical Analysis, Elsevier, Amsterdam, Netherlands.
31. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
32. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
33. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
34. ———, Editorial Board, Bernoulli Journal, International Statistical Institute/Bernoulli Society for Mathematical Statistics and Probability, The Hague, Netherlands.
35. ———, Series Editor, Pathways in Mathematics, Birkhäuser, Basel, Switzerland.
36. M. Radziunas, Editorial Board, Mathematical Modelling and Analysis, Vilnius Gediminas Technical University, Vilnius, Lithuania.
37. J.G.M. Schoenmakers, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
38. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
39. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
40. V. Spokoiny, Co-Editor, The Annals of Statistics, Institute of Mathematical Statistics, USA.
41. M. Thomas, Associate Editor, Discrete & Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences, Springfield, USA.
42. 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

Dynamic Spatial Random Systems
Berlin, January 29–31
Organized by: WIAS (LG DYCOMNET)
Supported by: DFG SPP 2265, MATH+

The workshop on interacting random systems with spatial and dynamical features was a resounding success, bringing together 44 researchers from across Europe to exchange ideas and explore new developments in this vibrant field. The event focused on advancing the understanding of systems with both theoretical and applied perspectives, addressing topics such as dynamical random graphs, interacting particle systems, percolation theory, and random walks, with applications spanning wireless networks, biological systems, and mathematical physics. Highlights included in-depth mini-courses and engaging invited talks, which spurred insightful discussions and fostered collaborations among participants. This workshop not only showcased cutting-edge research but also strengthened connections within the research community, paving the way for future advancements.

OT Berlin 2024 – Optimal Transport: From Theory to Applications
Berlin, March 11–15
Organized by: WIAS (RG 1, RG 6, WG DOC), TU Berlin
Supported by: DFG, MATH+, WIAS

The 2024 workshop on Optimal Transport (OT) theory brought together experts from mathematics, computer science, and applied sciences to explore the interplay between theory and applications of OT. With 25 invited talks and 27 poster contributions, the event fostered interdisciplinary collaboration among 103 global participants, including early-career researchers. The program spanned diverse topics, from PDEs, geometry, and gradient flows to advanced applications in machine learning, optimization, and statistics. Highlights included discussions on unbalanced OT, entropic regularization, and machine learning frameworks exploiting OT principles. Invited speakers addressed challenges in computation, data-driven modeling, and novel theoretical approaches. Poster sessions, complemented by concise pitches, encouraged vibrant scientific exchange. The workshop emphasized bridging theoretical insights with real-world applications, particularly in understanding complex systems and improving computational methodologies.

Women in Math – Introduction of the Iris Runge Postdoc Program
Berlin, March 18
Organized by: WIAS

This kick-off was a celebration of women in math: Along with the introduction of our first two program participants Anieza Maltsi and Jin Yan, the program featured a talk by Renate Tobies (Jena) on Iris Runge and the opening of the touring exhibition “Women of Mathematics from around the world – A gallery of portraits.” The exhibition, proudly hosted by WIAS in its library, offered a glimpse into the world of mathematics through photographs of female mathematicians by Noel Tovia Matoff and excerpts of interviews by Sylvie Paycha and Sara Azzali.

Leibniz MMS Days 2024
Kaiserslautern, April 10–12
Organized by: IVW Kaiserslautern, WIAS
Supported by: Leibniz Association (Grant for network activities)

The Leibniz MMS Days are the central annual workshop of the Leibniz Research Network “Mathematical Modeling and Simulation (MMS).” In 2024, this workshop took place from April 10 to 12 at the Leibniz-Institut für Verbundwerkstoffe GmbH (Leibniz Institute for Composite Materials, IVW) in Kaiserslautern. The meeting represented another important step in the further development of the network’s activities. It was attended by

78 scientists from 25 institutions. Two key-note talks were given by Nathan Kutz (University of Washington) “Revolutionizing science and engineering in the age of machine learning” and Claudia Redenbach (Universität Kaiserslautern-Landau, RPTU) on “Stochastic modelling of microstructures.” 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.

Quantum Optimal Control From Mathematical Foundations to Quantum Technologies
Berlin, May 21–24
Organized by: WIAS (RG 2 / SemQuTech), ZIB, FU Berlin, TU Berlin
Supported by: Einstein Foundation Berlin, MATH+

In May 2024, the workshop “Quantum Optimal Control – From Mathematical Foundations to Quantum Technologies” attracted numerous pioneers and young researchers in the field of optimal control of quantum systems. The program comprised a total of 30 talks and 36 posters on a broad range of current topics at the interface between applied mathematics and theoretical physics, e.g., numerical methods and algorithms for quantum optimal control problems, controllability of quantum systems, quantum thermodynamics and control of open quantum systems, quantum computing algorithms and quantum error correction as well as applications to specific model systems (cold atoms in optical lattices, Bose–Einstein condensates, superconductors). Video recordings of the talks are available on the MATH+ YouTube channel [1]. In addition, the participants were given the opportunity to learn about state-of-the-art software tools for quantum optimal control problems within the framework of an integrated software tutorial. The workshop received great interest and attracted about 100 registered on-site participants, so that the registration had to be terminated early. In response to the considerable international interest, a hybrid option was set up at short notice, whereupon a further 50 participants registered for the online stream. The workshop was organized by Tobias Breiten (Technische Universität Berlin), Patrick Gelß (Zuse Institute Berlin), Markus Kantner (WIAS), and Christiane Koch (Freie Universität Berlin) as a part of the Thematic Einstein Semester on “Mathematics for Quantum Technologies.”

[1] https://www.youtube.com/playlist?list=PLMG1in_rYUozabocEiHeUplvuUf1Nm2bs

19th Berlin-Oxford Young Researchers Meeting on Applied Stochastic Analysis
Berlin, June 24–26
Organized by: WIAS (RG 6), TU Berlin, University of Oxford
Supported by: WIAS, University of Oxford, TU Berlin, DFG IRTG 2544, DataSig

Around 50 participants attended the 19th Berlin-Oxford Workshop in April of this years, as in previous years participants were predominantly from the UK and Germany, but we also had several particpants from France. 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 18th meeting took place in Oxford in January 2024, a 20th meeting is again scheduled for Oxford.)

Developments in Computational Finance and Stochastic Numerics
Berlin, July 1
Organized by: WIAS (RG 6)
Supported by: WIAS

The workshop honoring John Schoenmakers’s successful career in computational finance and stochastic numerics and his service to WIAS was attended by around thirty participants, mainly from Germany and the Netherlands. Eight invited presentations were given by leaders in the field, who had important interactions with John Schoenmakers. Most of the speakers were former group members of WIAS. A wide variety of topics were presented, including models of water movement, regression, Hawkes processes, and machine learning.

The Director of WIAS, the head of RG 6, and several speakers praised John Schoenmakers for his impactful contributions to the institute and the research community, and wished him well for his retirement.

Workshop Junior Female Researchers in Probability
Berlin, July 3–5
Organized by: WIAS (RG 5), TU, FU and HU Berlin
Supported by: IRTG 2544, CRC 1114, MATH+, TU Berlin, HU Berlin, FU Berlin, and WIAS

The workshop was one of the activities of the International Research Training Group (IRTG) 2544 *Stochastic Analysis in Interaction*. The goal of the workshop was to offer junior female researchers in stochastics a platform to talk about their own research work and to get acquainted with important research topics presented by well-established female researchers. The talks covered a wide variety of topics: chemical reaction networks, convergence on high dimensional spaces, machine learning, risk measure theory, statistics within the context of deep learning, and introducing new research topics spreading over the last years such as cellular automaton with solitonic behavior. There were two keynote talks, four invited talks and 23 contributed from master's students, Ph.D. students, and postdoc researchers. The workshop hosted about 75–80 participants.

Two of the organizers were members of the RG 5 *Interacting Random Systems*.

Second NFDI Berlin-Brandenburg network meeting: Ontologies and Knowledge Graphs
Berlin, July 11
Organized by: WIAS, MaRDI
Supported by: MaRDI

The MaRDI (Mathematical Research Data Initiative) team at WIAS organized a second regional networking event, where all NFDI (National Research Data Infrastructure) consortia within the Berlin-Brandenburg area were invited to. The one-day workshop took place on July 11, 2024, at WIAS in Berlin. There was a total of 35 registered participants coming from 16 different consortia in the area. During the first NFDI in Berlin-Brandenburg (NFDI_BB) meeting, the topic "Ontologies and Knowledge Graphs" was identified as a central task overarching the consortia and which was chosen as the topic of this meeting. During the morning session, a general overview of that topic was given by four speakers, focusing—among others—on the newly installed NFDI basic services (Base4NFDI) as well as Wikidata and Wikibase technology stacks. In the afternoon session, the focus switched to individual ontologies and knowledge graphs developed/used within the different consortia of the NFDI. The topic was very interesting for the participants, thus opening up potential collaboration also across consortia from diverse disciplines while a strong interest was shown in continuing the series of NFDI_BB meetings in the future.

AMaSiS 2024: Applied Mathematics and Simulation for Semiconductor Devices
Berlin, September 10–13
Organized by: WIAS (RG 1, RG 2, LG NUMSEMIC), Josef Weinbub (Silvaco, Inc.)
Supported by: MATH+, Einstein Foundation, WIAS

The international workshop "AMaSiS 2024: Applied Mathematics and Simulation for Semiconductor Devices" was organized by Annegret Glitzky, Matthias Liero, Michael O'Donovan (RG 1), Markus Kantner (RG 2), Patricio Farrell (LG NUMSEMIC), and Josef Weinbub (Silvaco Vienna) as part of the event series "Thematic Einstein Semester: Mathematics for Quantum Technologies." It was held at the Humboldt-Universität zu Berlin and the Leibniz Headquarters from September 10 to 13. AMaSiS 2024 started with two full-day tutorial sessions and had its focus on quantum and semiclassical transport, electronic structure theory, computational materials science, and on upscaling from quantum mechanics and particle systems to continuum-scale models. A particular focus was on spin-qubit devices for applications in quantum information processing. With 19 invited talks, 19 contributions, and 57 participants from nine countries AMaSiS 2024 brought together experts from mathematics, physics, engineering, and material science to address new challenges in mathematical modeling and numerical simulation of semiconductor devices.

Exploring Calcium Channel Dynamics: From Molecular Insights to Macroscopic Ion Flow
Berlin, October 14–15
Organized by: WIAS (RG 3 and RG 7), CRC 1114, ZIB
Supported by: MATH+, CRC 1114, WIAS, ZIB

As part of the two MATH+ projects AA1-14 “Development of an ion-channel model-framework for in-vitro assisted interpretation of current voltage relations” and AA1-15 “Math-powered drug design,” the workshop “Exploring Calcium Channel Dynamics: From Molecular Insights to Macroscopic Ion Flow” took place at WIAS on October 14 and 15, 2024. Around 20 scientists took part, including mathematicians, theoreticians, and experimenters. Its aim was to discuss the mechanisms of ion channels from different perspectives, including molecular dynamics, continuum models, and experimental approaches. The workshop focused on three thematic areas: perception of ion channels, bridging scales, and combining theory and experiments. The invited speakers were Bob Eisenberg (Rush University), Christoph Stein (Charité), and Alexander Walter (Unversity of Copenhagen).

Third Annual Conference of the SPP 2265
Berlin, October 28–30
Organized by: WIAS (RG 5)
Supported by: DFG SPP 2265

This conference was one of the main activities of the Priority Program SPP 2265 *Random Geometric Systems*. It was the third edition of the annual meeting of all the members of this program. The conference offered a broad survey on all the topics of the SPP 2265, like spatial point processes, percolation, random polytopes, phase transitions, and much more. The program comprised two extended guest talks, the presentation of 12 of the 36 projects of the SPP 2265, and a series of crash courses for younger researchers on fundamental topics. One of the main purposes of the conference (as for the entire SPP) was to foster discussions across the language barrier between physics and mathematics and between different mathematical areas. There were 70 participants, two third of which were Ph.D. students or fresh postdocs. All talks were given in presence in the wonderful location of the Harnack House in Berlin-Dahlem.

The organizers were members of the RG 5 *Interacting Random Systems*.

Foundations of Modern Nonparametric Statistics
Berlin, November 13
Organized by: WIAS (RG 6)
Supported by: WIAS

Nonparametric methods have become essential in modern statistical theory and practice, offering flexibility and robustness in analyzing complex data structures without assuming a specific parametric form for the underlying distributions. The workshop brought together specialists from across Europe and Israel in the field to discuss recent advances in nonparametric statistics and related topics. Specific topics addressed were inverse problems, adaptive estimation, bandits, the Smoluchowski process, and panel models. The workshop took place on the occasion of Vladimir Spokoiny’s 65th birthday, and his significant influence on modern nonparametric statistics was a major theme of the workshop.

Probability meets Biology: Berlin Edition
Berlin, November 27—29
Organized by: WIAS (RG 5)
Supported by: MATH+, SFB 1114, WIAS

The aim of this workshop was to bring together young researchers, particularly Ph.D. students and early-career postdocs, to collaborate on topics at the intersection of probability theory and biology. The event was designed to foster a collaborative environment where current questions and innovative approaches from both fields could be explored. A total of 24 young researchers participated, traveling from various institutions and countries to attend. The workshop began with five short introductory talks (three by biologists and two by mathematicians), in which open problems involving stochastic modeling of certain biological phenomena were presented. Following these sessions, participants were divided into small working groups to collaboratively address these specific problems. Most of these groups showed their intention to continue their collaboration beyond the workshop.

The organizers were members of the RG 5 *Interacting Random Systems*.

A.4.2 Oberwolfach Workshops co-organized by WIAS

Directions in Rough Analysis
Mathematisches Forschungsinstitut Oberwolfach, November 3–8
Organized by: Thomas Cass (London), Christa Cuchiero (Vienna), Peter K. Friz (RG 6)

This workshop focused on the currently most active areas of the subject among two central strands: (1) the mathematics of the signature transform, including its applications to data science and finance, and (2) rough path theory applied to novel areas in stochastic analysis, such as homogenization, SLE, and rough PDEs.

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

1. A. Alphonse, M. Bongarti, organizers of the Minisymposium 07 "Modeling, Analysis and Optimal Control of Infinite Dimensional Problems and Applications", *31st IFIP TC7 Conference 2024 on System Modeling and Optimization*, Universität Hamburg, August 12–16.
2. U. Bandelow, co-organizer, *Workshop on Integrability for Higher-Order Optical Pulse Propagation associated with the meeting of the Australian and New Zeeland Association of Mathematical Physics (ANZAMP)*, Katoomba, Australia, February 6–9.
3. ———, co-organizer, *Workshop on Nonlinear Photonics and Metasurfaces*, Australian National University, Canberra, Australia, February 8.
4. U. Bandelow, M. Kantner, Th. Koprucki, co-organizers, *Thematic Einstein Semester 2024 "Mathematics for Quantum Technologies", among other things: Kick Off Event (April 16, TU Berlin), Quantum Optimal Control (May 21–24, FU/ZIB Berlin), Advanced Lecture Series by Prof. Ronnie Kosloff "Quantum Thermodynamics and Quantum Control" (May 16–29, FU Berlin), Advanced Lecture Series by Prof. Ulf Leonhardt "Forces of The Quantum Vacuum"(July 15–19, WIAS), AMaSiS 2024 (September 10–13, WIAS/Leibniz Association Headquarters)*, Einstein Foundation & MATH+, Berlin, April 8 – September 30.
5. P.K. Friz, co-organizer, *18th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis*, University of Oxford, Mathematical Institute, UK, January 4–6.
6. ———, co-organizer, *Recent Developments in Rough Paths*, BI Norwegian Business School, Nydalen, Norway, March 3–8.
7. ———, organizer, *Klagenfurt-Berlin-Meeting on Multiple Perspectives in Optimization*, Universität Klagenfurt, Institut für Mathematik, Austria, June 6–7.
8. ———, co-organizer, *Workshop "Directions in Rough Analysis"*, Mathematisches Forschungsinstitut Oberwolfach (MFO), November 3–8.
9. ———, co-organizer, *20th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis*, University of Oxford, Mathematical Institute, UK, December 9–11.
10. C. Geiersbach, co-organizer, *TRR 154 Summer School on Optimization, Uncertainty and AI*, Universität Hamburg, August 7–9.
11. M. Hintermüller, co-meeting director, *VARANA 2024 (Variational Analysis and Applications): 77th Course of the International School of Mathematics "Guido Stampacchia"*, Erice, Italy, September 1–7.
12. B. Jahnel, co-organizer, *Interacting Particles in the Continuum*, EURANDOM, Eindhoven, Netherlands, September 9–13.
13. B. Jahnel, J. Köppl, organizers of the Minisession OCPS 22 "Gibbs Measures – Continuum and Discrete", *Bernoulli-IMS 11th World Congress in Probability and Statistics*, Ruhr-Universität Bochum, August 13.
14. J. Kern, organizer, *Math.en JEANS*, Technische Universität Berlin, June 26.
15. A. Maltsi, member of the Scientific Committee, *Future WINS: Cross-sections and Interfaces in Science, Careers, and Communication*, Humboldt-Universität zu Berlin, November 21–22.
16. D. Sommer, co-organizer of the Minisymposium "Nonlinear Approximation of High-Dimensional Functions: Compositional, Low-Rank and Sparse Structures I–III", *SIAM Conference on Uncertainty Quantification (UQ24)*, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 27 – March 1.

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

A.6 Publications

A.6.1 Monographs

[1] V.A. Zagrebnov, H. Neidhardt, T. Ishinose, *Trotter–Kato Product Formulae*, vol. 296 of Operator Theory: Advances and Applications, Springer Nature, Cham, 2024, vii+873 pages. doi:10.1007/978-3-031-56720-9.

A.6.2 Outstanding Contributions to Monographs

[1] A. Caiazzo, L. Heltai, I.E. Vignon-Clementel, *Part 1/Chapter 2: Mathematical Modeling of Blood Flow in the Cardiovascular System, in: Quantification of Biophysical Parameters in Medical Imaging, Second Edition*, I. Sack, T. Schaeffter, eds., Springer, Cham, 2024, pp. 39–61. doi:10.1007/978-3-031-61846-8_3.

A.6.3 Articles in Refereed Journals[4]

[1] P. Bella, M. Kniely, *Regularity of random elliptic operators with degenerate coefficients and applications to stochastic homogenization*, Stoch. Partial Differ. Equ. Anal. Comput., 12 (2024), pp. 2246–2288. doi:10.1007/s40072-023-00322-9.

[2] M. Brokate, M. Ulbrich, *Corrigendum and Addendum: Newton differentiability of convex functions in normed spaces and of a class of operators*, SIAM J. Optim., 34 (2024), pp. 3163–3166. doi:10.1137/24M1669542.

[3] P. Colli, G. Gilardi, A. Signori, J. Sprekels, *Curvature effects in pattern formation: Well-posedness and optimal control of a sixth-order Cahn–Hilliard equation*, SIAM J. Math. Anal., 56 (2024), pp. 4928–4969. doi:10.1137/24M1630372.

[4] P. Colli, J. Sprekels, F. Tröltzsch, *Optimality conditions for sparse optimal control of viscous Cahn–Hilliard systems with logarithmic potential*, Appl. Math. Optim., 90 (2024), pp. 47/1–47/48. doi:10.1007/s00245-024-10187-6.

[5] R. Haller, H. Meinlschmidt, J. Rehberg, *Hölder regularity for domains of fractional powers of elliptic operators with mixed boundary conditions*, Pure Appl. Funct. Anal., 9 (2024), pp. 169–194.

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[10] J. Sprekels, F. Tröltzsch, *Second-order sufficient conditions in the sparse optimal control of a phase field tumor growth model with logarithmic potential*, ESAIM Control Optim. Calc. Var., 30 (2024), pp. 13/1–13/25. doi:10.1051/cocv/2023084.

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

[11] D. Abdel, A. Glitzky, M. Liero, *Analysis of a drift-diffusion model for perovskite solar cells*, Discrete Contin. Dyn. Syst. Ser. B, 30 (2025), pp. 99–131 (appeared online in June 2024). doi:10.3934/dcdsb.2024081.

[12] S. Amiranashvili, R. Čiegis, *Stability of the higher-order splitting methods for the generalized nonlinear Schrödinger equation*, Math. Model. Anal., 29 (2024), pp. 560–574. doi:10.3846/mma.2024.20905.

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A.7 Preprints, Reports

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[33] G. Dong, M. Hintermüller, C. Sirotenko, *Dictionary learning based regularization in quantitative MRI: A nested alternating optimization framework*, Preprint no. 3135, WIAS, Berlin, 2024.

[34] D. Hömberg, R. Lasarzik, L. Plato, *Existence of weak solutions to an anisotropic electrokinetic flow model*, Preprint no. 3104, WIAS, Berlin, 2024.

[35] K. Hopf, M. Kniely, A. Mielke, *On the equilibrium solutions of electro-energy-reaction-diffusion systems*, Preprint no. 3157, WIAS, Berlin, 2024.

[36] D. Brust, K. Hopf, J. Fuhrmann, A. Cheilytko, M. Wullenkord, Ch. Sattler, *Transport of heat and mass for reactive gas mixtures in porous media: Modeling and application*, Preprint no. 3139, WIAS, Berlin, 2024.

[37] K. Hopf, J. King, A. Münch, B. Wagner, *Interface dynamics in a degenerate Cahn–Hilliard model for viscoelastic phase separation*, Preprint no. 3149, WIAS, Berlin, 2024.

[38] T. Iyer, *Fixation of leadership in non-Markovian growth processes*, Preprint no. 3137, WIAS, Berlin, 2024.

[39] ———, *Persistent hubs in CMJ branching processes with independent increments and preferential attachment trees*, Preprint no. 3138, WIAS, Berlin, 2024.

[40] P.P. Ghosh, B. Jahnel, S.K. Jhawar, *Large and moderate deviations in Poisson navigations*, Preprint no. 3096, WIAS, Berlin, 2024.

[41] B. Jahnel, U. Rozikov, *Gibbs measures for hardcore-SOS models on Cayley trees*, Preprint no. 3100, WIAS, Berlin, 2024.

[42] ———, *Three-state p-SOS models on binary Cayley trees*, Preprint no. 3089, WIAS, Berlin, 2024.

[43] B. Jahnel, J. Köppl, *Time-periodic behaviour in one- and two-dimensional interacting particle systems*, Preprint no. 3092, WIAS, Berlin, 2024.

[44] B. Jahnel, J. Köppl, Y. Steenbeck, A. Zass, *The variational principle for a marked Gibbs point process with infinite-range multibody interactions*, Preprint no. 3126, WIAS, Berlin, 2024.

[45] B. Jahnel, L. Lüchtrath, M. Ortgiese, *Cluster sizes in subcritical soft Boolean models*, Preprint no. 3106, WIAS, Berlin, 2024.

[46] E. Jacob, B. Jahnel, L. Lüchtrath, *Subcritical annulus crossing in spatial random graphs*, Preprint no. 3148, WIAS, Berlin, 2024.

[47] V. John, X. Li, Ch. Merdon, *Pressure-robust L2 (Ω) error analysis for Raviart–Thomas enriched Scott–Vogelius pairs*, Preprint no. 3097, WIAS, Berlin, 2024.

[48] V. John, M. Matthaiou, M. Zainelabdeen, *Bound-preserving PINNs for steady-state convection-diffusion-reaction problems*, Preprint no. 3134, WIAS, Berlin, 2024.

[49] T. Bai, W. König, Q. Vogel, *Proof of off-diagonal long-range order in a mean-field trapped Bose gas via the Feynman–Kac formula*, Preprint no. 3119, WIAS, Berlin, 2024.

[50] E. Bolthausen, W. König, Ch. Mukherjee, *Self-repellent Brownian bridges in an interacting Bose gas*, Preprint no. 3110, WIAS, Berlin, 2024.

[51] L. Andreis, W. König, H. Langhammer, R.I.A. Patterson, *Spatial particle processes with coagulation: Gibbs-measure approach, gelation and Smoluchowski equation*, Preprint no. 3086, WIAS, Berlin, 2024.

[52] J. Köppl, N. Lanchier, M. Mercer, *Survival and extinction for a contact process with a density-dependent birth rate*, Preprint no. 3103, WIAS, Berlin, 2024.

[53] A. Kroshnin, V. Spokoiny, A. Suvorikova, *Generalized bootstrap in the Bures–Wasserstein space*, Preprint no. 3145, WIAS, Berlin, 2024.

[54] A. Kroshnin, A. Suvorikova, *Bernstein-type and Bennett-type inequalities for unbounded matrix martingales*, Preprint no. 3146, WIAS, Berlin, 2024.

[55] R. Lasarzik, E. Rocca, R. Rossi, *Existence and weak-strong uniqueness for damage systems in viscoelasticity*, Preprint no. 3129, WIAS, Berlin, 2024.

[56] L. Lüchtrath, *All spatial graphs with weak long-range effects have chemical distance comparable to Euclidean distance*, Preprint no. 3154, WIAS, Berlin, 2024.

[57] L. Lüchtrath, Ch. Mönch, *The directed age-dependent random connection model with arc reciprocity*, Preprint no. 3090, WIAS, Berlin, 2024.

[58] ———, *A very short proof of Sidorenko's inequality for counts of homomorphism between graphs*, Preprint no. 3120, WIAS, Berlin, 2024.

[59] M. Gösgens, L. Lüchtrath, E. Magnanini, M. Noy, É. de Panafieu, *The Erdős–Rényi random graph conditioned on every component being a clique*, Preprint no. 3111, WIAS, Berlin, 2024.

[60] E. Magnanini, G. Passuello, *Statistics for the triangle density in ERGM and its mean-field approximation*, Preprint no. 3102, WIAS, Berlin, 2024.

[61] E. Abi Jaber, Ch. Cuchiero, L. Pelizzari, S. Pulido, S. Svaluto-Ferro, *Polynomial Volterra processes*, Preprint no. 3098, WIAS, Berlin, 2024.

[62] J. Li, X. Liu, D. Peschka, *Local well-posedness and global stability of one-dimensional shallow water equations with surface tension and constant contact angle*, Preprint no. 3084, WIAS, Berlin, 2024.

[63] M. Radziunas, D.M. Kane, *Traveling wave mode analysis of coherence collapse regime semiconductor laser with optical feedback*, Preprint no. 3117, WIAS, Berlin, 2024.

[64] M. Radziunas, V. Raab, *Modeling and simulation of the cascaded polarization-coupled system of broad-area semiconductor lasers*, Preprint no. 3116, WIAS, Berlin, 2024.

[65] M. Radziunas, H. Wenzel, B. King, P. Crump, E. Kuhn, *Dynamical simulations of single-mode lasing in large-area all-semiconductor PCSELs*, Preprint no. 3156, WIAS, Berlin, 2024.

[66] J. Rehberg, *Regularity for non-autonomous parabolic equations with right-hand side singular measures involved*, Preprint no. 3150, WIAS, Berlin, 2024.

[67] T. Böhnlein, M. Egert, J. Rehberg, *Bounded functional calculus for divergence form operators with dynamical boundary conditions*, Preprint no. 3115, WIAS, Berlin, 2024.

[68] D. Belomestny, J.G.M. Schoenmakers, V. Zorina, *Weighted mesh algorithms for general Markov decision processes: Convergence and tractability*, Preprint no. 3088, WIAS, Berlin, 2024.

[69] P. Hagemann, J. Schütte, D. Sommer, M. Eigel, G. Steidl, *Sampling from Boltzmann densities with physics informed low-rank formats*, Preprint no. 3153, WIAS, Berlin, 2024.

[70] H. Shafigh, *A spatial model for dormancy in random environment*, Preprint no. 3136, WIAS, Berlin, 2024.

[71] C. Bellingeri, E. Ferrucci, N. Tapia, *Branched Itô formula and natural Itô–Stratonovich isomorphism*, Preprint no. 3083, WIAS, Berlin, 2024.

[72] L. Schmitz, N. Tapia, *Free generators and Hoffman's isomorphism for the two-parameter shuffle algebra*, Preprint no. 3087, WIAS, Berlin, 2024.

[73] A. Thayil, L. Ermoneit, M. Kantner, *Theory of valley-splitting in Si/SiGe spin-qubits: Interplay of strain, resonances and random alloy disorder*, Preprint no. 3158, WIAS, Berlin, 2024.

[74] W. van Oosterhout, *Linearization of finite-strain poro-visco-elasticity with degenerate mobility*, Preprint no. 3123, WIAS, Berlin, 2024.

[75] K. Panajotov, A.G. Vladimirov, M. Tlidi, *Polarized frequency combs in a mode-locked VECSEL*, Preprint no. 3109, WIAS, Berlin, 2024.

[76] O. Burylko, M. Wolfrum, S. Yanchuk, *Reversible saddle-node separatrix-loop bifurcation*, Preprint no. 3133, WIAS, Berlin, 2024.

A.7.2 Preprints/Reports in other Institutions

[1] S. Athreya, O. Butkovsky, K. Lê, L. Mytnik, *Analytically weak and mild solutions to stochastic heat equation with irregular drift*, arXiv:2410.06599, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2410.06599.

[2] O. Butkovsky, L. Mytnik, *Weak uniqueness for singular stochastic equations*, arXiv:2405.13780, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2405.13780.

[3] R. Araya, A. Caiazzo, F. Chouly, *Stokes problem with slip boundary conditions using stabilized finite elements combined with Nitsche*, arXiv:2404.08810, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2404.08810.

[4] C.K. MACNAMARA, I. RAMIS-CONDE, T. LORENZI, A. CAIAZZO, *An agent-based modelling framework for tumour growth incorporating mechanical and evolutionary aspects of cell dynamics*, bioRxiv:596685, Cold Spring Harbor Laboratory, New York, USA, 2024. doi:10.1101/2024.05.30.596685.

[5] P. DVURECHENSKY, Y. NESTEROV, *Improved global performance guarantees of second-order methods in convex minimization*, arXiv:2408.11022, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2408.11022.

[6] P. DVURECHENSKY, M. STAUDIGL, *Barrier algorithms for constrained non-convex optimization*, arXiv:2404.18724, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2404.18724.

[7] P. DVURECHENSKY, C. GEIERSBACH, M. HINTERMÜLLER, A. KANNAN, ST. KATER, G. ZÖTTL, *A Cournot–Nash model for a coupled hydrogen and electricity market*, arxiv:2410.20534, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2410.20534.

[8] E. GLADIN, P. DVURECHENSKY, A. MIELKE, J.-J. ZHU, *Interaction-force transport gradient flows*, arXiv:2405.17075, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2405.17075.

[9] M. EIGEL, J. SCHÜTTE, *Adaptive multilevel neural networks for parametric PDEs with error estimation*, arXiv:2403.12650, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2403.12650.

[10] G. ALÌ, P. FARRELL, N. ROTUNDO, *Forward lateral photovoltage scanning problem: Perturbation approach and existence-uniqueness analysis*, arXiv:2404.10466, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2404.10466.

[11] TH. BELIN, P. LAFITTE-GODILLON, V. LESCARRET, J. FUHRMANN, C. MASCIA, *Entropy solutions of a diffusion equation with discontinuous hysteresis and their finite volume approximation*, hal-04647129, HAL (Hyper Articles en Ligne) open science, National Center for Scientific Research (CNRS), Inria, and INRAE, France, 2024.

[12] L. ANDREIS, T. IYER, E. MAGNANINI, *Convergence of cluster coagulation dynamics*, arXiv:2406.12401, Cornell University, Ithaka, USA, 2024. doi:10.48550/arXiv.2406.12401.

[13] TH. ANANDH, D. GHOSE, H. JAIN, P. SUNKAD, S. GANESAN, V. JOHN, *Improving hp-variational physics-informed neural networks for steady-state convection-dominated problems*, arXiv:2411.09329, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2411.09329.

[14] P. GONÇALVES, J. KERN, L. XU, *A novel approach to hydrodynamics for long-range generalized exclusion*, arXiv:2410.17899, Cornell University, Ithaka, USA, 2024. doi:10.48550/arXiv.2410.17899.

[15] H. WENZEL, E. KUHN, B. KING, P. CRUMP, M. RADZIUNAS, *Theory of the linewidth-power product of photonic-crystal surface-emitting lasers*, arXiv:2024.11246, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2402.11246.

[16] I. PAPADOPOULOS, S. OLVER, *A sparse hierarchical hp-finite element method on disks and annuli*, arXiv.2402.12831, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2402.12831.

[17] K. KNOOK, S. OLVER, I. PAPADOPOULOS, *Quasi-optimal complexity hp-FEM for Poisson on a rectangle*, arXiv.2402.11299, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2402.11299.

[18] B. SCHEMBERA, F. WÜBBELING, H. KLEIKAMP, B. SCHMIDT, A. SHEHU, M. REIDELBACH, CH. BIEDINGER, J. FIEDLER, TH. KOPRUCKI, D. IGLEZAKIS, D. GÖDDEKE, *Towards a knowledge graph for models and algorithms in applied mathematics*, arXiv:2408.10003, Cornell University, Ithaca, 2024. doi:10.48550/arXiv.2408.10003.

[19] 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, 2024. doi:10.1101/2023.06.21.545891.

[20] I. CHEVYREV, J. DIEHL, K. EBRAHIMI-FARD, N. TAPIA, *A multiplicative surface signature through its Magnus expansion*, arXiv:2406.16856, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2406.16856.

[21] J.P. Thiele, *ideal.II: A Galerkin space-time extension to the finite element library deal.II*, arXiv:2408.08840, Cornell University, Ithaca, USA, 2024. doi:10.48550/arXiv.2408.08840.

[22] P.C. Africa, D. Arndt, W. Bangerth, B. Blais, M. Fehling, R. Gassmöller, T. Heister, L. Heltai, S. Kinnewig, M. Kronbichler, M. Maier, P. Munch, M. Schreter-Fleischhacker, J.P. Thiele, B. Turcksin, D. Wells, V. Yushutin, *The deal.II Library, Version 9.6*, Report, https://www.dealii.org/, 2024.

A.8 Talks and Posters

A.8.1 Main and Plenary Talks

1. A. Mielke, *Analysis of (fast-slow) reaction-diffusion systems using gradient structures*, Conference on Differential Equations and their Applications (EQUADIFF 24), June 10–14, Karlstad University, Sweden, June 14.
2. ———, *Asymptotic self-similar behaviour in reaction-diffusion systems on Rd*, Dynamical Systems Approaches towards Nonlinear PDEs, August 28–30, Universität Stuttgart, August 29.
3. Ch. Bayer, *Primal and dual optimal stopping with signatures (plenary talk)*, International Conference on Computational Finance (ICCF24), April 2–5, Utrecht University, Mathematical Institute, Netherlands, April 2.
4. ———, *RKHS regularization of singular local stochstic volatility McKean–Vlasov models*, Stochastics in Mathematical Finance and Physics Conference, October 21–25, Tunis El Manar University, Department of Mathematics, Hammamet, Tunisia, October 21.
5. P. Dvurechensky, *Hessian barrier algorithms for non-convex conic optimization (semi-plenary talk)*, Workshop on Nonsmooth Optimization and Applications (NOPTA 2024), April 8–12, University of Antwerp, Department of Mathematics, Belgium, April 10.
6. R. Henrion, *Optimization problems with probabilistic/robust (probust) constraints: Theory, numerics and applications*, 31th IFIP TC 7 Conference 2024 on System Modeling and Optimization, August 12–16, Universität Hamburg, August 12.

A.8.2 Scientific Talks (Invited)

1. M. Brokate, *Derivatives of the vector stop*, Seminar on Differential Equations and Integration Theory, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, Czech Republic, April 25.
2. ———, *Derivatives of rate-independent evolutions*, Seminar of the Mathematical Department, University of Trento, Prague, Italy, June 21.
3. ———, *Derivatives of rate-independent evolutions*, 31th IFIP TC7 Conference 2024 on System Modeling and Optimization, August 12–16, Universität Hamburg, August 15.
4. ———, *Differential sensitivity in rate independent problems*, Control of State-constrained Dynamical Systems, September 25–29, Università degli Studi di Padova, Italy, September 26.
5. A. Mielke, *On EVI flows for gradient systems on the (spherical) Hellinger–Kantorovich space*, Workshop "Applications of Optimal Transportation", February 5–9, Mathematisches Forschungsinstitut Oberwolfach, February 5.
6. ———, *Hellinger–Kantorovich (aka WFR) spaces and gradient flows*, Optimal Transport from Theory to Applications: Interfacing Dynamical Systems, Optimization, and Machine Learning, March 11–15, WAS Berlin, March 11.
7. ———, *Asymptotic self-similar behavior in reaction-diffusion systems*, Analysis Seminars, Heriot-Watt University, Mathematical and Computer Sciences, Edinburgh, UK, March 20.
8. ———, *Balanced-viscosity solutions for generalized gradient systems and a delamination problem*, Measures and Materials, March 25–28, University of Warwick, Coventry, UK, March 25.
9. ———, *Non-equilibrium steady states for port gradient systems*, 23rd Symposium on Trends in Applications of Mathematics to Mechanics (STAMM 2024), April 3–5, Julius-Maximilians-Universität Würzburg, April 4.
10. ———, *Non-equilibrium steady states for gradient systems with ports*, Analysis and Applied Mathematics Seminar, Università Commerciale Luigi Bocconi, Milano, Italy, May 15.

11. ———, *On the stability of NESS in gradient systems with ports*, Gradient Flows Face-to-Face 4, September 9–12, Technische Universität München, Raitenhaslach, September 10.

12. ———, *Balanced-viscosity solutions for generalized gradient systems in mechanics*, Frontiers of the Calculus of Variations, September 16–20, University of the Aegean, Karlovasi, Greece, September 17.

13. ———, *Asymptotic self-similar behavior in reaction-diffusion systems on* R^n , Applied Analysis Complex Systems & Dynamics Seminar, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, November 13.

14. ———, *On EVI flows for the spherical Hellinger distance and the spherical Hellinger–Kantorovich distance*, Optimal Transportation and Applications, December 2–6, Scuola Normale Superiore di Pisa, Centro di Ricerca Matematica Ennio De Giorgi, Italy, December 6.

15. J. Sprekels, *Optimality conditions in the sparse optimal control of viscous Cahn–Hilliard systems*, Seminari di Matematica Applicata, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, April 23.

16. V. Aksenov, *Learning distributions with regularized JKO scheme and low-rank tensor decompositions*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS153 “Low Rank Methods for Random Dynamical Systems and Sequential Data Assimilation”, February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 29.

17. ———, *Modelling distributions with Wasserstein proximal methods and low-rank tensor decompositions*, 94th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2024), Session 15.06 “UQ – Sampling and Rare Events Estimation”, March 18–22, Otto-von-Guericke-Universität Magdeburg, March 21.

18. A. Alphonse, *A quasi-variational contact problem arising in thermoelasticity*, Workshop “Interfaces, Free Boundaries and Geometric Partial Differential Equations”, February 12–16, Mathematisches Forschungsinstitut Oberwolfach, February 15.

19. ———, *Risk–averse optimal control of elliptic variational inequalities*, 94th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2024), Session 19.01 “Various Topics in Optimization of Differential Equations”, March 18–22, Otto-von-Guericke-Universität Magdeburg, March 19.

20. S. Amiranashvili, *Role of modulation instability in numerical analysis*, 6th International Conference on Application of Optics and Photonics, July 16–19, University of Aveiro, Portugal, July 16.

21. ———, *Role of modulation instability in numerical analysis*, XX Workshop on Instabilities and Nonequilibrium Structures, October 7–9, Institut de Physique de Nice, France, October 8.

22. U. Bandelow, *Hierarchies of integrable NLS-type equations and selected solutions*, Workshop “Nonlinear Optics: Physics, Analysis, and Numerics”, March 10–15, Mathematisches Forschungsinstitut Oberwolfach, March 11.

23. Ch. Bayer, *Efficient Markovian approximations of rough volatility models*, Finance and Stochastics Seminar, Imperial College London, Department of Mathematics, UK, January 30.

24. ———, *Primal and dual optimal stopping with signatures*, London Mathematical Finance Seminar, Imperial College London, Department of Mathematics, UK, February 1.

25. ———, *Signature methods in finance*, Bachelier Seminar, École Polytechnique (CMAP), Palaiseau, France, February 28.

26. ———, *Signatures for stochastic optimal control*, 2024 Conference on Modern Topics in Stochastic Analysis and Applications (in honour of Terry Lyons’ 70th birthday), April 22–26, Imperial College London, UK, April 22.

27. ———, *A reproducing kernel Hilbert space approach to singular local stochastic volatility McKean–Vlasov models*, Stochastic Numerics and Statistical Learning: Theory and Applications Workshop 2024, May 25 –

June 1, King Abdullah University of Science and Technology, Stochastic Numerics Research Group, Thuwal, Saudi Arabia, May 27.

28. ———, *Primal and dual optimal stopping with signatures*, International Conference on Scientific Computation and Differential Equations, July 15–19, National University of Singapore, Singapore, July 16.

29. ———, *A reproducing kernel Hilbert space approach to singular local stochastic volatility McKean–Vlasov models*, University of Oslo, Department of Mathematics, Norway, August 27.

30. ———, *A reproducing kernel Hilbert space approach to singular local stochastic volatility McKean—Vlasov models*, 24th MathFinance conference, September 19–20, Burg Reichenstein, Trechtingshausen, September 19.

31. ———, *An adaptive algorithm for rough differential equations*, Workshop "Directions in Rough Analysis", November 4–8, Mathematisches Forschungsinstitut Oberwolfach, November 8.

32. ———, *Markovian approximations to rough volatility models*, Research in Options: RiO 2024, December 4–8, School of Applied Mathematics of Fundação Getulio Vargas – FVG EMAp, Rio de Janeiro, Brazil, December 5.

33. CH. BAYER, P.K. FRIZ, *Path signatures and rough path analysis (minicourse)*, 2 talks, Spring School 2024, SFB 1481 "Sparsity and Singular Structures", May 13–17, Rheinisch-Westfälische Technische Hochschule Aachen.

34. O. BUTKOVSKY, *Weak and strong well-posedness and local times for SDEs driven by fractional Brownian motion with integrable drift (online talk)*, 18th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, University of Oxford, Mathematical Institute, UK, January 6.

35. ———, *Strong rate of convergence of the Euler scheme for SDEs with irregular drifts and approximation of additive time functionals*, Mathematics, Data Science, and Education, March 13–15, FernUniversität in Hagen, Lehrgebiet Angewandte Stochastik, March 14.

36. ———, *Optimal weak uniqueness for SDEs driven by fractional Brownian motion and for stochastic heat equation with distributional drift*, Stochastic Dynamics and Stochastic Equations, March 25–27, École Polytechnique Fédérale de Lausanne, Switzerland, March 25.

37. ———, *Weak uniqueness for singular stochastic equations (online talk)*, Klagenfurt-Berlin-Meeting on Multiple Perspectives in Optimization, June 6–7, Universität Klagenfurt, Institut für Mathematik, Austria, June 6.

38. ———, *Weak uniqueness for stochastic equations with singular drifts*, University of Leeds, School of Mathematics, UK, July 8.

39. ———, *Weak uniqueness for singular stochastic equations driven by fractional Brownian motion*, Stochastic Afternoon at Bielefeld, Universität Bielefeld, Fakultät für Mathematik, October 30.

40. ———, *Weak uniqueness for singular stochastic equations driven by fractional Brownian motion*, 20th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 9–11, University of Oxford, Mathematical Institute, UK, December 9.

41. P. DVURECHENSKY, *Decentralized local stochastic extra-gradient for variational inequalities*, French-German-Spanish Conference on Optimization 2024, June 20–21, University of Oviedo, Department of Mathematics, Spain, June 20.

42. ———, *Barrier algorithms for constrained non-convex optimization*, EUROPT 2024, 21st Conference on Advances in Continuous Optimization, June 26–28, Lund University, Department of Automatic Control, Sweden, June 26.

43. ———, *On some results on minimization involving self-concordant functions and barriers*, ALGOPT2024 Workshop on Algorithmic Optimization: Tools for AI and Data Science, August 27–30, Université Catholique de Louvain, School of Engineering, Louvain-la-Neuve, Belgium, August 27.

44. M. EIGEL, *An operator network architecture for functional SDE representations*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS6 “Operator Learning in Uncertainty Quantification”, February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 27.

45. ———, *Adaptive multilevel neural networks for parametric PDEs with error control*, 94th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2024), Session 15.05 “Methodologies for Forward UQ”, March 18–22, Otto-von-Guericke-Universität Magdeburg, March 20.

46. ———, *Generative modelling with tensor compressed HJB approximations*, 11th International Conference “Inverse Problems: Modeling and Simulation” (IPMS 2024), Minisymposium M7 “Bayesian, Variational, and Optimization Techniques for Inverse Problems in Stochastic PDEs”, May 26 – June 1, Paradise-Bay Hotel, Cirkewwa, Malta, May 31.

47. ———, *Sparse and compositional tensor formats for high-dimensional function approximation*, Workshop “High-dimensional Methods in Stochastic and Multiscale PDEs”, September 30 – October 2, Technische Universität Wien, Austria, October 2.

48. ———, *Topology optimisation under uncertainties, modern tensor compression & empirical SFEM*, UQ Colloquium, Bosch Research Campus, Renningen, October 11.

49. TH. EITER, *The effect of time-periodic boundary flux on the decay of viscous flow past a body*, Conference on Differential Equations and their Applications (EQUADIFF 24), Minisymposium 12 “Fluid-structure Interactions”, June 10–14, Karlstad University, Sweden, June 11.

50. ———, *Far-field behavior of oscillatory viscous flow past an obstacle*, Oberseminar Analysis und Angewandte Mathematik, Universität Kassel, July 15.

51. ———, *Far-field behavior of viscous flow past a body driven by time-periodic boundary flux*, Mathematical Analysis of Viscous Incompressible Fluid, December 2–4, Kyoto University, Japan, December 3.

52. ———, *Existence of time-periodic flow past a rotating body by uniform resolvent estimates*, Seminar on Mathematics of Fluids, Ochanomizu University, Tokyo, Japan, December 5.

53. ———, *On the spatially asymptotic structure of oscillating flow past a body*, Seminar “Funktionalanalysis und Stochastische Analysis”, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, December 19.

54. A. ERHARDT, *Mathematical modeling of cell-hydrogel interactions*, 23rd Symposium on Trends in Applications of Mathematics to Mechanics (STAMM 2024), April 3–5, Julius-Maximilians-Universität Würzburg, April 3.

55. P. FARRELL, *Charge transport in perovskites solar cells: Modeling, analysis and simulations*, Inria-ECDF Partnership Kick-Off Workshop, June 5–7, Inria and the Einstein Center for Digital Future, Berlin, June 7.

56. P.K. FRIZ, *Analyzing classes of SPDEs via RSDEs*, Stochastic Partial Differential Equations, February 12–16, Universtität Wien, Erwin Schrödinger International Institute for Mathematics and Physics (ESI), Austria, February 16.

57. ———, *Rough Paths with Jumps (Minicourse)*, Workshop “Recent Developments in Rough Paths”, March 3–8, BI Norwegian Business School, Oslo, Norway, March 4.

58. ———, *On the analysis of some SPDEs via RSDEs*, Stochastic Dynamics and Stochastic Equations, March 25–27, École Polytechnique Fédérale de Lausanne, Switzerland, March 25.

59. ———, *Rough analysis of rough volatility models*, 2024 Conference on Modern Topics in Stochastic Analysis and Applications (in honour of Terry Lyons’ 70th birthday), April 22–25, Imperial College London, UK, April 23.

60. ———, *Rough analysis of rough volatility models*, Stochastic Numerics and Statistical Learning: Theory and Applications Workshop 2024, May 24–27, King Abdullah University of Science and Technology, Stochastic Numerics Research Group, Thuwal, Saudi Arabia, May 26.

61. ———, *Some things related to signatures*, Conference "Signatures of Paths and Images", June 10–14, The Norwegian Academy of Science and Letters, Centre for Advanced Study (CAS), Oslo, Norway, June 11.

62. ———, *On signatures, log-signatures, moments and cumulants*, Advances in Probability Theory and Interacting Particle Systems: A Conference in Honor of S. R. Srinivasa Varadhan, August 26–28, Harvard University, Department of Mathematics, Cambridge, USA, August 26.

63. ———, *Brownian rough paths in irregular geometries*, Stochastics and Geometry Workshop, September 8–13, Banff International Research Station (BIRS), Canada, September 11.

64. ———, *Simulation and weak error bounds for local stochastic volatility models*, QuantMinds International 2024, November 18–21, London, UK, November 21.

65. M. Fröhlich, *Quantum noise characterization with a tensor network quantum jump method*, Workshop on Tensor Methods for Quantum Simulation 2024, June 3–7, Zuse-Institut Berlin (ZIB), June 7.

66. J. Fuhrmann, *Finite volume simulations of drift-diffusion problems in semiconductors and electrolytes*, Seminar, Laboratoire de Génie des Procédés et Matériaux, Chaire de Biotechnologie de CentraleSupélec, Pomacle, France, September 19.

67. ———, *Introduction to Julia and VoronoiFVM.jl*, Workshop "Finite Volumes and Optimal Transport", November 19–21, Université Paris-Saclay, Institut de Mathématiques d'Orsay, France, November 19.

68. J. Fuhrmann, J.P. Thiele, *Erfahrungen mit Softwarelizenzierung und Transfer am WIAS*, Leibniz Open Transfer Workshop, Leibniz Gemeinschaft, June 5.

69. C. Geiersbach, *Numerical solution of an optimal control problem with probabilistic or almost sure state constraints*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS63 "Efficient Solution Schemes for Optimization of Complex Systems Under Uncertainty", February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 28.

70. ———, *PDE-restringierte Optimierungsprobleme mit probabilistischen Zustandsschranken*, Women in Optimization 2024, April 10–12, Friedrich-Alexander-Universität Erlangen (FAU), April 10.

71. ———, *Stochastic approximation for PDE-constrained optimization under uncertainty*, Summer School on Numerical Methods for Random Differential Models, June 11–14, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland, June 12.

72. ———, *Optimality conditions with probabilistic state constraints*, ISMP 2024 – 25th International Symposium on Mathematical Programming, Session TB111 "PDE–constrained Optimization under Uncertainty", July 21–26, Montreal, Canada, July 23.

73. ———, *Basics of random algorithms*, TRR 154 Summer School on Optimization, Uncertainty and AI, August 7–8, Universität Hamburg, August 8.

74. ———, *Probabilistic state constraints for optimal control problems under uncertainty*, VARANA 2024 (Variational Analysis and Applications): 77th Course of the International School of Mathematics "Guido Stampacchia", September 1–7, Erice, Italy, September 2.

75. ———, *Optimization with probabilistic state constraints*, Workshop "Control and Optimization in the Age of Data", September 18–20, Universität Bayreuth, September 19.

76. A. Glitzky, *Analysis of a drift-diffusion model for perovskite solar cells*, 94th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2024), Session 14.07 "Various Topics in Applied Analysis", March 18–22, Otto-von-Guericke-Universität Magdeburg, March 21.

77. G. Heinze, *Discrete-to-continuum limit for reaction-diffusion systems via variational convergence of gradient systems*, Oberseminar Angewandte Analysis, Universität Ulm, Institut für Angewandte Analysis, November 25.

78. H. Heitsch, *Probabilistic maximization of time-dependent capacities in a gas network*, Conference "Mathematics of Gas Transport and Energy" (MOG 2024), October 10–11, Regensburg, October 11.

79. R. Henrion, *On a chance-constrained optimal control problem with turnpike property*, 3rd International Conference on Variational Analysis and Optimization, January 16–19, Universidad de Chile, Santiago, Chile, January 16.

80. ———, *Chance constraints in energy management and aspects of nonsmoothness*, Workshop "Variational Analysis and Applications for Modeling of Energy Exchange" (VAME 2024), May 13–14, Universität Trier, May 13.

81. ———, *An introduction to chance-constrained programming*, TRR 154 Summer School on Optimization, Uncertainty, and AI, Universität Hamburg, August 9.

82. ———, *An enumerative formula for the spherical cap discrepancy*, PGMO DAYS 2024, Session 11E "Stochastic and Robust Optimization", November 19–20, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF Lab Paris-Saclay, Palaiseau, France, November 20.

83. M. Hintermüller, *Risk-averse optimal control of random elliptic VIs*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS43 "Efficient Solution Schemes for Optimization of Complex Systems Under Uncertainty", February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 27.

84. ———, *PDE-constrained optimization with learning-informed structures*, Recent Advances in Scientific Computing and Inverse Problems, March 11–12, The Hong Kong Polytechnic University, China, March 11.

85. ———, *Quasi-variational inequalities: Semismooth Newton methods, optimal control, and uncertainties*, Workshop on One World Optimization Seminar in Vienna, June 3–7, Erwin Schrödinger International Institute for Mathematics and Physics and University of Vienna, Austria, June 4.

86. ———, *QVIs: Semismooth Newton, optimal control, and uncertainties*, RICAM Colloquium, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, June 27.

87. ———, *A hybrid physics-informed neural network based multiscale solver as a PDE constrained optimization problem*, ISMP 2024 – 25th International Symposium on Mathematical Programming, Session TA90 "Nonsmooth PDE-constrained Optimization", July 21–26, Montreal, Canada, July 23.

88. ———, *A neural network approach to learning solutions of a class of elliptic variational inequalities*, Nonsmooth Optimization and Variational Analysis, December 2–4, The Hong Kong Polytechnic University, China, December 4.

89. ———, *PINNs in multiscale materials as PDE-constrained optimization problem*, Forum for Mathematical Optimization with PDEs, Central South University, Changsha, China, December 9.

90. ———, *A neural network approach to learning solutions of a class of elliptic variational inequalities*, colloquium talk, Hunan Normal University, Department of Mathematics, Changsha, China, December 10.

91. ———, *QVIs: Semismooth Newton, optimal control and uncertainties*, colloquium talk, Hunan Normal University, Department of Mathematics, Changsha, China, December 10.

92. ———, *A neural network approach to learning solutions of a class of elliptic variational inequalities*, Chinese University of Hong Kong, Department of Mathematics, China, December 12.

93. D. Hömberg, *Two-scale topology optimization – Modeling, analysis and numerical results*, XIV International Conference of the Georgian Mathematical Union, September 2–7, Batumi Shota Rustaveli State University, Georgia, September 3.

94. K. Hopf, *On the equilibrium solutions in a model for electro-energy-reaction-diffusion systems*, Modelling, PDE Analysis and Computational Mathematics in Materials Science, September 22–27, Prague, Czech Republic, September 27.

95. ———, *On rank-deficient cross-diffusion and the interface dynamics in viscoelastic phase separation*, Applied Analysis, Complex Systems & Dynamics Seminar, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, November 13.
96. J. Hörmann, *Geometrische Dichten für nicht-isotrope Boolesche Modelle*, Hochschule Pforzheim, Fakultät für Technik, April 17.
97. T. Iyer, *Persistent hubs in generalised preferential attachment trees*, Seminar Series in Mathematical Statistics, Stockholm University, Department of Mathematics, Stockholm, Sweden, May 22.
98. ———, *Persistent hubs in generalised preferential attachment trees*, Seminar Series in Probability and Combinatorics, Uppsala University, Department of Mathematics, Uppsala, Sweden, May 23.
99. ———, *Persistent hubs in preferential attachment trees*, Oberseminar AG Stochastik, Technische Universität Darmstadt, Fachbereich Mathematik, June 20.
100. ———, *Fixiation of leadership in growth processes*, Probability Seminar, University of Melbourne, School of Mathematics and Statistics, Melbourne, Australia, October 1.
101. ———, *Persistent hubs in generalised preferential attachment trees*, Monash Probability and Statistics Seminar, Monash University, School of Mathematics, Melbourne, Australia, November 3.
102. B. Jahnel, *Time-periodic behavior in one- and two-dimensional interacting particle systems (online talk)*, International Scientific Conference on Gibbs Measures and the Theory of Dynamical Systems (online event), May 20–21, Ministry of Higher Education, Science and Innovations of the Republic of Uzbekistan, Romanovskiy Institute of Mathematics and University of Exact and Social Sciences, Tashkent, Uzbekistan, May 20.
103. ———, *Poisson approximation of fixed-degree nodes in weighted random connection models*, Bernoulli-IMS 11th World Congress in Probability and Statistics, Session OCPS 07 "Spatial Random Graphs", August 12–16, Ruhr-Universität Bochum, August 16.
104. ———, *Cluster sizes in subcritical soft Boolean models*, Long-range Phenomena in Percolation, September 23–27, Universität zu Köln, Mathematisches Institut, September 26.
105. ———, *Cluster sizes in subcritical soft Boolean models*, GrHyDy2024: Random Spatial Models, October 23–25, Université de Lille, Institut Mines-Télécom, Lille, France, October 24.
106. ———, *Gibbs point processes in random environment*, Random Geometric Systems, Third Annual Conference of SPP 2265, October 28–30, Harnack-Haus, Tagungsstätte der Max-Planck-Gesellschaft, October 29.
107. ———, *Subcritical annulus crossing in spatial random graphs*, Seminar, Institut für Mathematische Stochastik, Georg-August-Universität Göttingen, December 4.
108. V. John, *On using machine learning techniques for the numerical solution of convection-diffusion problems*, Seminar of Prof. Sashikumaar Ganesan, Indian Institute of Science Bangalore, Department of Computational and Data Sciences, Bangalore, India, February 13.
109. ———, *On two modeling issues in aortic blood flow simulations*, Seminar of Dr. Nagaiah Chamakuri, Scientific Computing Group (SCG), School of Mathematics, Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala, India, February 20.
110. ———, *Finite element methods respecting the discrete maximum principle for convection-diffusion equations*, International Conference on Latest Advances in Computational and Applied Mathematics (LACAM) 2024, February 21–24, Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala, India, February 21.
111. ———, *On using machine learning techniques for the numerical solution of convection-diffusion problems*, ALGORITMY 2024, Central-European Conference on Scientific Computing, Minisymposium "Numerical Methods for Convection-dominated Problems", March 16–20, Department of Mathematics and Descriptive Geometry, Slovak University of Technology in Bratislava, Podbanske, Slovakia, March 19.

112. ———, *Finite element methods respecting the discrete maximum principle for convection-diffusion equations*, Trends in Scientific Computing – 30 Jahre Wissenschaftliches Rechnen in Dortmund, May 21–22, Technische Universität Dortmund, Fakultät für Mathematik, LSIII, May 21.

113. ———, *Finite element methods respecting the discrete maximum principle for convection-diffusion equations*, Mathematical Fluid Mechanics In 2024, August 19–23, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, August 21.

114. M. Kantner, *Conveyor-mode electron shuttling in a Si/SiGe quantum bus: Modeling, simulation, optimization*, Focus Workshop on Theory of Spin-Qubit Shuttling, Rheinisch-Westfälische Technische Hochschule Aachen, September 18.

115. J. Kern, *Modelling populations with fluctuating size*, Mathematical Models in Ecology and Evolution (MMEE), July 15–18, Universität Wien, Fakultät für Mathematik, Vienna, Austria, July 15.

116. W. König, *Off-diagonal long-range order for the free Bose gas via the Feynman–Kac formula (online talk)*, Forschungsseminar Analysis, FernUniversität in Hagen, Fakultät für Mathematik und Informatik, April 24.

117. J. Köppl, *The long-time behaviour of interacting particle systems: A Lyapunov functional approach (online talk)*, Probability Seminar, University of California Los Angeles (UCLA), Department of Mathematics, Los Angeles, USA, February 15.

118. ———, *Dynamical Gibbs variational principles and applications to attractor properties (online talk)*, Postgraduate Online Probability Seminar (POPS), February 28.

119. ———, *Dynamical Gibbs variational principles and applications to attractor properties (online talk)*, Oberseminar Stochastik, Universität Paderborn, Institut für Mathematik, May 15.

120. D. Korolev, *A hybrid physics-informed neural network based multiscale solver as a partial differential equation constrained optimization problem*, Leibniz MMS Days 2024, Parallel Session "Computational Material Science", April 10–12, Leibniz Network "Mathematical Modeling and Simulation," Leibniz-Institut für Verbundwerkstoffe GmbH (IVW), Kaiserslautern, April 11.

121. A. Kroshnin, *Tropical optimal transport, Maslov dequantization, and large deviation principle*, Università degli Studi di Pisa, Dipartimento di Matematica, Italy, November 29.

122. M. Landstorfer, *Mathematical modeling of lithium-ion intercalation cells based on non-equilibrium thermodynamics*, Seminar, Università degli Studi di Brescia, Dipartimento di Ingegneria Meccanica e Industriale, Italy, September 11.

123. H. Langhammer, *Large deviations for a spatial particle progress with coagulation*, Seminar, Dipartimento di Matematica, Università di Roma "La Sapienza", Italy, September 25.

124. R. Lasarzik, *Evolutionary variational inequalities as generalized solution concepts*, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, November 27.

125. L. Lüchtrath, *The random cluster graph*, Workshop Frauenchiemsee 2024, January 14–17, Universität Augsburg, Mathematisch-Naturwissenschaftlich-Technische Fakultät, January 16.

126. ———, *A random cluster graph*, Oberseminar Stochastik, Universität zu Köln, Mathematisches Institut, October 23.

127. ———, *Cluster sizes in subcritical soft Boolean models*, Geneva Mathematical Physics Seminar, Université de Genève, Section de Mathématiques, Switzerland, December 2.

128. E. Magnanini, *Spatial coagulation and gelation*, Random Geometric Systems, Third Annual Conference of SPP 2265, October 28–30, Harnack-Haus, Tagungsstätte der Max-Planck-Gesellschaft, October 29.

129. A. Maltsi, *The mathematics behind imaging*, WINS School 2024: Cross Sections and Interfaces in Science and its Environment, May 31 – June 3, Humboldt-Universität zu Berlin, Blossin, May 31.

130. CH. MIRANDA, *Solving stochastic differential equations using deep operator networks*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS25 “Nonlinear Approximation of High-Dimensional Functions: Compositional, Low-Rank and Sparse Structures”, February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 27.

131. ———, *Functional SDE approximation inspired by a deep operator network architecture*, 94th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2024), Session 25.02 “Various Topics in Computational and Mathematical Methods in Datascience”, March 18–22, Otto-von-Guericke-Universität Magdeburg, March 19.

132. I. PAPADOPOULOS, *A frame approach for equations involving the fractional Laplacian*, Singular and Oscillatory Integration, June 24–26, University College London, Department of Mathematics, UK, June 25.

133. ———, *A semismooth Newton method for obstacle-type quasivariational inequalities*, Firedrake 2024 (8th Firedrake user and developer workshop), September 16–18, University of Oxford, UK, September 18.

134. L. PELIZZARI, *Primal and dual optimal stopping with signatures*, 18th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, January 4–6, University of Oxford, Mathematical Institute, UK, January 5.

135. ———, *Rough PDEs for local stochastic volatility*, Recent Developments in Rough Paths, March 3–8, BI Norwegian Business School, Nydalen, Norway, March 4.

136. ———, *Rough PDE for LSVM*, Klagenfurt-Berlin-Meeting on Multiple Perspectives in Optimization, June 6–7, Universität Klagenfurt, Institut für Mathematik, Austria, June 6.

137. D. PESCHKA, *Wetting of soft deformable substrate – Phase fields for fluid structure interaction with moving contact lines*, Colloquium on Interfaces, Complex Structures, and Singular Limits in Continuum Mechanics – Analysis and Numerics, Universität Regensburg, Fakultät für Mathematik, May 24.

138. ———, *Dissipative processes in thin film flows*, Liquid Thin Films, August 26–30, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, August 27.

139. L. PLATO, *Existence and weak-strong uniqueness of suitable weak solutions to an anisotropic electrokinetic flow model*, Universität Kassel, Institut für Mathematik, July 18.

140. M. RADZIUNAS, *Mode analysis in dynamical semiconductor laser models*, 25th Congress of the Australian Institute of Physics (AIP), Conference on Microelectronic Materials and Devices (COMMAD) 2024, December 2–6, Melbourne, Australia, December 2.

141. ———, *Modeling, simulation, and analysis of all-semiconductor photonic crystal surface-emitting lasers*, International Symposium on Semiconductor Optoelectronics and Nanotechnology (ISSON), December 8–11, Canberra, Australia, December 10.

142. A. RATHSFELD, *Analysis of scattering matrix algorithm for diffraction by periodic structures (online talk)*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 13.

143. J. REHBERG, *Estimates for operator functions*, Oberseminar Analysis und Theoretische Physik, Leibniz Universität Hannover, Institut für Analysis, October 15.

144. ———, *Parabolic equations with measure-valued right hand sides*, Forschungsseminar Analysis, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, October 23.

145. J.G.M. SCHOENMAKERS, *Optimal stopping with randomly arriving opportunities to stop*, DYNSTOCH 2024, May 22–24, Christian-Albrechts-Universität zu Kiel (CAU), May 22.

146. J. SCHÜTTE, *Bayes for parametric PDEs with normalizing flows*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS37 “Forward and Inverse Uncertainty Quantification for Nonlinear Problems”, February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 27.

147. ———, *Approximating Langevin Monte Carlo with ResNet-like neural network architectures*, 94th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2024), Session 25.02 “Various Topics in Computational and Mathematical Methods in Datascience”, March 18–22, Otto-von-Guericke-Universität Magdeburg, March 20.

148. D. Sommer, *Approximating Langevin Monte Carlo with ResNet-like neural network architectures*, SIAM Conference on Uncertainty Quantification (UQ24), Minisymposium MS25 “Nonlinear Approximation of High-Dimensional Functions: Compositional, Low-Rank and Sparse Structures”, February 27 – March 1, Savoia Excelsior Palace Trieste and Stazione Marittima, Italy, February 27.

149. ———, *Approximating Langevin Monte Carlo with ResNet-like neural network architecture (online talk)*, University of Tokyo, Graduate School of Mathematical Sciences, Japan, March 13.

150. V. Spokoiny, *Statistical inference for nonlinear inverse problems*, Statistical Aspects of Non-Linear Inverse Problems, September 17–19, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK.

151. ———, *Inference for nonlinear inverse problems*, The Mathematics of Data: Workshop on Optimal Transport and PDEs, January 21–26, National University of Singapore, Institute for Mathematical Sciences, Singapore, January 23.

152. ———, *Gaussian variational inference in high dimension*, Mohamed Bin Zayed University of Artificial Intelligence (MBZUAI), Department of Machine Learning, Abu Dhabi, United Arab Emirates, March 12.

153. ———, *Inference for nonlinear problems*, University of Electronic Science and Technology of China (UEST), School of Mathematical Sciences, Chengdu, China, May 14.

154. ———, *Non-asymptotic and non-minimax estimation of smooth functionals*, Workshop “Statistics and Learning Theory in the Era of Artificial Intelligence”, June 23–28, Mathematisches Forschungsinstitut Oberwolfach (MFO), June 28.

155. ———, *Uncertainty quantification under self-concordance*, ALGOPT2024 Workshop on Algorithmic Optimization: Tools for AI and Data Science, August 27–30, Université Catholique de Louvain, School of Engineering, Louvain-la-Neuve, Belgium, August 29.

156. ———, *Inference for nonlinear inverse problems*, New Challenges in High-dimensional Statistics, December 16–20, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, December 16.

157. A. Suvorikova, *Bernstein type inequality for unbounded martingales*, Workshop “Statistics and Learning Theory in the Era of Artificial Intelligence”, June 23–28, Mathematisches Forschungsinstitut Oberwolfach (MFO), June 28.

158. N. Tapia, *Stabilitiy of deep neural networks via discrete rough paths*, Mathematics, Data Science, and Education, March 13–15, FernUniversität in Hagen, Lehrgebiet Angewandte Stochastik, March 13.

159. ———, *Stability of deep neural networks via discrete rough paths*, Mathematics of Data Streams: Signatures, Neural Differential Equations, and Diffusion Models, April 10–13, Universität Greifswald, Institut für Mathematik, April 12.

160. ———, *Branched Itô formula and natural Itô-Stratonovich isomorphism*, Klagenfurt-Berlin-Meeting on Multiple Perspectives in Optimization, June 6–8, Universität Klagenfurt, Institut für Mathematik, Austria, June 6.

161. ———, *Unified signature cumulants and generalized Magnus expansions*, 70 Years of Magnus Series, July 1–5, Universitat Jaume I, Castellón, Spain, July 2.

162. ———, *Branched Itô formula*, Workshop “Directions in Rough Analysis”, November 4–8, Mathematisches Forschungsinstitut Oberwolfach, November 6.

163. ———, *A multiplicative surface signature through its Magnus expansion*, Multi-Parameter Signatures, December 5–6, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, December 5.

164. ———, *Branched Itô formula and intrinsic RDEs*, 20th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 9–11, University of Oxford, Mathematical Institute, UK, December 10.

165. J.P. Thiele, *RSE and RDM: Code and perish?! How about publishing your software (and data)?*, Oberseminar Numerik und Optimierung, Institut für Angewandte Mathematik, Leibniz Universität Hannover, May 2.

166. ———, *The Research Software Engineer (RSE): Who is that? And what skills do they have to help you?*, European Trilinos & Kokkos User Group Meeting 2024 (EuroTUG 2024), June 24–26, Helmut-Schmidt-Universität, Universität der Bundeswehr Hamburg, June 24.

167. ———, *RSE training and professional development BoF*, Research Software Engineering Conference, RSECon24, September 3–5, Society of Research Software Engineering (SocRSE), a charitable incorporated organisation based in the UK, Newcastle, UK, September 5.

168. M. Thomas, *Analysis of a model for visco-elastoplastic two-phase flows in geodynamics*, Seminar on Nonlinear Partial Differential Equations, Texas A&M University, Department of Mathematics, College Station, USA, March 19.

169. ———, *Analysis of a model for visco-elastoplastic two-phase flows in geodynamics*, 23rd Symposium on Trends in Applications of Mathematics to Mechanics (STAMM 2024), April 3–5, Julius-Maximilians-Universität Würzburg, April 5.

170. ———, *Analysis of a model for visco-elastoplastic two-phase flows in geodynamics*, 9th European Congress of Mathematics (9ECM), Minisymposium 27 “New Trends in Calculus of Variations”, July 15–19, Universidad de Sevilla, Spain, July 16.

171. S.M. Toukam Tchoumegne, *Stochastic maximum principle for McKean–Vlasov SDEs with rough drift coefficients*, 20th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, December 9–11, University of Oxford, Mathematical Institute, UK, December 9.

172. A.G. Vladimirov, *Dynamics of neutral delay differential equation model of a dispersive Kerr cavity*, Dynamics Day in Shangai, China, September 8.

173. ———, *Short pulse interaction in delay differential equation models of mode-locked lasers*, China-Russia Dynamics Days in Jinhua, September 10–15, China, September 11.

174. ———, *Modeling dispersive nonlinear optical cavities using delay differential equations*, XX Workshop on Instabilities and Nonequilibrium Structures, October 7–9, Institut de Physique de Nice, France, October 8.

175. B. Wagner, *Dynamics of cellular patterns on hydrogel sheets*, University of Oxford, Mathematical Institute, UK, November 22.

176. C. Zarco Romero, *Large deviations for inhomogeneous random graphs*, Berlin-Oxford Summer School in Mathematics of Random Systems 2024, September 9–13, Oxford University, Mathematical Institute, Oxford, UK, September 10.

177. A. Zass, *A model for colloids: Diffusion dynamics for two-type hard spheres and the associated depletion effect*, Colloquium, Institut für Mathematische Stochastik, Technische Universität Braunschweig, January 17.

178. ———, *Discrete and continuous Widom–Rowlinson models in random environment*, A Lifelong Journey in Stochastic Analysis: From Branching Processes to Statistical Mechanics, May 27–28, Institut Henri Poincaré, Paris, May 28.

179. ———, *Discrete and continuous Widom–Rowlinson models in random environment*, 52th Probability Summer School Saint-Flour, July 1–13, Université Clermont Auvergne, Saint-Flour, France, July 10.

180. ———, *A model for colloids: Diffusion dynamics for two-type hard spheres and the associated depletion effect*, Colloquium in Probability, Technische Universität München, Department of Mathematics, November 11.

181. J.-J. Zhu, *Approximation and kernelization of gradient flow geometry: Fisher–Rao and Wasserstein*, The Mathematics of Data: Workshop on Optimal Transport and PDEs, January 17–23, National University of Singapore, Institute for Mathematical Sciences, Singapore, January 22.

182. ———, *Kernelization, approximation, and entropy dissipation of gradient flows*, 3 talks, RIKEN Center for Advanced Intelligence Project (AIP), Saitama, Japan, January 24–26.

183. ———, *Gradient flows and kernelization in the Hellinger–Kantorovich (a.k.a. Wasserstein–Fisher–Rao) space*, EUROPT 2024, 21st Conference on Advances in Continuous Optimization, June 26–28, Lund University, Department of Automatic Control, Sweden, June 28.

184. ———, *Transport and flow: The modern mathematics of distributional learning and optimization*, Universität des Saarlandes, Saarland Informatics Campus, Saarbrücken, July 5.

185. ———, *Flow and transport: Modern mathematical foundation for statistical machine learning*, University of St. Gallen, Department of Economics, Switzerland, October 17.

186. ———, *Kernel approximation of Wasserstein–Fisher–Rao gradient flows*, DFG SPP 2298 Annual Meeting, November 10–12, Ludwig-Maximilians-Universität München, Department Mathematik, Tutzingen, November 11.

187. ———, *Kernel approximation of Wasserstein and Fisher–Rao gradient flows*, Probability and Stochastic Analysis Seminar, École Polytechnique Fédérale de Lausanne, Switzerland, November 27.

188. ———, *From distributional ambiguity to gradient flows: Wasserstein, Fisher–Rao, and kernel approximation*, Seminar, College of Management of Technology, École Polytechnique Fédérale de Lausanne, Switzerland, November 28.

189. ———, *Kernel approximation of Wasserstein and Fisher–Rao gradient flows*, The Thirty-Eighth Annual Conference on Neural Information Processing Systems (NeurIPS 2024), December 10–15, Neural Information Processing Systems Foundation, Vancouver, Canada, December 16.

A.8.3 Talks for a More General Public

1. Th. Eiter, *Unendlichkeiten vergleichen*, Tag der Mathematik, Universität Kassel, February 16.

2. ———, *Unendlichkeit im Großen und im Kleinen*, 27. Berliner Tag der Mathematik (27th Berlin Day of Mathematics), Technische Universität Berlin, May 4.

3. C. Geiersbach, *Optimierung und Anwendungen*, Girls' Day 2024, WIAS Berlin, April 25.

4. A. Glitzky, *Elektrothermische Beschreibung von organischen Halbleiterbauelementen*, Girls' Day 2024, WIAS Berlin, April 25.

5. M. Heida, *Als Voronoi den Raum zerteilte*, 27. Berliner Tag der Mathematik (27th Berlin Day of Mathematics), Technische Universität Berlin, May 4.

6. R. Henrion, *Optimisation de l' incertain*, MATh.en.JEANS – Von der Forschung in die Schule und zurück!, WIAS Berlin, February 21.

7. J. Hörrmann, *Punktprozesse und Voronoi-Mosaike oder die beste Lage für eine neue Eisdiele*, WIAS Berlin, June 20.

8. B. Jahnel, *Stochastische Methoden für Kommunikationsnetzwerke*, 27. Berliner Tag der Mathematik (27th Berlin Day of Mathematics), Technische Universität Berlin, May 4.

9. J. Kern, *Warum der Zufall nicht zufällig ist*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2024, WIAS at Leibniz Association Headquarters, Berlin, June 22.

10. A. Pešić, *Studying in Berlin*, Visit of the specialized Computer Science High School from Serbia to ZIB, Zuse-Institut Berlin, November 21.

11. H. Shafigh, *Überlebenswahrscheinlichkeit eines Hasen unter Wölfen*, WIAS Berlin, June 20.

A.8.4 Posters

1. V. Aksenov, *Learning distributions with regularized JKO scheme and low-rank tensor decompositions*, Workshop on Optimal Transport from Theory to Applications, Berlin, March 11–15.

2. Ch. Bayer, W. Kenmoe Nzali, D. Kreher, M. Landstorfer, *Volatile electricity markets and battery storage: A model-based approach for optimal control*, MATH+ Day, Urania Berlin, October 18.

3. D. Dolinina, *Desynchronization of temporal solitons in Kerr cavities with pulsed injection*, XLIV Dynamics Days Europe, Bremen, July 29 – August 2.

4. T. Dörffel, M. Landstorfer, M. Liero, *Modeling battery electrodes with mechanical interactions and multiple phase transistions upon ion insertion*, MATH+ Day, Urania Berlin, October 18.

5. P. Dvurechensky, *Barrier algorithms for constrained non-convex optimization*, The International Conference on Machine Learning (ICML), Vienna, Austria, July 21–26.

6. ———, *High-probability convergence for composite and distributed stochastic minimization and variational inequalities with heavy-tailed noise*, The International Conference on Machine Learning (ICML), Vienna, Austria, July 21–26.

7. N. Ciroth, A. Sala, L. Ermoneit, Th. Koprucki, M. Kantner, L. Schreiber, *Numerical simulation of coherent spin-shuttling in silicon devices across dilute charge defects*, Silicon Quantum Electronics Workshop 2024, Davos, Switzerland, September 4–6.

8. L. Ermoneit, B. Schmidt, J. Fuhrmann, A. Sala, N. Ciroth, L. Schreiber, T. Breiten, Th. Koprucki, M. Kantner, *Optimal control of a Si/SiGe quantum bus for scalable quantum computing architectures*, Quantum Optimal Control: From Mathematical Foundations to Quantum Technologies, MATH+, Berlin, May 21.

9. L. Ermoneit, B. Schmidt, Th. Koprucki, T. Breiten, M. Kantner, *Coherent transport of semiconductor spin-qubits: Modeling, simulation and optimal control*, MATH+ Day 2024, Urania Berlin, October 2.

10. L. Ermoneit, B. Schmidt, A. Sala, N. Ciroth, L. Schreiber, T. Breiten, Th. Koprucki, M. Kantner, *Simulation and optimal control of single-electron shuttling in a SiGe quantum bus*, Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024), Berlin, September 10–13.

11. J. Fuhrmann, *Development of numerical methods and tools for drift-diffusion simulations*, Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024), Berlin, September 10–13.

12. J. Fuhrmann, St. Maass, St. Ringe, *Monolithic coupling of a CatMAP based microkinetic model for heterogeneous electrocatalysis and ion transport with finite ion sizes*, ModVal 2024 – 20th Symposium on Modeling and Validation of Electrochemical Energy Technologies, Villigen, Switzerland, March 13–14.

13. ———, *Monolithic coupling of a CatMAP based microkinetic model for heterogeneous electrocatalysis and ion transport with finite ion sizes*, Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024), Berlin, September 10–13.

14. 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, Urania Berlin, October 18.

15. A. Glitzky, *Electrothermal models for organic semiconductor devices*, Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024), Berlin, September 10–13.

16. Y. Hadjimichael, *Strain distribution in zincblende and wurtzite GaAs nanowires bent by a one-sided (In,Al)As shell*, Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024), Berlin, September 10–13.
17. G. Heinze, *Graph-based nonlocal gradient systems and their local limits*, Aggregation-Diffusion Equations & Collective Behavior: Analysis, Numerics and Applications, Marseille, France, April 8–12.
18. R. Henrion, D. Hömberg, N. Kliche, *Optimal operation of mini-grids including battery management under uncertainty*, 5th Workshop "Women in Optimization 2024", Friedrich-Alexander-Universität Erlangen, April 10–12.
19. ———, *Optimal operation of mini-grids including battery management under uncertainty*, Summer School "Data-driven Dynamical Systems", Universität Bremen, July 24–26.
20. M. Kantner, L. Ermoneit, B. Schmidt, A. Sala, N. Ciroth, L. Schreiber, Th. Koprucki, *Optimal control of conveyor-mode electron shuttling in a Si/SiGe quantum bus in the presence of charged defects*, Silicon Quantum Electronics Workshop 2024, Davos, Switzerland, September 4–6.
21. Ch. Keller, *A drift-diffusion model to describe ion channel dynamics*, Applied Mathematics and Simulation for Semiconductor Devices (AMaSiS 2024), Berlin, September 10–13.
22. W. Kenmoe Nzali, *Volatile electricity market and battery storage*, 7th Berlin Workshop on Mathematical Finance for Young Researchers, September 2–6.
23. O. Klein, *On a model for a magneto mechanical device: Forward and inverse uncertainty quantification*, 2nd Workshop of the MATH+ Thematic Einstein Semester "Mathematics of Small Data Analysis", Berlin, January 17–19.
24. ———, *A model for a magneto mechanical device: Forward and inverse uncertainty quantization*, Leibniz MMS Days 2024, Kaiserslautern, April 10–12.
25. M. Landstorfer, T. Dörffel, *Mathematical modeling of intercalation batteries with non-equilibrium thermodynamics and homogenization theory*, Oxford Battery Modelling Symposium 2024, UK, April 15–17.
26. R. Lasarzik, *Minimizing movements for damped Hamiltonian systems*, Workshop on Optimal Transport from Theory to Applications, Berlin, March 11–15.
27. Ch. Merdon, *Mass-conservative reduced basis approach for heterogeneous catalysis*, Leibniz MMS Days 2024, Kaiserslautern, April 10–12.
28. L. Mertenskötter, M. Kantner, *Narrow-linewidth lasers*, CLEO Conference, North Carolina, USA, May 5–10.
29. M. O'Donovan, *Theoretical investigations on different scales towards novel III-N materials and devices*, Roundtable discussion of the SPP 2477 "Nitrides4Future", Magdeburg, September 24–25.
30. L. Pelizzari, *Non-Markovian optimal stopping with signatures*, Stochastic Numerics and Statistical Learning: Theory and Applications Workshop 2024, Thuwal, Saudi Arabia, May 19–30.
31. F. Romor, *Registration-based data assimilation of aortic blood flow*, Leibniz MMS Days 2024, Kaiserslautern, April 10–12.
32. D. Runge, *Mass-conservative reduced basis approach for heterogeneous catalysis*, Leibniz MMS Days 2024, Kaiserslautern, April 10–12.
33. F. Sauer, *Equilibria for distributed multi-modal energy systems under uncertainty*, MATH+ Day, Urania Berlin, October 18.
34. J. Schütte, M. Eigel, *Adaptive multilevel neural networks for parametric PDEs with error estimation*, ICLR Workshop on AI4DifferentialEquations In Science, Vienna, Austria, May 11.
35. A. Thayil, L. Ermoneit, M. Kantner, *Towards optimization of valley splitting in Si/SiGe quantum wells*, Silicon Quantum Electronics Workshop 2024, Davos, Switzerland, September 4–6.

36. W. van Oosterhout, *Finite-strain poro-visco-elasticity with degenerate mobility*, Spring School 2024 "Mathematical Advances for Complex Materials with Microstructures", Universität Würzburg, April 8–12.
37. Q. Wang, *Robust multilevel training of artificial neural networks*, MATH+ Day, Urania Berlin, October 18.
38. C. Zarco Romero, *Statistical mechanics for spatial dense random graphs*, DFG SPP 2265 Summer School on Particle Systems in Random Environments, Frankfurt am Main, August 26–30.
39. J.-J. Zhu, P. Dvurechensky, *Analysis of kernel mirror prox for measure optimization*, 27th Conference on Artificial Intelligence and Statistics (AISTATS), Valencia, Spain, May 2–4.

A.9 Visits to other Institutions[6]

1. A. Mielke, Heriot-Watt University, Mathematical and Computer Sciences, Edinburgh, UK, March 17–24.
2. ———, Università Commerciale Luigi Bocconi, Department of Decision Sciences, Milano, Italy, May 13–17.
3. J. Sprekels, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, April 20–26.
4. Ch. Bayer, Imperial College London, Department of Mathematics, UK, January 22 – February 8.
5. ———, École Polytechnique (CMAP), Palaiseau, France, February 27 – March 8.
6. ———, University of Oslo, Department of Mathematics, Norway, August 26–29.
7. O. Butkovsky, University of Leeds, School of Mathmatics, UK, July 5–9.
8. ———, Imperial College London, Department of Mathematics, UK, July 26–30.
9. A. Caiazzo, Politecnico di Torino, Department of Mathematical Sciences, Italy, August 5–9.
10. C. Cárcamo, Pontificia Universidad Católica de Valparaíso, School of Civil Engineering, Chile, January 22–26.
11. Th. Eiter, Czech Academy of Sciences, Institute of Mathematics, Prague, Czech Republic, May 28 – June 1.
12. A. Erhardt, Universität Wien, Institut für Mathematik, Austria, February 12–16.
13. P.K. Friz, Technische Universität Wien, Finanz- und Versicherungsmathematik, Austria, August 19–22.
14. J. Fuhrmann, CentraleSupélec, Chaire de Biotechnologie, Pomacle, France, April 28 – May 11.
15. ———, September 16 – October 4.
16. G. Heinze, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, August 18–22.
17. M. Hintermüller, Central South University, Department of Mathematics, Changsha, and Chinese University of Hong Kong, Department of Mathematics, China, December 7–15.
18. D. Hömberg, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, January 15–26.
19. ———, April 8–12.
20. ———, September 30 – October 6.
21. K. Hopf, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, November 12–15.
22. T. Iyer, Uppsala University, Department of Mathematics, Uppsala, Sweden, May 21–24.
23. ———, University of Melbourne, School of Mathematics and Statistics, Melbourne, Australia, September 30 – October 4.
24. V. John, Scientific Computing Group (SCG), School of Mathematics, Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala, India, February 12–20.
25. ———, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, March 11–14.
26. J. Kern, Universität Wien, Fakultät für Mathematik, Vienna, Austria, July 18–22.
27. W. König, Centre for Theoretical Studies, Prague, Czech Republic, November 10–13.
28. J. Köppl, Arizona State University, School of Complex Adaptive Systems, Tempe, USA, March 11–22.

[6] Only stays of more than three days are listed.

29. A. Kroshnin, University of Pisa, Department of Mathematics, Italy, November 26 – December 6.
30. M. Landstorfer, Università degli Studi di Brescia, Dipartimento di Ingegneria Meccanica e Industriale, Italy, September 9–13.
31. H. Langhammer, Università di Roma "La Sapienza", Dipartimento di Matematica, Rome, Italy, September 23–27.
32. L. Lüchtrath, Universität zu Köln, Mathematisches Institut, October 17–24.
33. E. Magnanini, Politecnico Milano, Dipartimento di Matematica, Milano, Italy, April 29 – May 2.
34. E. Magnanini, Università degli Studi di Padova, Dipartimento di Matematica, Padova, Italy, September 24–27.
35. J. Rehberg, Universität Graz, Institut für Mathematik, Austria, October 22–25.
36. J. Schütte, Ecole Polytechnique Fédérale de Lausanne, Institut de Mathématiques, Switzerland, October 14–18.
37. V. Spokoiny, University of Electronic Science and Technology of China (UEST), School of Mathematical Sciences, Chengdu, China, May 12–19.
38. M. Thomas, Texas A&M University, Department of Mathematics, College Station, USA, March 17–27.
39. ———, University of Cambridge, Centre for Mathematical Sciences, UK, November 6–11.
40. W. van Zuijlen, Radboud University Nijmegen, Department of Mathematics, Nijmegen, Netherlands, November 21–25.
41. B. Wagner, University of Oxford, Mathematical Institute, UK, November 4 – December 3.
42. A. Zass, Technische Universität München, Department of Mathematics, November 11–15.
43. J.-J. Zhu, RIKEN Center for Advanced Intelligence Project (AIP), Tokyo, Japan, January 23–27.
44. ———, KTH Royal Institute of Technology, Department of Mathematics, Stockholm, Sweden, November 19 – December 21.
45. ———, École Polytechnique Fédérale de Lausanne, Section de Mathématiques/College of Management of Technology, Switzerland, November 23–28.

A.10 Academic Teaching[7]

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. P.K. Friz, *Rough Stochastic Differential Equations* (lecture), Technische Universität Berlin, 2 SWS.
10. ———, *Oberseminar Rough Paths, SPDEs and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
11. ———, *Seminar Optimal Transport and Mean Field Games* (seminar), Technische Universität Berlin, 2 SWS.
12. J. Fuhrmann, *Advanced Topics from Scientific Computing* (lecture), Technische Universität Berlin, 2 SWS.
13. C. Geiersbach, *Stochastische Optimierung (M20)* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
14. ———, *Stochastische Optimierung (M20)* (practice), Humboldt-Universität zu Berlin, 1 SWS.
15. 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.
16. M. Hintermüller, *Ausgewählte Kapitel der Mathematik (M40): Semismooth Newton Method* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
17. ———, *Hybrid: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
18. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
19. B. Jahnel, *Bachelor Seminar Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
20. ———, *Einführung in die Stochastik* (lecture), Technische Universität Braunschweig, 4 SWS.
21. ———, *Markov Processes* (lecture), Technische Universität Braunschweig, 4 SWS.
22. ———, *RampUp for Data Scientists: Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
23. W. König, *Wahrscheinlichkeitstheorie II* (lecture), Technische Universität Berlin, 4 SWS.
24. R. Lasarzik, *Partielle Differentialgleichungen II* (lecture), Freie Universität Berlin, 4 SWS.
25. ———, *Partielle Differentialgleichungen II* (practice), Freie Universität Berlin, 2 SWS.

[7] SWS = semester periods per week

26. R. Lasarzik, M. Thomas, *Sobolev- und BV-Räume* (seminar), Freie Universität Berlin, 2 SWS.
27. J. Ginster, M. Liero, *Mathematische Prinzipien der Kontinuumsmechanik (M1)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
28. ———, *Mathematische Prinzipien der Kontinuumsmechanik (M1)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
29. B. Moreau, *Computational Fluid Dynamics* (lecture), Beuth Hochschule für Technik Berlin, 4 SWS.
30. B. Keller, B. Schmidt, *Einführung in die Theoretische Chemie* (lecture), Freie Universität Berlin, 2 SWS.
31. C. Sirotenko, *Ausgewählte Kapitel der Mathematik (M40): Semismooth Newton Method* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
32. ———, *Ausgewählte Kapitel der Mathematik (M40): Semismooth Newton Method* (practice), Humboldt-Universität zu Berlin, 2 SWS.
33. 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.
34. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
35. V. Spokoiny, J.-J. Zhu, *Nonparametric Statistics (M29)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
36. ———, *Nonparametric Statistics (M29)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
37. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
38. M. Thomas, *Analysis III* (lecture), Freie Universität Berlin, 4 SWS.
39. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/Technische Universität Berlin, 2 SWS.

Summer Semester 2024

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. Th. Eiter, *Harmonische Analysis* (lecture), Universität Kassel, 4 SWS.
3. ———, *Seminar Analysis* (seminar), Universität Kassel, 2 SWS.
4. ———, *Harmonische Analysis* (practice), Universität Kassel, 2 SWS.
5. P.K. Friz, *Wahrscheinlichkeitstheorie III* (lecture), Technische Universität Berlin, 4 SWS.
6. ———, *Signatures and Data Science* (seminar), Technische Universität Berlin, 2 SWS.
7. 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.
8. M. Hintermüller, *Hybrid: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
9. D. Hömberg, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
10. D. Hömberg, *Online and on site: Optimization II – PDE-Constrained Optimal Control* (lecture), Norwegian University of Science and Technology, Trondheim, 4 SWS.
11. B. Jahnel, *Markov Processes* (lecture), Technische Universität Braunschweig, 4 SWS.
12. ———, *Master Seminar Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.

13. ———, *Probability Theory and Discrete Financial Mathematics* (lecture), Technische Universität Braunschweig, 4 SWS.
14. ———, *RampUp for Data Scientists: Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
15. V. John, *Numerik I* (lecture), Freie Universität Berlin, 4 SWS.
16. O. Klein, *Ausgewählte Themen der Angewandten Analysis (M38): Mathematische Modellierung von Hystereseeffekten* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. ———, *Ausgewählte Themen der Angewandten Analysis (M38): Mathematische Modellierung von Hystereseeffekten* (practice), Humboldt-Universität zu Berlin, 1 SWS.
18. W. König, et al., *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin/Technische Universität Berlin/WIAS Berlin, 4 SWS.
19. R. Lasarzik, *Nonlinear Evolution Equations* (lecture), Freie Universität Berlin, 2 SWS.
20. ———, *Partielle Differentialgleichungen III* (lecture), Freie Universität Berlin, 2 SWS.
21. ———, *Partielle Differentialgleichungen III* (practice), Freie Universität Berlin, 2 SWS.
22. R. Lasarzik, M. Thomas, *Gewöhnliche Differentialgleichungen* (seminar), Freie Universität Berlin, 2 SWS.
23. 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.
24. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
25. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
26. N. Tapia, *Stochastik für Informatik* (lecture), Technische Universität Berlin, 4 SWS.
27. M. Thomas, *Partielle Differentialgleichungen I* (lecture), Freie Universität Berlin, 4 SWS.
28. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/Technische Universität Berlin, 2 SWS.
29. A. Zass, *Gibbs Measures in Statistical Mechanics* (seminar), Technische Universität Berlin, 2 SWS.

Winter Semester 2024/2025

1. A. Alphonse, *Ausgewählte Themen der Optimierung (M23): Obstacle Problems and Optimal Control* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
2. ———, *Ausgewählte Themen der Optimierung (M23): Obstacle Problems and Optimal Control* (practice), Humboldt-Universität zu Berlin, 1 SWS.
3. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
4. M. Eigel, D. Sommer, *Analysis of Neural and Tensor Networks for High Dimensional Approximations* (lecture), Technische Universität Berlin, 4 SWS.
5. Th. Eiter, *Introduction to Mathematical Modeling with Partial Differential Equations* (lecture), Freie Universität Berlin, 2 SWS.
6. ———, *Introduction to Mathematical Modeling with Partial Differential Equations* (practice), Freie Universität Berlin, 2 SWS.
7. P.K. Friz, *Senior Seminar "Rough Analysis and Stochastic Dynamics"* (senior seminar), Technische Universität Berlin, 2 SWS.

8. J. Fuhrmann, *Advanced Topics from Scientific Computing* (lecture), Technische Universität Berlin, 2 SWS.
9. 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.
10. M. Hintermüller, *Hybrid: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
11. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
12. B. Jahnel, *Bachelor Seminar Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
13. ———, *Einführung in die Stochastik und Statistik (für Lehramt)* (lecture), Technische Universität Braunschweig, 4 SWS.
14. ———, *Point Processes* (lecture), Technische Universität Braunschweig, 4 SWS.
15. ———, *RampUp for Data Scientists: Stochastics* (lecture), Technische Universität Braunschweig, 2 SWS.
16. V. John, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
17. O. Klein, *Spezielle Themen der Mathematik (M39): Einführung in die Quantifizierung von Unsicherheiten (Uncertainty Quantification, UQ)* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
18. ———, *Spezielle Themen der Mathematik (M39): Einführung in die Quantifizierung von Unsicherheiten (Uncertainty Quantification, UQ)* (practice), Humboldt-Universität zu Berlin, 1 SWS.
19. M. Liero, *Ausgewählte Themen der Angewandten Analysis (M38): Optimaler Transport und Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
20. ———, *Ausgewählte Themen der Angewandten Analysis (M38): Optimaler Transport und Anwendungen* (practice), Humboldt-Universität zu Berlin, 1 SWS.
21. L. Lüchtrath, *Versicherungsmathematik* (lecture), Technische Universität Berlin, 4 SWS.
22. Ch. Merdon, *Numerik partieller Differentialgleichungen I* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
23. B. Keller, B. Schmidt, *Einführung in die Theoretische Chemie* (lecture), Freie Universität Berlin, 2 SWS.
24. 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.
25. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
26. K. Tabelow, *Mathematik* (seminar), Beuth Hochschule für Technik Berlin, 4 SWS.
27. M. Thomas, *Analysis I* (lecture), Freie Universität Berlin, 4 SWS.
28. ———, *Topics in Measure and Integration Theory* (seminar), Freie Universität Berlin, 2 SWS.
29. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/Technische Universität Berlin, 2 SWS.

A.11 Visiting Scientists[8]

A.11.1 Guests

1. L. Andreis, Politecnico di Milano, Dipartimento di Matematica, Milano, Italy, October 27 – November 2.
2. S. Bechtel, Université Paris-Saclay, Laboratoire de Mathématiques d'Orsay, France, December 9–13.
3. G. Bellot, Université de Lille, Laboratoire Paul Painlevé, Lille, France, August 5–9.
4. D. Belomestny, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, June 26 – July 1.
5. S. Ben Naamia, Rheinisch-Westfälische Technische Hochschule Aachen, Aachen Institute for Advanced Study in Computational Engineering Science, May 6–10.
6. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, July 7–13.
7. ———, December 8–15.
8. M. Brokate, Technische Universität München, Department of Mathematics, Garching, January 1 – December 31.
9. F. Brosa Planella, University of Warwick, Mathematics Institute, Coventry, UK, August 6–9.
10. P. Colli, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, April 12–19.
11. N. Doikov, École Polytechnique Fédérale de Lausanne, Machine Learning and Optimization Laboratory, Lausanne, Switzerland, December 1–6.
12. A. Drewitz, Universität zu Köln, Mathematisches Institut, Köln, August 5–9.
13. K. Ebrahimi-Fard, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, March 24–27.
14. R. Eisenberg, Rush University Chicago, Department of Physiology & Biophysics, USA, October 12–18.
15. A. Faggionato, Università di Roma "La Sapienza", Dipartimento di Matematica, Rome, Italy, January 23–28.
16. E. Ferrucci, University of Oxford, Mathematical Institute, Oxford, UK, March 24–30.
17. C. Geiersbach, Universität Hamburg, Fachbereich Mathematik, Hamburg, October 7–11.
18. E. Gladin, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School (BMS), January 17 – December 31.
19. S. Hermann, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, Freiburg im Breisgau, January 28 – February 3.
20. E. Jacob, École Normale Supérieure de Lyon, Unité de Mathématiques Pures et Appliquées, Lyon, France, May 19–24.
21. A. Katsevich, Massachusetts Institute of Technology, Department of Mathematics, Cambridge, USA, June 28 – July 11.
22. G. Kitavtsev, Middle East Technical University, Northern Cyprus Campus, Mathematics Research and Teaching Group, Kalkanlı, Güzelyurt, September 3–13.
23. J. Komjáthy, Delft University of Technology, Department Electrical Engineering, Mathematics and Computer Science (EWI), Netherlands, November 18–21.
24. B. Krauskopf, The University of Auckland, Department of Mathematics, New Zealand, July 1–4.
25. G. Last, Karlsruher Institut für Technologie, Institut für Stochastik, Karlsruhe, October 24 – December 5.

[8] Only stays of more than three days are listed.

26. U. Leonhardt, Weizmann Institute of Science, Faculty of Physics, Rehovot, Israel, July 12–28.
27. Y. Li, Fudan University, School of Mathematical Science, Shanghai, China, July 22–25.
28. D. Loutchko, University of Tokyo, Institute of Industrial Science, Japan, September 16–25.
29. H. Meinlschmidt, Friedrich-Alexander Universität Erlangen-Nürnberg, Dynamics, Control, Machine Learning and Numerics, March 11–15.
30. Th. Möllenhoff, RIKEN Center for Advanced Intelligence Project, Approximate Bayesian Inference Team, Nihonbashi,Chuo-ku, Tokyo, Japan, May 13–18.
31. Ch. Mönch, Johannes Gutenberg-Universität Mainz, Institut für Mathematik, Mainz, February 12–16.
32. L.O. Muller, University of Trento, Department of Mathematics, Povo, Italy, November 26–29.
33. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, March 13–28.
34. ———, May 27–31.
35. A. Nouy, Ecole Centrale de Nantes, Département Mathématiques, Laboratoire de Mathématiques Jean Leray, Nantes, France, April 14–17.
36. H.M. Osinga, The University of Auckland, Department of Mathematics, New Zealand, July 1–4.
37. A. Pasco, Ecole Centrale de Nantes, Département Mathématiques, Laboratoire de Mathématiques Jean Leray, Nantes, France, April 14–19.
38. T. Pereira, University of São Paulo, Departamento de Matematica Aplicada e Estatistica, Brazil, November 17, 2023 – February 5, 2024.
39. P. Perez-Aros, Universidad de Chile, Departamento de Ingeniería Matemática, Santiago de Chile, Chile, December 1–7.
40. Ch. Renaud Chan, Université Grenoble Alpes, Informatique, Mathématiques et Mathématiques Appliquées, Saint-Martin-d'Hères, France, October 7–12.
41. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, October 23 – November 23.
42. U. Rozikov, Academy of Sciences of Uzbekistan, V.I. Romanovskiy Institute of Mathematics, Tashkent, Uzbekistan, January 15 – March 15.
43. M. Schmidt, Universität Trier, Fachbereich Mathematik, Trier, February 18–21.
44. A. ter Elst, University of Auckland, Department of Mathematics, New Zealand, February 29 – March 17.
45. Z. Tomovski, Palacký University Olomouc, Department of Mathematical Analysis and Applications of Mathematics, Czech Republic, October 7–11.
46. H.-S. Tran, National University of Singapore, Department of Mathematics, Singapore, June 9–14.
47. W. van Ackooij, Electricité de France R&D, Palaiseau, France, May 20–24.
48. Q. Vogel, Ludwig-Maximilians-Universität München, Mathematisches Institut, München, May 27–30.
49. ———, August 5–9.
50. S. Wang, Humboldt-Universität zu Berlin, Institut für Mathematik, February 12 – December 31.
51. J. Weber, Universität Wien, Mathematische Fakultät, Austria, July 1–5.
52. E. Wiedemann, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, July 21–26.
53. L.C. Wirth, Georg-August-Universität Göttingen, Felix-Bernstein-Institut für Mathematische Stochastik in den Biowissenschaften, Göttingen, December 9–12.

54. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, September 13–18.

A.11.2 Scholarship Holders

1. A. Hryn, University of Grodno, Mathematical Analysis, Differential Equations and Algebra, Belarus, DAAD Scholarship, July 8 – August 27.
2. M. Kniely, Universität Graz, Austria, Erwin Schrödinger-Auslandsstipendium, March 1, 2022 – February 29, 2024.
3. H. Li, Shandong University, School of Mathematics, Jinan, China, Ph.D. Mobility Program, November 15, 2024 – November 14, 2025.
4. 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 – August 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. L. Abel, Humboldt-Universität zu Berlin, Institut für Mathematik, *A scaling law for a model of epitaxial growth with dislocations*, November 13.
2. S. Bechtel, Université Paris-Saclay, Laboratoire de Mathématiques d'Orsay, France, *What we know about square roots of elliptic systems – And a bit more!*, December 11.
3. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, *Pruning in DNNs via regularization and the Marchenko–Pastur distribution: Fully connected and ViT networks*, July 9.
4. T. Bodnár, Czech Technical University in Prague, Department of Technical Mathematics, Czech Republic, *On the use of viscoelastic fluids flows models in hemolysis prediction*, November 7.
5. T. Böhnlein, Technische Universität Darmstadt, Fachbereich Mathematik, *Bounded functional calculus and dynamical boundary conditions*, April 10.
6. M. Brokate, Technische Universität München, Department of Mathematics, *Rate independent evolutions: Some basics, some progress*, May 7.
7. F. Brosa Planella, University of Warwick, Mathematics Institute, Coventry, UK, *Asymptotic methods for lithium-ion battery models*, August 8.
8. F. Bugini, Technische Universität Berlin, Institut für Mathematik, *Rough SDEs: Connections to rough PDEs and Malliavin calculus*, November 12.
9. K. Buryachenko, Humboldt-Universität zu Berlin / Vasyl' Stus Donetsk National University, Institut für Mathematik / Department of Applied Mathematics and Cybersecurity, Vinnytsia, Ukraine, *Regularity problems for anisotropic models*, February 14.
10. J. Chhor, Toulouse School of Economics, France, *Locally sharp goodness-of-fit testing in sup norm for high-dimensional counts*, November 27.
11. E. Chzhen, Université Paris-Saclay, Laboratoire de Mathématiques d'Orsay, Paris, France, *Small total-cost constraints in contextual bandits with knapsacks*, February 7.
12. P. Colli, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, *Curvature effects in pattern formation: Analysis and control of a sixth-order Cahn–Hilliard equation*, April 17.
13. C. Daversin-Catty, Simula Research Laboratory, Numerical Analysis and Scientific Computing, Oslo, Norway, *Mixed-dimensional coupled finite elements in FEniCS(x) (online talk)*, April 9.
14. N. Doikov, École Polytechnique Fédérale de Lausanne, Machine Learning and Optimization Laboratory, Switzerland, *Stochastic second-order optimization with momentum*, December 3.
15. C. Duval, Université de Lille, Département de Mathématiques, France, *Geometry of excursion sets: Computing the surface area from discretized points*, July 3.
16. H. Engler, Georgetown University, Department of Applied Mathematics, Washington DC, USA, *The Lorenz system of 1996 (hybrid talk)*, July 16.
17. A. Faggionato, Università di Roma "La Sapienza", Dipartimento di Matematica, Italy, *Transport in weighted Delaunay triangulations*, January 24.
18. E. Ferrucci, University of Oxford, Mathematical Institute, Oxford, UK, *Constraint-based causal discovery in stochastic dynamical systems*, March 26.
19. G. Finocchio, Universität Wien, Institut für Statistik und Operations Research, Austria, *An extended latent factor framework for ill-posed linear regression*, January 31.
20. M. Ganet Some, University of Ghana, African Institute for Mathematical Sciences, Accra, Ghana, *Stochastic optimal control of a prosumer in a district heating system*, April 16.

21. J. GIESSELMANN, Technische Universität Darmstadt, Fachbereich Mathematik, *A posteriori error estimates for systems of hyperbolic conservation laws modeling compressible flows*, July 18.
22. M. GIORDANO, Università degli Studi di Torino, Dipartimento di Scienze Economico-sociali e Matematico-statistiche, Italy, *Likelihood methods for low frequency diffusion data*, January 17.
23. E. GLADIN, Humboldt-Universität zu Berlin, Berlin Mathematical School, *Cutting plane methods and dual problems*, July 30.
24. A. GONZALEZ CASANOVA, Universidad Nacional Autónoma de México and University of California, Berkeley, USA, *A random model of Poissonian interacting trajectories inspired by the Lenski experiment*, May 15.
25. M. GÖSGENS, Eindhoven University of Technology, Department of Mathematics and Computer Science, Eindhoven, Netherlands, *The Erdős–Rényi random graph conditioned on every component being a clique*, September 5.
26. M. GUGAT, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, Erlangen, *Optimal control problems with probabilistic constraints*, October 31.
27. C. HEISS, École Polytechnique Fédérale de Lausanne, School of Basic Sciences, Switzerland, *Plasmas, fusion and some math behind it*, August 27.
28. B. HÖVELER, Technische Universität Berlin, Institut für Mathematik, *An analogue for the Gramian of a linear quadratic regulator for nonlinear control systems and its approximability by finite rank operators*, September 24.
29. A. HRYN, University of Grodno, Mathematical Analysis, Differential Equations and Algebra, Belarus, *Continuum of limit cycles in a class of quadratic polynomial systems of three differential autonomous equations*, August 15.
30. T. HSING, University of Michigan, Department of Statistics, Ann Arbor, USA, *A functional-data perspective in spatial data analysis*, May 29.
31. G. IOMMAZZO, Zuse Institute Berlin, Mathematical Algorithmic Intelligence, *Linearly converging conditional gradients over intersecting polytopes*, June 11.
32. E. IPOCOANA, Freie Universität Berlin, Institut für Mathematik, *Non-isothermal phase-field models for tumor growth*, May 15.
33. H. ISHII, University of Tokyo, Graduate School of Frontier Sciences, Department of Complexity Science and Engineering, Nonlinear Physics Group, Japan, *Employing dynamical modeling to understand complex phenomena: From interacting bistable systems to football ball possession*, November 21.
34. E. JACOB, Ecole Normale Supérieure de Lyon, Unité de Mathématiques Pures et Appliquées, France, *Local weak limit of dynamical random graphs*, May 22.
35. S. JANSEN, Universität München, Mathematisches Institut, *Infinite-dimensional Lie algebras, Lévy random fields and stochastic processes*, February 7.
36. Y. KATO, University of Tokyo, Graduate School of Frontier Sciences, Department of Complexity Science and Engineering, Nonlinear Physics Group, Japan, *Introduction of two studies: (1) analysis of oscillation quenching by periodic perturbation and (2) parameter estimation of Kuramoto model*, November 21.
37. G. KEILBAR, R. MITFACHOV, Humboldt-Universität zu Berlin, Institut für Mathematik, *Shapley curves: A smoothing perspective*, May 8.
38. H. KERN, Technische Universität Berlin, International Research Training Group (IRTG) 2544, *Application of stochastic multiparameter sewing to regularity of local times associated to Gaussian sheets*, January 9.
39. H. KERSTING, Yahoo! Research, *Log neural controlled differential equations: The Lie brackets make a difference*, February 13.

40. O. Klopp, ESSEC Business School, Department of Information Systems, Data Analytics and Operations, Cergy, France, *Adaptive density estimation under low-rank constraints*, October 30.
41. B. Krauskopf, The University of Auckland, Department of Mathematics, New Zealand, *To blend or not to blend?*, July 2.
42. G. Kur, Eidgenössische Technische Hochschule Zürich, Departement Mathematik, Switzerland, *Connections between minimum norm interpolation and local theory of Banach spaces*, April 17.
43. P. Lappicy, Universidad Complutense de Madrid, Departamento de Análisis Matemático y Matemática Aplicada, Spain, *An energy formula for fully nonlinear degenerate parabolic equations in one spatial dimension (hybrid talk)*, July 9.
44. C. Lasser, Technische Universität München, Fakultät für Mathematik, *Variational Gaussian approximation for quantum dynamics*, July 10.
45. G. Last, Karlsruher Institut für Technologie, Institut für Stochastik, Karlsruhe, *Decorrelation and mixing properties of some Gibbs processes*, December 4.
46. J.N. Latz, Czech Academy of Sciences & Charles University, Institute of Information Theory and Automation (UTIA), Prague, Czech Republic, *Monotone interacting particle systems: Survival and the upper invariant law*, February 1.
47. Y. Li, Fudan University, School of Mathematical Science, Shanghai, China, *Function and derivative approximation by shallow neural networks*, July 23.
48. D. Loutchko, University of Tokyo, Institute of Industrial Science, Japan, *Information geometrical entropy production decompositions in chemical reaction networks*, September 18.
49. A. Majumdar, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Solution landscapes in the Landau–de Gennes theory for nematic liquid crystals: Analysis, computations and applications*, April 16.
50. D. Matthes, Technische Universität München, School of Computation, Information and Technology, Garching, *Covariance modulated optimal transport: Geometry and gradient flows*, July 17.
51. St. Metzger, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, Erlangen, *An augmented SAV scheme for the stochastic Allen–Cahn equation*, July 2.
52. Th. Möllenhoff, RIKEN Center for Advanced Intelligence Project, Approximate Bayesian Inference Team, Nihonbashi,Chuo-ku, Tokyo, Japan, *Variational learning for large deep networks*, May 14.
53. Ch. Mönch, Johannes-Gutenberg-Universität Mainz, Institut für Mathematik, *Inhomogeneous long-range percolation: Recent results*, February 14.
54. É. Moulines, Ecole Polytechnique, Centre de Mathématiques Appliquées, UMR 7641, Palaiseau, France, *Score-based diffusion models and applications*, January 10.
55. L.O. Muller, University of Trento, Department of Mathematics, Povo, Italy, *Towards real-life computional haemodynamics*, November 28.
56. E. Nijholt, Imperial College London, Department of Mathematics, UK, *Emergent hypernetworks in weakly coupled oscillators*, January 25.
57. A. Nouy, Ecole Centrale de Nantes, Laboratoire de Mathématiques Jean Leray, Nantes, France, *Moment methods for some optimal transport problems and parameter-dependent equations*, April 15.
58. I. Nuñez Morales, Centro de Investigación en Matemáticas A.C. Calle Jalisco, Department of Probability and Statistics, Mexico, *Alpha-stable branching and beta-frequency processes, beyond the iid assumption*, September 25.
59. H.M. Osinga, The University of Auckland, Department of Mathematics, New Zealand, *Isochron geometry and its influence on phase resets for higher-dimensional oscillators*, July 2.

60. T. Pereira, University of São Paulo, Departamento de Matematica Aplicada e Estatistica, Brazil, *Chaotic behaviour in the Turing–Smale problem*, January 25.
61. P. Perez-Aros, Universidad de Chile, Departamento de Ingeniería Matemática, Santiago de Chile, Chile, *The boosted double-proximal subgradient algorithm for nonconvex optimization*, December 3.
62. A. Pešić, Humboldt-Universität zu Berlin, Institut für Mathematik, *Variational models for pattern formation in biomembranes*, January 24.
63. Ł. Płociniczak, Wrocław University of Science and Technology, Faculty of Pure and Applied Mathematics, Poland, *From hydrology, through climatology to hemo- and lymphodynamics: Mathematical modelling approaches*, June 4.
64. A.J. Pool, Deutsches Zentrum für Luft- und Raumfahrt e.V., Universität Stuttgart Campus Vaihingen, *Non-linear dynamics as a ground-state solution on quantum computers*, September 18.
65. N. Ranwan, Indian Institute of Science Education and Research Thiruvananthapuram, Kerala, School of Mathematics, India, *Existence of a weak solution to the fluid-structure interaction problem of blood flow in coronary artery*, July 16.
66. Ch. Renaud Chan, Université Grenoble Alpes, Informatique, Mathématiques et Mathématiques Appliquées, Grenoble, France, *Liquid-gas phase transition for Gibbs point process with saturated interaction*, October 9.
67. J. Riebesehl, Technical University of Denmark, Department of Electrical and Photonics Engineering, Kgs. Lyngby, *Kalman filtering for noise characterization in optical frequency combs*, June 26.
68. A. Rodomanov, CISPA Helmholtz Center for Information Security, Saarbrücken, *Optimizing (L_0, L_1)-smooth functions by gradient methods*, December 3.
69. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, *Time discretization in visco-elastodynamics at large displacements and strains in the Eulerian frame*, October 30.
70. Ch. Rouyer, Universität Potsdam, Institut für Mathematik, Potsdam OT Golm, *Foundations of online learning for easy and worst-case data*, December 11.
71. J. Royset, University of Southern California, Department of Industrial and Systems Engineering, Los Angeles, USA, *Approximations of Rockafellians, Lagrangians, and dual functions*, April 22.
72. U. Rozikov, Academy of Sciences of Uzbekistan, V.I. Romanovskiy Institute of Mathematics, Tashkent, Uzbekistan, *Gibbs measures of Potts model on trees*, February 20.
73. A. Sander, Technische Universität München, School of Computation, Information and Technology, Chair for Design Automation, München, *Verifying the equivalence or non-equivalence of quantum circuits with tensor networks*, September 10.
74. M. Schmidt, Universität Trier, Fachbereich Mathematik, Trier, *A primer on bilevel optimization under uncertainty*, February 20.
75. M. Schmidtchen, Technische Universität Dresden, Institut für Wissenschaftliches Rechnen, *Gradient flow solutions for porous medium equations with nonlocal Lévy-type pressure*, May 8.
76. I. Schneider, Freie Universität Berlin, Institut für Mathematik, *Symmetry groupoids of dynamical systems*, January 10.
77. R. Schneider, Technische Universität Berlin, Institut für Mathematik, Berlin, *Numerical solution of high-dimensional Hamilton Jacobi Bellmann (HJB) equations, mean field games and compositional tensor networks*, February 13.
78. M. Sega, University College London, Department of Chemical Engineering, UK, *Microscopic and mesoscopic simulations of fluid interfaces*, February 13.
79. B. Stankewitz, Universität Potsdam, Institut für Mathematik, *Contraction rates for conjugate gradient and Lanczos approximate posteriors in Gaussian process regression*, November 20.

80. B. Szabo, Bocconi University, Department of Decision Sciences, Milan, Italy, *Privacy constrained semiparametric inference*, October 16.
81. F. Telschow, Humboldt-Universität zu Berlin, Institut für Mathematik, *Estimation of the expected Euler characteristic of excursion sets of random fields and applications to simultaneous confidence bands*, May 15.
82. A. ter Elst, University of Auckland, Department of Mathematics, New Zealand, *The Dirichlet problem for elliptic equations without the maximum principle*, March 4.
83. R. Tobies, Jena, *Iris Runge. A life at the crossroads of mathematics, science, and industry*, March 18.
84. Z. Tomovski, Palacký University Olomouc, Department of Mathematical Analysis and Applications of Mathematics, Czech Republic, *Anomalous and ultraslow diffusion of a particle driven by distributed-order noises*, October 9.
85. A. Topalovic, Humboldt-Universität zu Berlin, Angewandte Mathematik mit Schwerpunkt Optimierung komplexer Systeme, Berlin, *Model predictive control for generalized Nash equilibrium problems*, June 26.
86. A. Tribuzio, Universität Bonn, Institut für Angewandte Mathematik, *Scaling laws for multi-well nucleation problems*, February 7.
87. D. Turaev, Imperial College London, Faculty of Natural Sciences, Department of Mathematics, UK, *4-winged Lorenz attractors*, April 4.
88. G. Uribe Bravo, Universidad Nacional Autónoma de México, Instituto de Matemáticas, Coyoacán, Mexico, *A pathwise approach to time-change*, June 5.
89. W. van Ackooij, Electricité de France R&D, Palaiseau, France, *A bilevel perspective on optimization with probability constraints*, May 21.
90. F. van der Plas, Massachusetts Institute of Technology, Julia Lab, Cambridge, USA, *Julia and Pluto.jl – Is scientific computing accessible?*, February 15.
91. N. Verzelen, Institut National de Recherche pour l'Agriculture, l'Alimentation et l'Environnement (INRAE), Statistics and Machine Learning, Montpellier, France, *Computational trade-offs in high-dimensional clustering*, April 24.
92. A. Vikelis, Universität Wien, Fakultät für Mathematik, Austria, *Measure-valued solutions for non-associative finite plasticity*, July 3.
93. S. von der Gracht, Universität Paderborn, Faculty of Computer Science, Electrical Engineering and Mathematics, *Exploring exotic symmetries to explain exotic behavior of network dynamical systems (hybrid talk)*, July 16.
94. I. Voulis, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, *An adaptive stochastic FEM method for the Poisson problem*, April 30.
95. M. Wahl, Universität Bielefeld, Fakultät für Mathematik, *Heat kernel PCA with applications to Laplacian eigenmaps*, February 14.
96. B. Walker, University of Oxford, Mathematical Institute, UK, *Log neural controlled differential equations: The Lie brackets make a difference*, January 16.
97. W. Wang, University of Groningen, Faculty of Business and Economics, AV Groningen, Netherlands, *Conditional nonparametric variable screening by neural factor regression*, October 23.
98. J. Weber, Universität Wien, Mathematische Fakultät, Austria, *Axisymmetric capillary water waves with vorticity and swirl*, July 4.
99. E. Wiedemann, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, *Measure-valued solutions in fluid dynamics*, July 24.

100. L.C. Wirth, Georg-August-Universität Göttingen, Felix-Bernstein-Institut für Mathematische Stochastik in den Biowissenschaften, Göttingen, *Stein's method for spatial random graphs*, December 11.

101. W. Wollner, Universität Hamburg, Fakultät für Mathematik, Informatik und Naturwissenschaften, *Gradient-robustness in the context of optimal control*, October 24.

102. S. Wood, University of Edinburgh, School of Mathematics, UK, *On neighbourhood cross validation*, January 24.

103. M. Yamamoto, University of Tokyo, Graduate School of Mathematical Sciences, Japan, *Inverse problems for time-fractional diffusion-wave equations*, September 17.

104. R. Zhang, Technische Universität Berlin, Institut für Mathematik, *Direct and inverse problems in periodic waveguides*, April 24.

105. X. Zuo, National University of Singapore, Risk Management Institute, Singapore, *Cryptos have rough volatility and correlated jumps*, January 15.

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 (partial differential equations with random data), methods for (sample-free) Bayesian inverse problems are available.

More information: https://www.wias-berlin.de/software/index.jsp?lang=1&id=ALEA

AWS – Adaptive Weights Smoothing (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

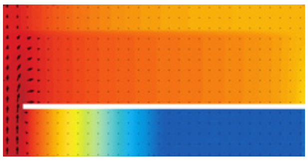
`AWS` is a contributed package within the R-Project for Statistical Computing containing a reference implementation of the **A**daptive **W**eights **S**moothing algorithms for local constant likelihood and local polynomial regression models. Binaries for several operating systems are available from 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/



Current density for single photon system

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.

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/.

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

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 https://www.wias-berlin.de/software/ParMooN/.

Important features of ParMooN are

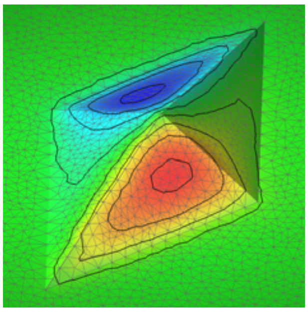
- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, non-conforming, discontinuous, higher-order, vector-valued, isoparametric, with bubbles),
- the use of implicit time-stepping schemes (θ-schemes, DIRK schemes, Rosenbrock–Wanner schemes),
- the application of a multiple-discretization multi-level (MDML) preconditioner in Krylov subspace methods,
- tools for using reduced-order models based on proper orthogonal decomposition (POD) are available,
- hybrid parallelization with MPI and OpenMP.

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

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

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

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.

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.

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-PDELib.jl (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, P. Jaap, phone: +49 30/20372-525, e-mail: patrick.jaap@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 `ExtendableFEM.jl` implementing gradient-robust finite element methods in Julia.

Please see also https://github.com/WIAS-PDELib.

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).