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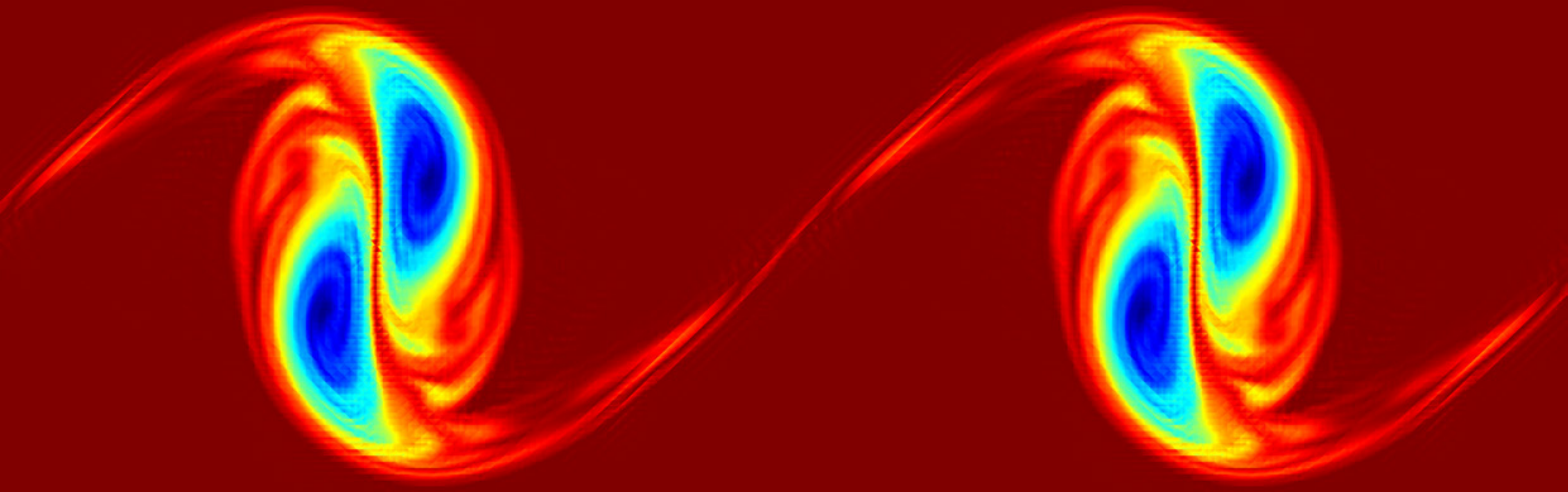
Intelligent solutions for complex problems

Annual Research Report 2022



Cover figure: Plot of the vorticity from a simulated evolution of a Kelvin–Helmholtz instability. This is a challenging benchmark example in computational fluid dynamics and was used to test the capabilities of a novel divergence-free discretization for the time-dependent Navier–Stokes equations (see page 81).

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Edited by Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
D – 10117 Berlin
Germany

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Fax: + 49 30 20372 303
E-Mail: contact@wias-berlin.de
World Wide Web: `https://www.wias-berlin.de/`

Prof. Michael Hintermüller, Director

The Weierstrass Institute for Applied Analysis and Stochastics, Leibniz Institute in Forschungsverbund Berlin e.V. (WIAS, member of the Leibniz Association), presents its Annual Research Report 2022. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2022.

The year 2022 was, with the war in the Ukraine and the energy and climate crises, again a very demanding one for our institute and our society as a whole. Fortunately, WIAS members made many constructive, creative, and very valuable contributions to help achieve the aims of our institute. Finally, we also overcame most effects of the COVID-19 pandemic.

New outstanding successes were recorded and excellent projects brought to the WIAS in 2022. Many newly acquired MATH+ projects, the Leibniz MMS network, and MaRDI show the enormous creativity and radiance of the institute.

The WIAS deepened its research in Quantum Technology, Data-driven Applications: Machine Learning and Optimization, and Electrochemistry. Newly launched projects are, e.g., the MATH+ incubator project “Electronic properties of gate-confined quantum dots in Si-Ge heterostructures for qubit generation” in cooperation with the Institut für Kristallzüchtung, the DFG project “Adaptive neural tensor networks for parametric PDEs” in DFG SPP 2298, and “Invertible neural networks for applications in metrology” within the EU project ATMOC. As a partner of the network *Artificial Intelligence in Digital Health (AIDHeal)* in the Berlin-Brandenburg region, it contributes to strengthen the expertise in the areas of data science, machine learning, and digital health in Germany.

The institute passed the audit by its Scientific Advisory Board (SAB) in September with very good results. The SAB congratulated the WIAS staff for the excellent preparation. In its oral statement at the end of the Audit, the SAB acknowledged that the institute continued performing world-class research and developed further exciting research areas. An open discussion following a recent survey among the WIAS staff was positively seen to have the potential to enhance the work environment and paving the way for further success.

The WIAS also successfully passed its re-audit in the *audit berufundfamilie*, documenting our commitment to a sustainable family- and life-phase-conscious personnel policy for making our institute a highly attractive working place. The extremely carefully prepared dialog day in this framework showed that we satisfy most of the goals set and that we are on the right track.

A Research Data Management unit was established in the directorate of the WIAS comprising the library, the *Mathematical Research Data Initiative* MaRDI (consortium of mathematics in the National Research Data Infrastructure NFDI) coordinated at WIAS and a position for research software engineering, to develop a future-oriented research data culture.

In the Leibniz Competition 2023, the project “Excellence in Photonic Crystal Surface Emitting Lasers (PCSELence)” submitted by Ferdinand-Braun-Institut within the funding program “Leibniz Collaborative Excellence” in cooperation with Kyoto University and the WIAS, was recommended for funding.

WIAS is among the five cooperation partners of the Cluster of Excellence Berlin Mathematics Research Center MATH+, with its Director its new Chair since November 2022. Two MATH+ Distinguished Fellowships went to WIAS members: Prof. Alexander Mielke and Prof. Peter K. Friz. The reporting year brought WIAS four new MATH+ projects starting 2023.

Prof. Marita Thomas, the head of the Weierstrass Group *Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes* at WIAS, recently received and accepted an offer of a professorship at the Freie Universität Berlin and was elected to the speaker team of DFG CRC 1114 *Scaling Cascades in Complex Systems* for its next round of funding.

Prof. Benedikt Jahnel, the head of the Leibniz Group *Probabilistic Methods for Dynamic Communication Networks* received and accepted an offer of a professorship at Universität Braunschweig.

WIAS co-organized two of the distinguished conferences of the Society for Industrial and Applied Mathematics (SIAM) in 2022: The SIAM Conference on Analysis of Partial Differential Equations (PD22; March 14–18, 2022) and the The SIAM Conference on Imaging Science (IS22; March 21–25, 2022) were happening virtually due to the Corona situation.

The Secretariat of the International Mathematical Union (IMU), hosted since 2011 at WIAS, supported the IMU in organizing the virtual International Congress of Mathematicians 2022 (ICM 2022) as well as the 19th IMU General Assembly (GA) and the IMU Award Ceremony 2022. The GA passed a resolution where it "expresses its deep gratitude to Germany, and in particular to the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) for their generous support of the IMU Secretariat. The General Assembly reaffirms its endorsement of the Stable Office for the International Mathematical Union as hosted at WIAS."

WIAS's primary aim remains unchanged: to combine fundamental research with application-oriented research, and to contribute to the advancement of innovative technologies through new scientific insights.

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

Berlin, in March 2023

M. Hintermüller

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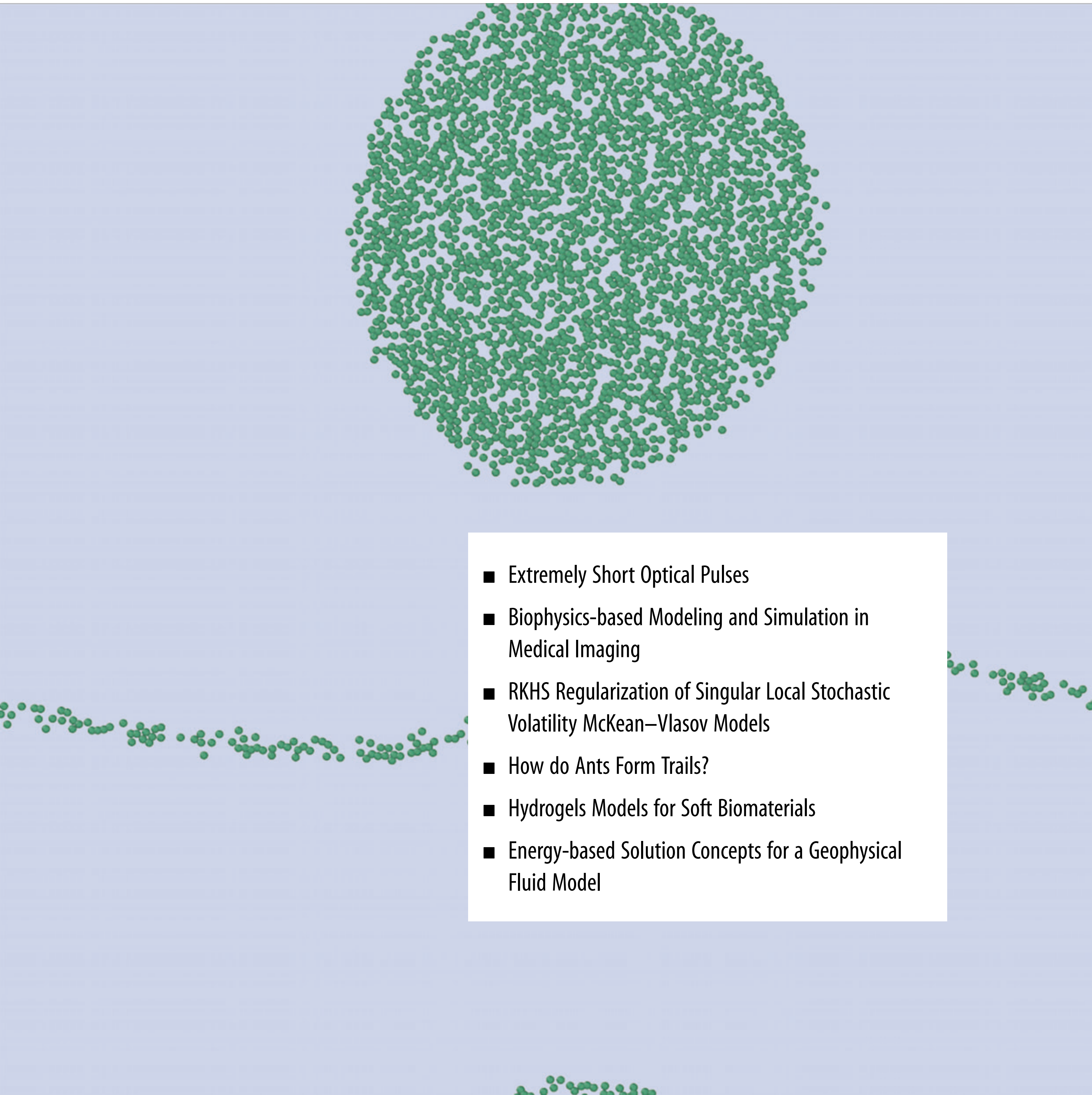
1 Scientific Highlights



- Extremely Short Optical Pulses
- Biophysics-based Modeling and Simulation in Medical Imaging
- RKHS Regularization of Singular Local Stochastic Volatility McKean–Vlasov Models
- How do Ants Form Trails?
- Hydrogels Models for Soft Biomaterials
- Energy-based Solution Concepts for a Geophysical Fluid Model

1.1 Extremely Short Optical Pulses

"You must go on and find out all about that light, and what it is for, and if all is perfectly safe. . . " J.R.R. Tolkien

Shalva Amiranashvili

Light signals have been used to transmit information since the earliest days of human history, for instance, in the form of "signal bombs" (flares), which were used by the Chinese to report on the movements of the Mongol army during the siege of Yangzhou in 1276. The Mongols also mastered the technique of light signals: They used large lanterns to control their troops at nighttime. Better command and control was one of the reasons why the Mongols' invasion of the rest of the Asian world was so successful. At about the same time, attempts to defend against the Viking attacks on the other side of the continent in Europe suffered from the slow exchange of information between the unprotected coastal settlements and the military authorities.

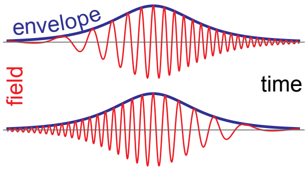


Fig. 1: *Two wave packets with the same envelope. To distinguish between them, a complex-valued envelope is used.*

Mankind has come a long way since the time of signal fires and nowadays information is transmitted in a more effective manner: via short pulses consisting of electromagnetic waves, so-called *wave packets*, like in Figure 1. The Morse code distress signal $\overline{\text{SOS}}$, established in 1906, is a combination of nine such pulses of just two types (short and long or, mathematically speaking, 0 and 1), which is sufficient to encode any message. The most ambitious project that employs short pulses to exchange information is without a doubt the World Wide Web, where a typical data center network is capable to transmit 40 Gb/s. In plain language, one would need one hour to create a full backup of the United States Library of Congress, of course, only after its complete digitization. As the digitization is progressing slowly, and the technology is rapidly evolving, the actual time will be much less than one hour.

Both old-fashioned signal lights and modern wave packets, the latter of which are invisible to the naked eye, transmit information using the same electromagnetic waves. All such waves are subject to one common set of equations discovered by James Clerk Maxwell in the mid-19th century. The main practical difference between these pulses is their duration: The modern pulses in optical networks are, to put it mildly, much shorter than the signals from the Chinese signal bombs. It is no wonder that especially the shortest possible pulses are ideally suited for the quick transfer of information, even taking into account all the difficulties associated with their *generation*, made possible by the invention of lasers, and *transmission*, made possible by the invention of optical fibers. This is how the *ultrashort pulses* came into play.

". . . the most significant event of the 19th century will be judged as Maxwell's discovery of the laws of electrodynamics." R. Feynman

It is important to note that both short (with the duration of one trillionth of a second) and ultrashort (up to 1,000 times shorter) optical pulses have numerous practical and potential applications in addition to the transmission of information. In the field of popular science, for instance, they allow for the filming of a bullet piercing an apple, as in a famous sequence of photos made by Harold E. Edgerton. To give a more practical example, let an external electromagnetic pulse with the duration t_0 hit and go through a small target, which reacts by emitting its own radiation. On the time scale $t > t_0$, the emitted target's radiation is separated from the initial pulse, which is already gone, what is not the case for $t < t_0$. Ultrashort pulses make it possible to initiate and observe certain very fast processes, those that are fully accomplished and thus unobservable on a larger time scale. A close analogy is found in mathematics: If we know how a (linear) system reacts on a short-but-strong perturbation, which physicists associate with Paul Dirac and call *Dirac's delta function*, we can calculate how the system reacts on any perturbation. A prominent application of this approach was the observation of a chemical reaction on molecular level (the 1999 Nobel Prize in chemistry).

One more possibility to make use of ultrashort optical pulses is to take advantage of similarities between different physical systems, whose behavior is determined by the propagation and interaction of waves. It may happen that *mathematically* such systems are described by the same equation. *Optical black holes*, for instance, appear in a specially designed optical system that simulates solutions of Einstein's equations of general relativity. Such an analog black hole is represented by one edge of a short, extremely intense optical pulse propagating in a fiber. Just as a true black hole absorbs the matter from the surrounding space, the optical one absorbs the energy from other pulses, with the main pulse gradually becoming shorter and stronger. The analogy is destroyed when the hole-presenting pulse becomes too extreme and certain optical effects, which have no equivalent in the theory of gravity, come into play. Before that happens, the optical black hole gives laboratory access to mysterious phenomena such as event horizons and Hawking radiation, which are believed to play their part somewhere in deep space [1].

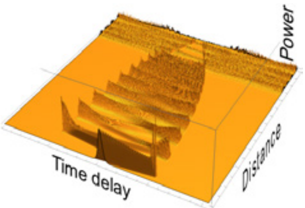


Fig. 2: *A trapped pulse that propagates bouncing between two invisible extreme pulses, like between two mirrors in a laser cavity*

Optical white holes also exist; they are represented by the second edge of the same ultrashort pulse, and they, in turn, feed other pulses with energy. Both edges of the seed ultrashort pulse serve as impermeable barriers for the ordinary radiation (in a range of wavelengths that, by the way, was calculated at WIAS, see [2] and the references cited therein). Among other things, the impermeable extreme pulses might replace physical mirrors in certain fantastical devices such as an all-optical laser cavity in Figure 2. Alternatively, the external radiation can be applied to the "black" and "white" sides of an extreme optical pulse to switch the pulse on and off, just like it happens with the electric current in a transistor. This is a possible approach to all-optical switching and optical transistors.

Another example comes from fluid dynamics. Ocean waves have much in common with electromagnetic waves in fibers: To a certain extent, both wave systems are governed by the same nonlinear Schrödinger equation (NLSE). Here, an important issue is the statistical distribution of the heights of individual ocean waves and especially the probability with which the most dangerous killer waves appear. Sailors often reported on the spontaneous appearance of huge ocean waves, which were two and even three times larger than their neighbors; most accidents with large ships were attributed to such waves. Physicists have argued that the extreme waves are also extremely rare. Their assumed distribution, derived by Lord Rayleigh, had a Gaussian tail. The probability of a large wave was then considered to be negligibly small. In plain language, an observer of stormy weather would have to wait about 27 years before a wave that is three times larger than the average wave height appears.

By the way, the nonlinear Schrödinger equation has no relation to Erwin Schrödinger and his famous equation. Being different, they just look similar and the name has stuck.

The first fully recorded 25.6 m killer wave, which was more than twice as tall as its neighbors and which damaged a sea platform in the North Sea in 1995, put an end to the arguments. The question arose about the practical measurement of an unknown statistical distribution. If wave statistics is difficult to collect in a rough sea, why not to collect it in a fiber with its millions of pulses per second? It was done by Solli et al., and indeed demonstrated that the extreme waves appear much more often than previously thought by Lord Rayleigh and his followers; the scientists were wrong, and the sailors were telling the truth [3].

"Waves that appear from nowhere and disappear without a trace." N. Akhmediev

Direct observations of ocean waves were made using satellites covering large areas simultaneously. As a result, the equivalent of 27 years for an individual observer could be made in 14 minutes for one million of the digital observations. These observations confirmed both the existence of killer waves and the non-Gaussian distribution of the wave heights. Needless to say, the use of the satellites was much more expensive and yet necessary because human lives were at stake.

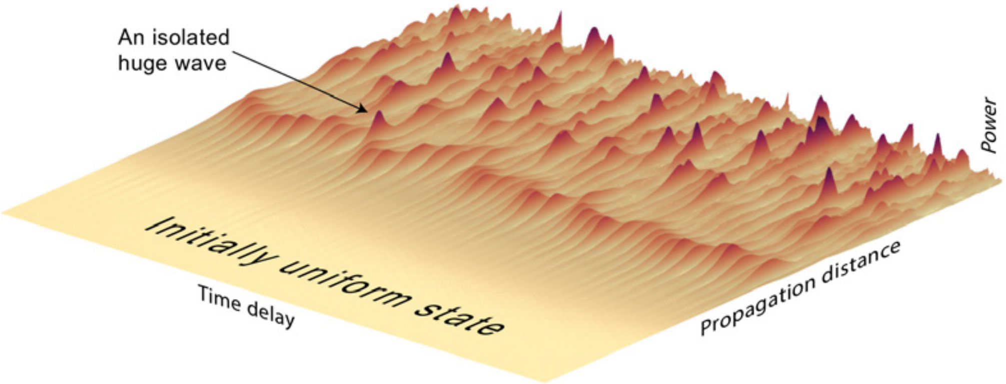


Fig. 3: *A numerical solution of the nonlinear Schrödinger equation that demonstrates how a small-amplitude uniform wave is destroyed and replaced by a turbulent state with the spontaneous extreme events*

What is important from a purely scientific standpoint: Solli's experiments demonstrated universality of extreme waves, which should be expected and indeed have been found in many nonlinear systems later on. Like the theory of catastrophes, killer waves have become very popular and are used to explain just about anything, even economic shocks. Staying on solid scientific ground, an exemplary numerical solution of the above-mentioned NLSE, which equally applies to both fibers and oceans, is shown in Figure 3. What is actually plotted is the squared magnitude of the envelope from Figure 1, which is proportional to the power. One can see how a complex turbulent "rough sea" develops from an initially uniform state and how huge isolated waves appear here and there. To prove their non-Gaussian nature, one has to make several thousands of such calculations to collect statistics of the potential extreme events.

Considering all of the above, there is little doubt that physics of ultra-fast phenomena is a fascinating area of modern science and that the generation of short pulses is a complex technical task. Are there any mathematical problems with their propagation? An accurate description of pulses in fibers seems to be simple. As opposed to string theory or quantum gravity, the fundamental equations governing all electromagnetic waves in nature have been known for almost 200 years. Moreover, pulses in optical fibers propagate in one spatial dimension, making their mathematical description even simpler. Given the equations and availability of powerful computers, why not solve the pulse propagation problem by brute force? The devil is in the separation of scales.

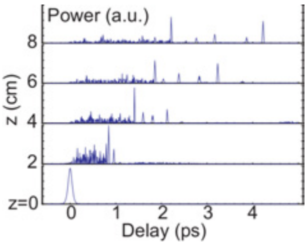


Fig. 4: *As pulses propagate differently, the numerical solution domain may become too small*

The smallest spatial scale for an optical pulse is its carrier wavelength with the typical value around 1.4 μm, which is close to the minimal attenuation in a silica fiber. This spatial scale is much smaller than the propagation distance, because the maximal length of a fiber optic cable is around 100 km. A direct calculation that resolves each wavelength all along the fiber is impossible. All useful pulse propagation models, including NLSE in the first place, employ approximations, namely:

(I) A pulse or a sequence of pulses is considered on a relatively small and comoving computational domain. As all pulses change their velocities and do it *differently* depending on their parameters, the domain may become too narrow and the calculation will have to be repeated (Figure 4).

(II) All normal evolution problems in physics predict a system's state at (time) $t > 0$ from the initial state at $t = 0$. In fiber optics, a system's state is "known" at (position along the fiber) $z = 0$ for all t and should be calculated for the evolution coordinate $z > 0$ for all t. Here, the causality principle is sacrificed (!!) to get the most simple propagation equation.

(III) All pulses move in one common direction along the fiber, and the backward waves are ignored. Moreover, these pulses are not too intense and propagate in a weakly nonlinear limit. We then have a small parameter that makes it possible to expand and simplify the equations.

(IV) As a typical picosecond pulse at 1.4 μm contains about 200 field oscillations, it is properly described by its carrier frequency ω_0 and envelope ψ. The *slowly varying envelope approximation* (SVEA) assumes that ψ is smooth and does not change much on the time scale $1/\omega_0$.

In the simplest case, the envelope (like in Figure 1) does not change at all and just moves along the fiber with the velocity $V = \text{const}$. The envelope ψ depends only on the delay variable $\tau = t - z/V$, and the propagation equation simply states that $\partial_z \psi(z, \tau) = 0$. If the simplest scenario is destroyed (by dispersion, nonlinearity, attenuation, and so on), the propagation equation takes the form

$$\partial_z \psi(z, \tau) = \text{dispersionOperator}(\psi) + \text{nonlinearOperator}(\psi) + \cdots, \tag{1}$$

where each term on the right-hand side accounts for a certain physical process. They act independently of each other because of the weak nonlinearity and SVEA; the list of the involved operators can be found in any textbook on fiber optics.

The simplest representative of (1) is the (normalized, focusing) NLSE

$$\partial_z \psi = i \partial_\tau^2 \psi + i |\psi|^2 \psi, \tag{2}$$

which is integrable. This is why numerous explicit solutions for all kinds of solitary pulses and spontaneous killer waves were found. By choosing both the dispersion and nonlinear operators in a special and very sophisticated manner, one can get further integrable envelope equations [4], but in practice, the general applications-relevant Eq. (1) is solved numerically. This is usually done by the split-step method, where the change from $\psi(z, \tau)$ to $\psi(z + \Delta z, \tau)$ occurs by the successive accounting of contributions of all involved operators one by one (Figure 5).

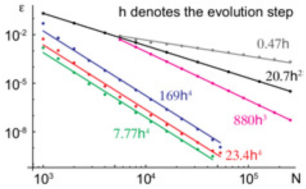


Fig. 5: *Relative error* ε *versus discretization* N *for different splitting methods. The two best methods (green and red lines) were found at WIAS [5].*

RG 2's research in the context of the application topic "Optical pulses in nonlinear media" is focused on pulses, which are so extreme that at least one of the assumptions from the list (I–IV) is violated. In the first place, this applies to the ultra-short few-cycle pulses with a duration of several femtoseconds, such that instead of 200 field oscillations within the pulse, we have only 1 or 2 of them.

Speaking of few-cycle pulses, is there any useful replacement of the envelope concept, one that avoids the costly solution of the full Maxwell system? The SVEA-independent definition of the envelope that is currently accepted in optics employs the so-called *analytic signal* and applies to any pulse, whether short or not. And yet the definition (a signal that is analytic in the upper half-plane of complex times) looks like a trick and comes from nowhere. Instead, we employ the so-called *classical creation-annihilation fields*, which are borrowed from the continuous Hamiltonian mechanics. The complex envelope is chosen to transform the Hamiltonian to its normal form. The definition is equivalent to the standard one for a longer pulse and is different from and better than the standard one for a few-cycle pulse. Among other things, the use of the creation-annihilation fields reduces the costs of the split-step solution.

Another area of research that is closely related to ultrashort pulses deals with an accurate description of medium dispersion, which is encoded in the $\mathrm{dispersionOperator}(\psi)$ in (1). Most commonly, the dispersion effect is approximated by a differential operator, e.g., by $i\partial_\tau^2$ in the simplest Eq. (2) and by a higher-order differential operator in a more general Eq. (1). Being unbounded, these operators lead to stiff numerical solutions. The situation with the ultrashort pulses is especially dangerous, as they have wide spectra such that higher-order derivatives of quickly oscillating frequency components ($e^{-i\omega\tau}$ with large ω) come into play. The difficulty is considerably relaxed by replacing the polynomial approximations with rational ones.

Throughout the lifetime of the application topic “Optical pulses in nonlinear media”, a considerable effort was invested in the numerical solutions of (1) and more specific pulse propagation models that avoid the use of the envelope. In addition to the conventional splitting methods, special attention was given to additive methods, such as the Burstein & Mirin splitting

$$e^{h(L+N)} = \frac{2}{3}\left(e^{\frac{h}{2}L}e^{hN}e^{\frac{h}{2}L} + e^{\frac{h}{2}N}e^{hL}e^{\frac{h}{2}N}\right) - \frac{1}{6}\left(e^{hN}e^{hL} + e^{hL}e^{hN}\right) + O(h^4), \tag{3}$$

where the evolution operator e^{hL} (e^{hN}) yields the solution of the linear (nonlinear) subproblem in (1) on $z \in (0, h)$. The splitting (3) consists of four threads that can be calculated in parallel. We found a new class of the additive splittings, a far-reaching generalization of (3); see [5].

Last but not least, we studied situations where excitation of backward waves cannot be ignored because it takes place in a resonant way in the course of wave mixing. We found a kind of Brillouin’s scattering that takes place due to optical nonlinearities without any involvement of the material waves. The new theory describes non-envelope pulses propagating in both directions ([6], Figure 6).

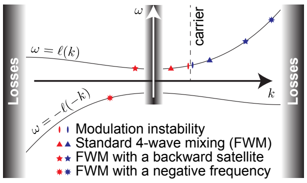


Fig. 6: *Four possible wave mixing scenarios. One with a backward wave and one with a negative frequency wave are new, see [6]*

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1.2 Biophysics-based Modeling and Simulation in Medical Imaging

Alfonso Caiazzo, Sarah Katz, and Karsten Tabelow

Modern image acquisition technologies allow clinicians to record detailed information not only on patient anatomy, but also related to biophysical processes, such as fluid and tissue mechanics water diffusion, and metabolic activities. Those data can support clinicians in the quantitative estimation of relevant biomarkers for identifying and staging pathologies, as well as non-invasive patient monitoring, making medical imaging a pillar of non-invasive clinical diagnostics.

This article focuses on three selected applications of mathematical methods in the context of medical imaging: the estimation of pressure-related biomarkers from tissue displacement data, the estimation of tissue properties from magnetic resonance imaging (MRI) images, and usage of computational fluid dynamics to quantify complex blood flow behavior in the aorta, to highlight how different biophysical models and suitable computational frameworks can be used to exploit the information contained in the available data.

Data assimilation for magnetic resonance elastography

Magnetic resonance elastography (MRE) is an imaging acquisition technique sensitive to tissue mechanical properties. During the examination, the living tissue undergoes a mechanical excitation (10–100 Hz) whose response is recorded via motion-sensitive (phase-contrast MRI) images, resulting in a three-dimensional displacement field on selected tissue regions. Combined with suitable physical models, these displacement data allow to obtain non-invasive estimates of tissue mechanical parameters.

Elastography has been widely used for the quantitative estimation of biomarkers (e.g., stiffness, tissue fluidity, viscoelasticity) related to different tissue pathologies, supporting the diagnosing and staging of diseases, such as cancer and fibrosis. This section discusses the applicability of elastography for quantifying an increase of brain intracranial pressure (ICP), i.e., the pressure of the cerebrospinal fluid (CSF) within the brain, a condition that might be responsible for different neurological diseases or cerebral damages. This application is particularly challenging, for at least two reasons. Firstly, data are only available on a portion of the domain (typically a thin slice of the brain), which does not necessarily include the regions where the pressure shall be quantified. Secondly, these data are limited to the displacement field, i.e., the pressure is not observed. These aspects make the application of standard variational frameworks unsuitable, due to the high dimension of the unknown state and to the absence of consistent boundary conditions for the state variables.

We address this *state estimation* combining the numerical solutions of suitable partial differential equations (PDEs) with an optimization problem solved on a low-dimensional space. Namely, assuming to be given a set of displacement data over a few slices of the computational domain – mimicking the setting of an MRE acquisition – our goals are to (i) reconstruct suitable displacement and pressure fields on the whole brain, and (ii) to provide quantitative estimation of the pressure difference between the ventricles and the outer domain [2].

A computational model of a human brain was generated using full brain anatomical MRI images, segmented into a triangulated surface and filled with an unstructured tetrahedral mesh. Denoting with $\Omega \subset \mathbb{R}^3$ the resulting computational domain, the dynamics of the tissue is assumed to be described in terms of a displacement field $\mathbf{u} : \Omega \to \mathbb{R}^3$ and a pressure field $p : \Omega \to \mathbb{R}$ in a time interval $[0, T]$:

$$\begin{aligned} \rho\, \partial_{tt} \mathbf{u} - \boldsymbol{\nabla} \cdot \left(\frac{E}{1+\nu} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right) + \nabla \cdot \frac{E\nu}{(1+\nu)(1-\nu)} \nabla \cdot \mathbf{u} + \boldsymbol{\nabla} p = 0 \quad &\text{in } \Omega \times [0, T]\,, \\ S_\epsilon\, \partial_t p + \boldsymbol{\nabla} \cdot \partial_t \mathbf{u} - \frac{\kappa}{\mu} \nabla^2 p = 0 \quad &\text{in } \Omega \times [0, T]\,. \end{aligned} \tag{1}$$

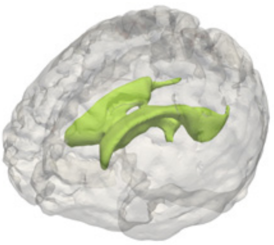

Fig. 1: *Surface of the computational model including the outer CSF (gray) and the ventricles (green)*

The system of PDE (1)[1] couples a linear, elastic solid phase with the motion of the fluid phase in the porous tissue. It depends on biophysical and mechanical parameters, such as tissue density (ρ), Young modulus (E), Poisson modulus (ν), tissue permeability (κ), fluid viscosity (μ), and mass-storage parameter (S_ϵ). Moreover, it depends on the boundary conditions to be imposed on the solid displacement and on the fluid pressure on the external and on the internal surfaces (the ventricles; see Figure 1).

The joint solution $v = (\mathbf{u}, p)$ is sought in a Hilbert *ambient* space V_h (e.g., piecewise linear finite elements for $\mathbf{u}$ and p), and we model the available measurements as m independent linear functionals $\ell_i : V_h \to \mathbb{R}$ $(i = 1, \dots, m)$, acting on the space V_h. In the target application, the images represent a three-dimensional displacement field on N_v voxels in the upper part of the brain, i.e., a total of $m = 3 \times N_v$ scalar measurements. As next, we construct an m-dimensional subspace that models how the solution is observed, as

$$W_m = \text{Span}(w_i, \dots, w_m) \subset V_h\,, \tag{2}$$

spanned by the unique Riesz representers of the functionals ℓ_i, $i = 1, \dots, m$, i.e., such that it holds $\ell_i(v) = \langle w_i, v \rangle$, for all $v \in V_h$ and for all $i = 1, \dots, m$. The space W_m is also called the *space of observations*.

We employ the physical model (1) to generate a *training set* $\mathcal{M}$, i.e., a manifold of solutions, by solving numerically (1) for different values of the biophysical parameters κ, E, ν, and $p_{\text{ventricles}}$ (CSF pressure at the ventricle boundary). The parameter ranges for the sampling can be chosen according to available literature, accounting automatically for parameter uncertainty. Moreover, including the pressure as parameter in the training set allows for considering different scenarios, such as distinguishing between healthy and increased pressure cases. As next, we compute an n-dimensional reduced-order subspace $V_n \subset V_h$ that approximates sufficiently well the training set $\mathcal{M}$ and whose dimension is much lower than the original ambient space (typically $n = O(10)$, while $\dim V_h = O(10^5)$). The space V_n encodes the physics of the model within the relevant parameter range, as it is spanned by solutions of system (1).

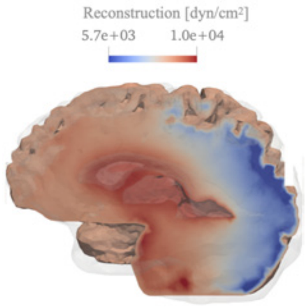

Fig. 2: *Snapshot (cross section) of the reconstructed pressure field p^*, obtained solving (3)*

The considered state reconstruction problem reads: For a given set of observations $\hat{\lambda} \in \mathbb{R}^m$, find a state $v^* = (\mathbf{u}^*, p^*) \in V_h$, with

$$v^* = \operatorname{arginf}_{v \in V_h} \left\| v - \Pi_{V_n} v \right\|^2, \text{ with } \langle w_i, v \rangle = \hat{\lambda}_i,\ i = 1, \dots, m\,. \tag{3}$$

(Π_{V_n} stands for the orthogonal projection on V_n). Namely, we look for a solution in the whole space V_h that minimizes the distance from the V_n, i.e., $\left\| v - \Pi_{V_n} v \right\|$, but fits the available measurements.

Problem (3) can be formulated as a saddle-point problem of dimension $n+m$, whose well-posedness is ensured if $n \leq m$ and if the following condition is satisfied. The quantity $\beta(V_n, W_m)$ can be estimated numerically solving a singular value problem, and it can be seen as the *angle* between the reduced-order space V_n and the space of the observations W_m, and it quantifies the observability of the state with respect to the considered observation space.

$$\beta(V_n, W_m) := \inf_{v \in V_n} \frac{\left\| \Pi_{W_m} v \right\|}{\|v\|} > 0\,. \tag{4}$$

Figure 2 shows an example of the reconstructed pressure using partial displacement measurements, while Figure 3 shows the application for pressure increase characterization. Namely, the pressure difference between ventricle and outer CSF for reconstructed pressure p^* is used to assess whether it refers to a normal or to an increased pressure case. The algorithm is validated using synthetic measurements, comparing the classification to the one obtained using the true pressure field, showing that it is able to separate correctly the two regimes.

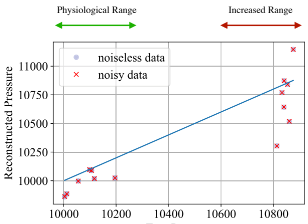

Fig. 3: *Characterization of normal and increased ventricle pressure, comparing the reconstructed and the synthetic true solutions*

Estimation of tissue parameters from inversion recovery MRI

Biological tissues are characterized by complex structures, whose dynamics reflects the interaction of fluid and solid compartments at very small spatial scales. Understanding this microscale properties is therefore of utmost importance in order to characterize mechanical and constitutive parameters that are used in tissue mechanical models at larger scales (e.g., the poroelastic models used in the previous section). Inversion recovery MRI (IRMRI) is an image acquisition technique that allows to obtain a time-dependent image intensity, sensitive to the presence of fluid in the tissue. This section focuses on mathematical methods to obtain improved tissue property estimation from brain IRMRI data, taking into account the inherent noise present in the images.

We consider a two-compartment model with a fluid and a solid phase. For each phase, the noise-free MR signal ξ depends on the time at which the sequence is acquired (the *inversion time*) and on the longitudinal relaxation rate $R_1 = 1/T_1$ (the reciprocal of the longitudinal relaxation time T_1) of the tissue within a voxel. In this simple model, the combined noise-free MR signal ξ can be described by a mixture model [3]

$$\xi(TI; f, I^f, R_1^f, I^s, R_1^s) = \Big| \underbrace{f I^f \left(1 - 2\mathrm{e}^{-TI \cdot R_1^f}\right)}_{\text{fluid contribution}} + \underbrace{(1-f) I^s \left(1 - 2\mathrm{e}^{-TI \cdot R_1^s}\right)}_{\text{solid contribution}} \Big|, \tag{5}$$

as a function of the inversion time TI, of the partial voxel volume containing the fluid phase f, and the parameters for the base signal intensity (I^f, I^s for fluid and solid, respectively) and the longitudinal relaxation rate in the fluid and solid phases (R_1^f and R_1^s, respectively). We distinguish between two main types of brain solid tissue, i.e., white and grey matter (WM and GM), while the fluid phase is constituted by the cerebrospinal fluid (CSF). The parameters related to the solid phase depend on the type of tissue (WM or GM). Furthermore, within the CSF, f is considered to be 1.

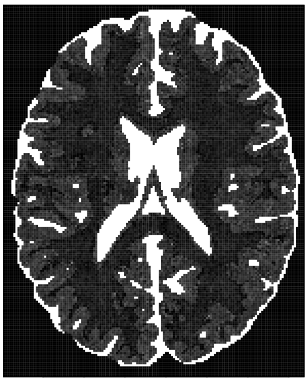

Fig. 4: *Results for smoothed estimated compartment parameter f for simulated data*

Parameter estimation of $\theta = (f, I^f, R_1^f, I^s, R_1^s)$ from available data is done by a quasi-likelihood estimation method. To this purpose, let $I(TI)$ denote the distribution of the MRI signal magnitude, and let σ denote the standard deviation of the noise. The rescaled magnitude $I(TI)/\sigma$ is assumed to be approximately χ-distributed with the non-centrality parameter ξ/σ and $2L'$ degrees of freedom. Estimates $\hat{\theta}$ can be obtained in each voxel relating the observed magnitude intensities $I(TI)$ with their expectations $\mu(\xi)$ by solving the optimization problem

$$\hat{\theta} = \arg\min_{\theta} \sum_{i} [I(TI_i) - \mu(\xi(TI_i, \sigma, L'; \theta)]^2 , \tag{6}$$

where $\mu(\xi) = \sigma\sqrt{\frac{\pi}{2}} L_{1/2}^{(L'-1)}\left(-\frac{\xi^2}{2\sigma^2}\right)$ is the expected value of signal distribution, and $L_{1/2}^{(L'-1)}$ is a generalized Laguerre polynomial. The analysis pipeline consists in the following steps (see Figure 4). Firstly, we segment the imaged brain tissue into the common three segments CSF, WM, and GM. Secondly, we estimate the parameters $\tilde{I}^f$ and $\tilde{R}_1^f$ for each voxel x within the CSF (using $f = 1$). Thirdly, we estimate $f(x)$, $I^s(x)$, and $R_1^s(x)$ in each voxel x of the GM and WM segments using model (5) and the parameters $\tilde{I}^f$ and $\tilde{R}_1^f$ from the previous step. Then, we perform local (adaptive) smoothing of $\tilde{I}(x)$ and $\tilde{R}_1(x)$ restricted to WM and GM (separately), to obtain estimates $\tilde{I}^s(x)$ and $\tilde{R}_1^s(x)$ with a reduced variance. Finally, the mixture parameter $f(x)$ of the model (5) is estimated again using the newly computed estimates $\tilde{I}^f$, $\tilde{R}_1^f$, $\tilde{I}^s(x)$, and $\tilde{R}_1^s(x)$.

Biomarkers estimation in blood flow

Aortic coarctation denotes a congenital heart condition characterized by the narrowing of a section of the aorta. The severity of the coarctation can be assessed using invasive measurement of the pressure gradient across the narrowed region. Non-invasive diagnosis based on medical imaging mainly consists in estimating the diameter of the narrowed area from anatomical data and the aortic pressure gradient from velocity images, e.g., acquired via cardiac MRI or ultrasound echocardiography. Other relevant biomarkers are related to abnormal flow conditions, such as increased flow asymmetries, and abnormal oscillatory behaviors of the wall shear stresses (WSS). Due to the limited resolution of image data, these quantities can only be quantified directly from medical imaging with reduced accuracy.

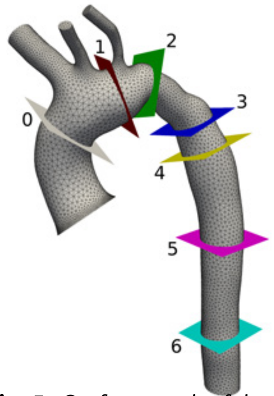

Fig. 5: *Surface mesh of the segment of aorta considered for the simulation. The cross sections were used to monitor averaged flow indicators.*

Computational hemodynamics plays an important role in supporting available medical data by performing patient specific simulations tuned to the particular physiological setting, which allows to obtain quantitative biomarkers estimations using anatomical images and flow data. The blood flow regime in the ascending aorta and the disturbances caused by aortic narrowing can yield to a transition to turbulence, which has to be properly taken into account in the computational model. The smallest scales of the turbulent dynamics cannot be neglected, for reasons of physical accuracy of the results, but full-scale numerical simulations of the whole scale spectrum are prohibitive. These challenges are addressed via *turbulence modeling*, i.e., with mathematical and numerical techniques to model the impact of the unresolved (small) scales onto the (large) resolved ones, so that important properties of the flow are preserved. The goal of this research is to study the impact of different turbulence modeling choices on selected quantities of interests, which are clinically relevant for the assessment of flow conditions in aortic coarctation [4].

Let $\Omega \subset \mathbb{R}^3$ denote a computational model of ascending and thoracic aorta, which can be obtained from medical images. The domain is bounded by the physical vessel wall Γ_{wall}, an inlet surface Γ_{in} – close to the left ventricle – and four outlet surfaces $\Gamma_{\text{out},i}$, $i = 1, 2, 3, 4$ (brachiocephalic, left common carotid, and left subclavian arteries, and downstream descending aorta), see Figure 5. The blood flow in Ω is modeled as an incompressible, Newtonian fluid, whose dynamics is described in terms of a velocity field $\mathbf{u} : \Omega \to \mathbb{R}^3$ and a pressure field $p : \Omega \to \mathbb{R}$ satisfying, in a given time interval $(0, T]$, the incompressible Navier–Stokes equations

$$\begin{aligned} \rho\partial_t\mathbf{u} - 2\mu\nabla\cdot\mathbb{D}(\mathbf{u}) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{0} \quad \text{in } (0,T]\times\Omega, \\ \nabla\cdot\mathbf{u} &= 0 \quad \text{in } (0,T]\times\Omega. \end{aligned} \tag{7}$$

In (7), ρ stands for the blood density, μ is the blood dynamic viscosity, and $\mathbb{D}(\mathbf{u}) = \big(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\big)/2$ denotes the velocity deformation tensor (i.e., the symmetric part of the velocity gradient). Boundary conditions for equations (7) are imposed using a measured inlet velocity profile on Γ_{in} and a resistive Neumann-type boundary condition on the outlet boundaries, of the form

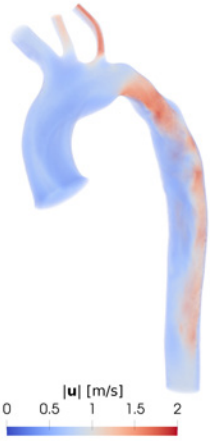

Fig. 6: *Snapshot of the numerical solution (velocity magnitude) at a selected instant, for the σ -turbulence model*

$$P_i(t) = R_i \int_{\Gamma_{\text{out},i}} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}\mu_{\Gamma_{\text{out},i}}, \; i = 1,\dots,4\,, \tag{8}$$

where $\mathbf{n}$ stands for the outgoing normal vector. Equation (8) relates the boundary pressures to the outgoing fluxes via resistance parameters $R_1, \dots R_4$, which model the resistance of the downstream circulation. The R_i are estimated to match observed systolic flow rates through each outlet.

Equations (7) and the boundary conditions are discretized using finite element spaces $\mathbf{V}_h$ and Q_h for velocity and pressure, introducing the variational form

$$\begin{aligned} A\left((\mathbf{u}_h, p_h), (\mathbf{v}_h, q_h)\right) :=& 2\nu\left(\mathbb{D}(\mathbf{u}_h), \mathbb{D}(\mathbf{v}_h)\right) + \left((\mathbf{u}_h\cdot\nabla)\mathbf{u}_h, \mathbf{v}_h\right) \\ & - (\nabla\cdot\mathbf{v}_h, p_h) + (\nabla\cdot\mathbf{u}_h, q_h) - f(\mathbf{u}_h, \mathbf{v}_h) \end{aligned} \tag{9}$$

(where $f(\mathbf{u}_h, \mathbf{v}_h)$ contains the outflow boundary condition terms), and solving the problem: Find $(\mathbf{u}_h, p_h) : [0, T] \to \mathbf{V}_h \times Q_h$, satisfying the initial and the boundary conditions, such that

$$(\partial_t\mathbf{u}_h, \mathbf{v}_h) = -A\left((\mathbf{u}_h, p_h), (\mathbf{v}_h, q_h)\right), \text{ for all } t \in (0, T) \text{ and for all } (\mathbf{v}_h, q_h) \in \mathbf{V}_h \times Q_h. \tag{10}$$

We consider then two types of turbulence models. The first class are *Large Eddy Simulation* (LES) methods, such as the original Smagorinsky model, the Vreman model, and the more recent σ -model. These attempt to model the large turbulent scales surrogating the effect of the small scales into explicit models for the stress tensor. In this case, the bilinear form (9) is modified as

$$\hat{A}_\theta\left((\mathbf{u}_h, p_h), (\mathbf{v}_h, q_h)\right) = A\left((\mathbf{u}_h, p_h), (\mathbf{v}_h, q_h)\right) + \left(\nu_t\,\mathbb{D}(\mathbf{u}_h), \mathbb{D}(\mathbf{v}_h)\right)\,, \tag{11}$$

where ν_t denotes the *eddy viscosity*, i.e., additional modeled dissipation due to the smallest, not resolved, scales, and θ stands for a set of model parameters to be properly chosen. A different approach is the *residual-based variational multiscale method* (RB-VMS), which is based on a two-scale decomposition of the analytic function spaces for velocity and pressure, surrogating the influence of the small scales into additional terms in the finite element formulation. For the RB-VMS, the bilinear form (9) is modified taking into account the momentum residue of the coarse scale solution.

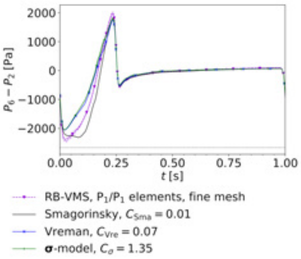

Fig. 7: *Pressure difference across the narrowing for different models, compared with critical value used in clinical assessment (dashed)*

Figure 6 shows a snapshot of the simulated blood flow for the σ -model. Depending on the considered biomarkers, the obtained results for different turbulence models are either quite similar (see Figure 7) or they are notably different. In summary, our results confirm that modeling and discretization choices have an important impact on the time-dependent dynamics. An extension of this study to several non-Newtonian blood flow models can be found in [5].

Conclusions and outlook

In medical imaging, data quality and information density are closely linked. Increasing spatial resolution, for example, requires longer acquisition times, which in turn can lead to inaccuracies arising from intrinsic organ and patient motion. At WIAS, this research area is based on joint research activities across different research groups as well as with interdisciplinary collaborations with clinical and experimental partners, ensuring that the lines of research tackle relevant challenges, both from the mathematical and from the clinical perspectives.

This article showed few examples on how biophysics-based data assimilation approaches can compensate for the limited availability of data by combining the available data with advanced mathematical models, numerical methods, and efficient algorithms. In the first example, reduced-order modeling and linear poroelasticity were used to reconstruct a full solution of an unknown pressure field using limited displacement data. The second example showed how statistical image intensity models can be used to exploit the influence of tissue properties, such as porosity, on tissue image intensity. The last example focused on the impact of different choices for turbulence modeling in the context of patient-specific modeling of aortic coarctation. Future directions will explore how these approaches can be used not only to enhance the physical consistency and clinical relevance of imaging data, but also to support long-term prediction in conjunction with follow-up imaging examination.

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1.3 RKHS Regularization of Singular Local Stochastic Volatility McKean–Vlasov Models

Christan Bayer, Oleg Butkovsky, and John Schoenmakers

Introduction

In financial markets, including stock and energy markets, options on future prices of stocks, interest rates, and different kinds of energy are very popular and intensively traded. In this note, we focus on call or put options in stock markets. Suppose S_t is the price of a stock at time $t \geq 0$. The dynamics of S is generally considered as a random process that satisfies so-called *no-arbitrage conditions*. Then, for example, a standard call option with strike price K and maturity time T is the option to receive $S_T - K$ if $S_T \geq K$, and 0, or nothing, if $S_T < K$. By standard financial theory, the value of the option at time $t = 0$, i.e., today, equals

$$C(T, K) = \mathbb{E}\left[\max\left(S_T - K, 0\right)\right], \quad T \geq 0, \quad K \geq 0, \tag{1}$$

under the simplifying assumption that interest rates are zero.

The call prices $C(T, K)$ are quoted for various T and K on the stock market. We here assume the idealized situation where $C(T, K)$ is available for all $0 \leq T \leq T_{\max}$ and all $K \geq 0$. Now, the crucial problem, also called *the calibration problem*, is to find a suitable model for S such that (1) holds, at least approximately but with high accuracy, for all $0 \leq T \leq T_{\max}$ and all $0 \leq K \leq K_{\max}$. One of the most striking results of the late nineties in finance was that (1) can be achieved exactly with a so-called *local volatility model*,

$$dS_t = S_t \sigma_{\text{Dupire}}\left(t, S_t\right) dW_t \tag{2}$$

with W being a standard Brownian motion, provided that the function $(T, K) \to C(T, K)$ is sufficiently smooth. In particular, σ_{Dupire} in (2) is given by *Dupire's formula,*

$$\sigma_{\text{Dupire}}(T, K) = \frac{1}{K}\sqrt{\frac{2\partial_T C(T, K)}{\partial_{KK} C(T, K)}}.$$

Unfortunately, while Dupire's model (2) is a model that solves (1), i.e., perfectly fits to market prices of call options, it is well understood that it exhibits unrealistic random price behavior. On the other hand, *stochastic volatility models*

$$dS_t = S_t \sqrt{v_t} dW_t,$$

for a suitably chosen stochastic variance process v_t, may lead to realistic (in particular, time-homogeneous) dynamics, but are typically difficult or impossible to calibrate to the observed market prices (1).

As a natural way out, one may combine a local volatility model with a stochastic volatility model to a *local stochastic volatility model* that combines the advantages of both local and stochastic volatility models. Indeed, if the stock price is given by

$$dS_t = S_t \sigma(t, S_t) \sqrt{v_t} dW_t, \tag{3}$$

then it exactly fits the observed market option prices via (1), provided that

$$\sigma_{\text{Dupire}}(t, x)^2 = \sigma(t, x)^2 \mathbb{E}[v_t \mid S_t = x]. \tag{4}$$

This is a consequence of the celebrated Markovian projection theorem by Gyöngy [4, Theorem 4.6]. By solving for σ in (4) and inserting the result in (3), we get the stochastic dynamics

$$dS_t = S_t \sigma_{\text{Dupire}}(t, S_t) \sqrt{\frac{v_t}{\mathbb{E}[v_t \mid S_t]}} dW_t. \tag{5}$$

As recognized by Guyon and Henry-Labordère [3], in principle, the stock price dynamics (5) is the solution of a *McKean-Vlasov Stochastic Differential Equation* (MVSDE) due to the presence of the conditional expectation $\mathbb{E}[v_t \mid S_t]$, which can be regarded as a complicated functional of the joint distribution of (S_t, v_t). MVSDEs are usually solved by Monte Carlo simulation of a particle system, and so was done in [3]. In a nutshell, in [3], one simulates, for $i = 1, \ldots, N,$ the "particles,"

$$dS_t^i = S_t^i \sigma_{\text{Dupire}}(t, S_t^i) \sqrt{\frac{v_t^i}{\frac{\sum_{j=1}^N v_t^j \phi_\delta(S_t^j - S_t^i)}{\sum_{j=1}^N \phi_\delta(S_t^j - S_t^i)}}} dW_t^i, \quad i = 1, \ldots, N, \tag{6}$$

where ϕ_δ is some "delta-shaped" density function with band width $\delta > 0.$ For example, $\phi_\delta(x) = \delta^{-1}\phi(x/\delta),$ where ϕ is the standard normal density. The conditional expectation in the MVSDE (5) is thus approximated by the blue expression in the particle system (6), a kind of weighted Nadaraya-Watson estimator, for some small (but not too small) δ.

Although the approach in [3] was well received in the financial community, there are two main issues:

(I) The MVSDE (5) is singular in the sense that it does not satisfy the standard regularity conditions in [2] that guarantee a unique solution. In particular, the general existence of a solution to (5) is still an open question.

(II) The choice of the band width in (6) is very delicate and, generally, the simulation of (6) is rather costly. A more efficient numerical approach is called for.

Both issues were addressed in our recent study [1], and below we will sketch the main lines.

Regularizing the MVSDE

In the MVSDE (5), the conditional expectation

$$m(x, \mu) := \mathbb{E}_{(S,v)\sim\mu}[v \mid S = x], \qquad x > 0, \tag{7}$$

is not Lipschitz continuous with respect to μ in the Wasserstein metric, and therefore the existence of a solution to (5) is not guaranteed by the usual conditions in [2]. As a remedy, we regularize (7) in the framework of a *reproducing kernel Hilbert space* (RKHS).

Let $\mathcal{H}$ be an $RKHS$ of functions on $\mathbb{R}_+$ (state space of the stock price model) that is generated by a positive definite symmetric kernel $k(\cdot,\cdot)$ on $\mathbb{R}_+ \times \mathbb{R}_+$. Assuming that $m(\cdot,\mu) \in \mathcal{H}$ for fixed μ, we may formally write

$$\begin{aligned} c^{\mu}(\cdot) &:= \int_{\mathbb{R}_+ \times \mathbb{R}_+} k(\cdot, x) y \mu(dx, dy) \\ &= \int_{\mathbb{R}_+} k(\cdot, x) \mu(dx, \mathbb{R}_+) \int_{\mathbb{R}_+} y \mu(dy|x) \\ &= \int_{\mathbb{R}_+} m(x, \mu) k(\cdot, x) \mu(dx, \mathbb{R}_+) =: \mathcal{C}^{\mu} m(\cdot, \mu). \end{aligned}$$

That is, formally, $m(\cdot,\mu) = \left(\mathcal{C}^{\mu}\right)^{-1} c^{\mu}$. Unfortunately, the symmetric operator $\mathcal{C}^{\mu}$ is generally not invertible. As $\mathcal{C}^{\mu}$ is positive definite, it is, however, possible to *regularize* the inversion by replacing $\mathcal{C}^{\mu}$ by the invertible operator $\mathcal{C}^{\mu} + \lambda I_{\mathcal{H}}$ for (small) $\lambda > 0$. Furthermore, it turns out that

$$m^{\lambda}(\cdot, \mu) := \left(\mathcal{C}^{\mu} + \lambda I_{\mathcal{H}}\right)^{-1} c^{\mu} \tag{8}$$

is the solution to the minimization problem

$$m^{\lambda}(\cdot, \mu) = \operatorname*{arg\,min}_{f \in \mathcal{H}} \left(\mathbb{E}_{(S,v)\sim\mu} \left[(v - f(S))^2 \right] + \lambda \, \| f \|_{\mathcal{H}}^2 \right),$$

and therefore, since conditional expectation is an L_2 projection in fact, it is natural to expect that if λ is small enough and $\mathcal{H}$ is large enough, then $m^{\lambda}(\cdot,\mu)$ will be close to the true conditional expectation $m(\cdot,\mu)$.

Significantly, we were able to prove in [1] that the MVSDE, obtained by replacing in (5) the conditional expectation with its regularized version (8),

$$dS_t = S_t \sigma_{\mathrm{Dupire}}(t, S_t) \sqrt{\frac{v_t}{m^{\lambda}(S_t, \mu_t)}} dW_t, \qquad \text{where} \qquad (S_t, v_t) \sim \mu_t, \tag{9}$$

is well posed in the sense of [2], and thus has a unique strong solution.

Particle system with ridge regression

In comparison to (6), the particle system corresponding to (9) now reads

$$\begin{aligned} dS_t^i &= S_t^i \sigma_{\mathrm{Dupire}}(t, S_t^i) \sqrt{\frac{v_t^i}{m^{\lambda}(S_t^i, \mu_t^N)}} dW_t^i, \quad i = 1, \dots, N, \\ \mu_t^N(dx, dy) &= \frac{1}{N} \sum_{j=1}^{N} \delta_{S_t^j}(dx) \delta_{v_t^j}(dy), \end{aligned} \tag{10}$$

where for any Borel measurable C, $\delta_x(C) := 1_C(x)$, i.e. δ_x denotes the Dirac measure at point x. In (10),

$$m^{\lambda}(\cdot, \mu_t^N) = \operatorname*{arg\,min}_{f \in \mathcal{H}} \left(\frac{1}{N} \sum_{j=1}^{N} \left(v_t^j - f(S_t^j) \right)^2 + \lambda \, \| f \|_{\mathcal{H}}^2 \right) \tag{11}$$

is computed via a ridge regression procedure. It follows from the representer theorem for RKHS [5, Theorem 1] that the solution to (11) has a representation

$$m^\lambda(\cdot, \mu_t^N) = \sum_{i=1}^{N} \alpha_i k(\cdot, S_t^i), \tag{12}$$

for some $\alpha_i \in \mathbb{R}$, $i = 1, \dots, N$, which can be found by plugging the ansatz 12 into the minimization problem 11.

Numerical example

For any numerical implementation of the approach suggested above, the regularized MV problem (10) together with (11) needs to be discretized in time, for which we use a straight-forward Euler–Maruyama method. In this short note, we do not further consider time discretization, since no phenomena specific to our approximation method seem to occur.

A more important practical concern directly related to (12) is the high cost of solving the minimization problem (11): As the ansatz corresponds to a regression problem with N basis functions and N samples, the expected asymptotic cost is $O(N^2)$, which is prohibitively expensive given that the number of samples may be very large. Hence, instead of using all basis functions $k(\cdot, S_t^i)$, $i = 1, \dots, N$, we pick a representative ensemble $k(\cdot, Z_t^j)$, $j = 1, \dots, L \ll N$. The *representative samples* Z_t^j can be chosen in many different ways, for instance, as the jL/N th order statistic of $(S_t^i)_{i=1}^N$ or even as points on a deterministic grid.

In order to test our method, we chose a synthetic, but nonetheless realistic calibration problem. In order to obtain realistic option prices, we fix a particular stochastic volatility model as a "ground-truth model," in which option prices are computed. In the second step, we choose a different stochastic volatility model as our "backbone model," which needs to be calibrated to the option prices computed in the first step by adding a suitable local volatility factor.

In practice, both our ground-truth model and our backbone model are instances of the popular *Heston model*, i.e.,

$$\begin{aligned} dS_t &= \sqrt{v_t} S_t dW_t, \\ dv_t &= \kappa(\theta - v_t)dt + \xi\sqrt{v_t} dB_t, \end{aligned}$$

driven by standard Brownian motions W, B with correlation ρ. However, different sets of parameters are chosen for the models. The concrete parameter choices are reported in Table 1.

	κ	θ	ξ	ρ	v_0
market	2.19	0.17023	1.04	−0.83	0.0045
backbone	1.0	0.0144	0.5751	−0.9	0.0144

Table 1: *Parameter choices for the Heston models (market) used for generating option prices and the backbone model to be calibrated. Both sets of parameters are realistic in the sense that they are reported in the literature as calibrated Heston parameters.*

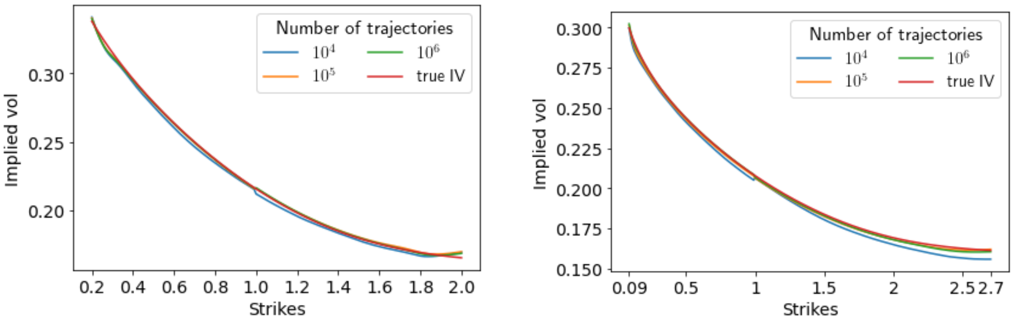

Fig. 1: *Implied volatilities for the calibrated Heston model for maturities $T = 4$ years (left) and $T = 10$ years (right)*

We consider the RKHS associated with the Gaussian kernel $k(x, y) := \exp(-|x-y|^2/(2\sigma^2))$ with $\sigma^2 = 5$. The representative samples Z_t^j are chosen as the $\frac{j \cdot 100}{L+1}$ percentiles of the empirical distribution of the samples $(S_t^i)_{i=1}^N$ based on the total number of samples $N \in \{10^4, 10^5, 10^6\}$. The weight λ for the ridge regression is chosen to be $\lambda = 10^{-5}$. In order to further mollify the singularity in (10), we truncate the denominator at $\varepsilon = 10^{-3}$, i.e., we choose

$$dS_t^i = S_t^i \sigma_{\text{Dupire}}(t, S_t^i) \frac{\sqrt{v_t^i}}{\sqrt{m^\lambda(S_t^i, \mu_t^N) \vee \varepsilon}} dW_t^i.$$

We plot implied volatility surfaces at different maturities for the calibrated Heston model by the described procedure in Figure 1. We note that the calibration is essentially exact for $N \geq 10^5$ samples.

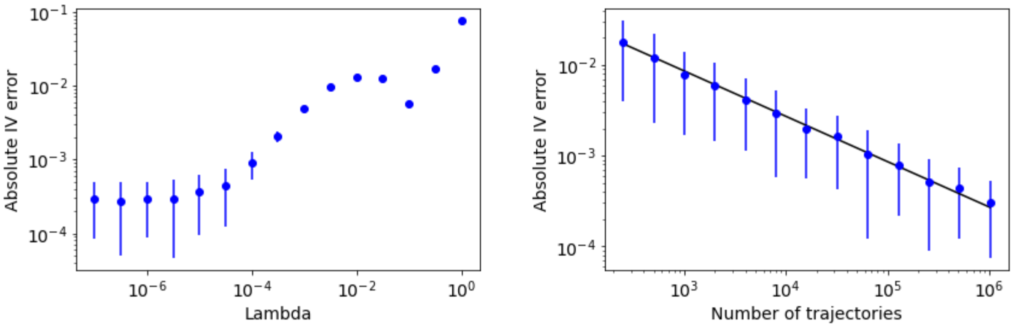

Fig. 2: *Error of the implied volatility smile for the calibrated Heston model as a function of λ (left) and as a function of the number of samples N (right)*

Figure 2 shows the dependence of the error in the calibrated Heston model (i.e., difference between the prices in the ground-truth model and the model (10)) in terms of the weight parameter λ in the ridge regression and the number of samples N. For the former, we note that the choice of λ is not important as long as it is small enough, which might indicate that the problem is actually more robust than suggested by the theoretical analysis. On the other hand, the results converge with rate $1/2$ in terms of N, faster than rate $1/4$ obtained in the error analysis.

Conclusions and outlook

We suggest a novel RKHS-based regularization method for the problem of calibrating local stochastic volatility models and prove that this regularization guarantees well-posedness of the underlying MVSDE. Our numerical results suggest that the proposed approach is quite efficient for the calibration of various local stochastic volatility models and can outperform widely used local kernel methods as in [3]. Nonetheless, it remains unclear whether the regularized MVSDE remains well posed when the regularization parameter λ tends to zero. This limiting case needs a subsequent study. Another important issue for future research is the choice of the RKHS kernel that ideally should be adapted to the problem at hand.

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1.4 How do Ants Form Trails?

Robert I.A. Patterson

In a joint project with Felix Höfling and Zahra Mokhtari from the Freie Universität Berlin work has been taking place at WIAS to identify simple mathematical models that explain how active particles or agents can interact with each other to form large-scale structures and patterns. In particular, we are studying models that are appropriate on the time and space scales of insects such as ants and where agents interact with each other by depositing chemical messages that can be detected by all agents that pass by in a short period of time. Our initial results suggest that these simple models explain the formation of large-scale trails in a way analogous to phase transitions known in physics.

Fig. 1: *Ant. Photo by Sian Cooper on Unsplash.*

Mathematical insights into collaborative behavior

Ants are well known for their ability for act collectively in order to obtain supplies by forming trails to enable large numbers of ants to visit a food source in close succession with each ant then carrying some of the food back to the colony. This is all achieved without any real-time command and control or long-range communication; however, various species of ants are known to deposit chemical markers, known as *pheromones*, as they move around. At this point, we note that there are many species of ants showing a wide range of behaviors; however, the trail-forming collective behavior seems especially relevant for mathematical study, because it is a good example of distributed self-organization. Studying it serves two purposes: Firstly, to gain mathematical insights into how individuals like ants can collaborate on an equal footing and how external actors might be able to influence the results of such collaborations, and secondly, to develop mathematical methods for studying collaborative motion that arises in other settings.

Key challenges

It is clear that ants and other kinds of agents or active particles do not always move along large-scale trails, but sometimes move in irregular, apparently random ways, for example, when searching for new sources of food. Any useful mathematical model of collective behavior will therefore have to incorporate both uncoordinated idiosyncratic motion and large-scale collaborative trails. Mathematical models that exhibit qualitatively distinct properties depending on the exact values of their parameters are said to have “phase transitions.” This means that the goal of the ongoing work is to find a mathematical model that is reasonable given the known physical properties of ants, in particular, their ability to deposit pheromones, and that shows at least one phase transition between disordered motion and trail-based motion. From a mathematical perspective, this topic is closely related to the work of the RG 5 on phase transitions and particle models in physics.

One strand of existing knowledge deals with the Patlak–Keller–Segel equations [1] and applies primarily to physical settings such as micro-swimmers in a fluid, where the pheromones can diffuse quite rapidly, and is not immediately relevant for applications such as ant behavior where pheromone diffusion is expected to be minimal on the time scale of the motion. The Patlak–Keller–Segel equations describe a system of organisms that tend to move towards higher concentrations of a pheromone they produce themselves. Such a model can lead to a phase transition where the organizing effect of the pheromone gradient leads to a large proportion of all the organisms gathering together in a small area despite random dispersive influences; however, it does not seem rich enough to generate collective motion along a "trail," for this one requires a more sophisticated model. A major innovation in the work currently taking place at WIAS and the Freie Universität (FU) Berlin is the use of vector pheromones, that is to say, pheromones that are deposited in a way that gives information about the direction of travel of the ant as it deposited the pheromone.

Pheromones with direction

As an initial model, we assume that each agent (ant) deposits one pheromone every τ_d seconds and that each pheromone evaporates after τ_p seconds. Each pheromone has an orientation that is the same as the direction of motion of the ant as it deposits the pheromone and does not change until it evaporates. The environment of a single ant can be thought of as shown in Figure 2.

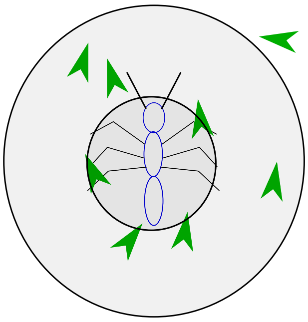

Fig. 2: *Inner disc of radius R_0 represents the ant, the large disc is the sensing radius, and the directed pheromones are shown in green*

In our model, every ant is treated as a disc of radius R_0 that moves with a constant speed v_0. However, the direction of each ant undergoes diffusion (small random perturbations) on the unit circle with a bias towards aligning with the average orientation of all the pheromones within a sensing radius. After choosing parameters to approximately represent the known physiological properties of the ant *Lasius niger* [2], two important degrees of freedom remain. The first is the ratio of the alignment strength to the orientational diffusion, which we denote s. The second is the concentration of ants or, equivalently, pheromones, which we quantify via the average number of pheromones in the sensing disc of a single ant N_p. Increasing either (or both) of these parameters increases the tendency of nearby ants to move in a common direction.

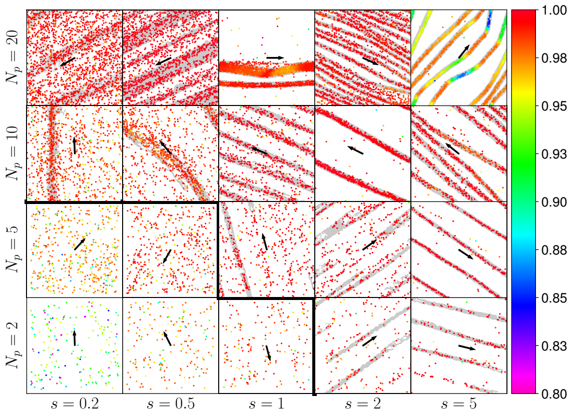

Fig. 3: *Ant positions color-coded by degree of alignment with the global average (black arrow)*

Computer simulations reported in Figure 3 show that this model is capable of capturing both uncoordinated motion (when s and N_p are both small in the bottom left of the figure) and the formation of trails (towards the top and right of the figure where at least one of s and N_p are large). The thick black line in Figure 3 separates the plots with smaller s and MN_p values where there is a drift in a common direction, but no detectable concentration of ants on a trail from the plots where it was possible to identify long trails. The exact position of the thick black line is to some extent a subjective decision, and a more quantitative approach to detecting regimes of trail formation is discussed below; however, the possibility of drawing such a line motivates a more precise mathematical search for a phase transition.

The model introduced above is also capable of reproducing a completely different type of collective behavior, which has long been observed in army ants namely the *ant mill* [5]. In an ant mill, a large rotating disc of ants is formed; this requires a high density of ants in order to produce a very strong pheromone signal and a strong response to the pheromones on the part of the ants, that is, both parameters N_p and s must be relatively large. We were able to observe this phenomenon with $N_p \approx 30$ and $s = 10$ as is shown in Figure 4, where one sees a mill and a mildly undulating trail, which at a later time (not shown) was even absorbed into the mill.

From these initial results, we are able to conclude that our model is capable of reproducing some important and significant features of the collective behavior of ants. They show that changing the parameter values leads to qualitative changes in the collective behavior; it is less clear whether the changes are continuous or abrupt in nature.

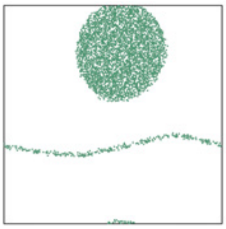

Fig. 4: *Ant positions are shown as green dots on a square domain with periodic boundary conditions*

Quantifying changes in collective behavior

In this section, we concentrate on distinguishing between the uncoordinated motion shown in the bottom left of Figure 3 and the trails visible in the panels towards the top and right of the same figure. The formation of mills as in Figure 4 is neglected as this occurs in a more extreme parameter regime.

Practically, we define a trail to be a region of continuously high pheromone density that extends from one side of the domain to the other. We then consider the ratio

$$p_\infty = \frac{\text{number of pheromones in trails}}{\text{total number of pheromones}},$$

which varies between 0 when there are no trails and 1 when all pheromones (and therefore all ants) are on trails. The value of p_∞ was then sampled repeatedly during simulations with different values of s in order to numerically estimate its probability distribution. The results are shown in Figure 5, which is consistent with Figure 3 in that for $s = 1$ it is rare to find many pheromones in trails (because even small trails are rare), whereas for $s = 10$ it is likely that a significant proportion of pheromones (and therefore ants) are concentrated on trails. The remainder of this highlight article concentrates on attempts to understand which parameter values lead to significant trail formation and which do not.

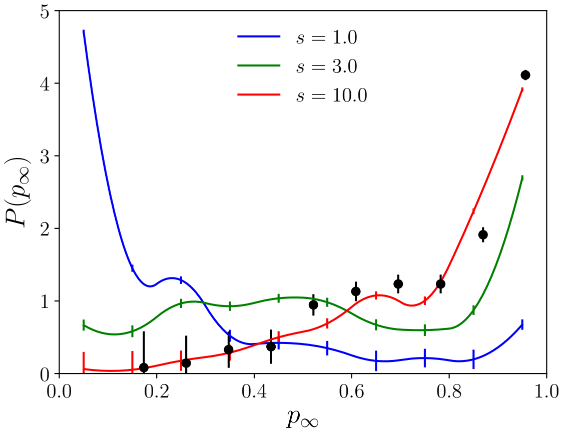

Fig. 5: *Probability distributions for p_∞ sampled with $N_p = 5$ and three different values of s. The black dots are an additional data set for $s = 10$ sampled using an even larger domain.*

The statistics in Figure 5 were derived from simulations carried out by Zahra Mokhtari at FU Berlin and required the development of a complex pipeline of tools to process the simulation results [4]. The image and data processing is not discussed further in this article for reasons of length, although it is an interesting topic in its own right. We note that the trails detected with these methods are shown in light grey in Figure 3.

Critical values for a reduced model

If one passes to the mean field limit on a fixed spatial domain $U \subset \mathbb{R}^2$, that is to say, one looks at the behavior of a very large number of agents leaving very weak pheromones (both scaling with the number of agents), one finds formally the following equations for the evolution in time t of the concentration of agents/ants α and pheromones ϕ on $U \times [0, 2\pi)$ representing position in the plane denoted r and orientation denoted θ:

$$\frac{\partial}{\partial t}\alpha + \nabla_r \cdot (v_\theta \alpha) = -\mu \frac{\partial}{\partial \theta}(\alpha\,(F * \phi)) + D_{\text{rot}} \frac{\partial^2}{\partial \theta^2}\alpha$$
$$\frac{\partial}{\partial t}\phi = -\frac{1}{\tau_p}\phi + \frac{1}{\tau_d}\alpha,$$

where v_θ is the unit vector in direction θ and $[0, 2\pi)$ is given periodic boundary conditions. The parameter μ measures the strength of the aligning force and D_{rot} the strength of the random fluctuations (rotational diffusion) of the ant orientations (the parameter s introduced above is μ/D_{rot}). The function $F = 2\pi \sin\theta$ is an interaction kernel, and $F * \phi$ is the convolution in the orientation variable θ with the pheromone field which gives the local force that the pheromones exert on the ants in order to align their direction with that of the pheromone field.

As an initial step towards identifying critical parameter values for changes in qualitative behavior, one can first consider what happens at a single point in space neglecting the advective part of the above equations. At a single point, the concentration of ants and that of pheromones depends only on their orientation, which is 2π-periodic, and so a Fourier decomposition is natural. The 0-th Fourier mode is simply the total concentration (of ants or pheromones), and the first Fourier mode gives a measure of the existence and prominence of a preferred direction (the direction itself would be given by the phase angle of the mode, which is not studied here). Higher Fourier modes provide a finer description of the distribution of orientations on the circle. Under some simplifying assumptions and extending the approach of [3] to include pheromones, one can derive the following equation for the first Fourier modes of α and ϕ with respect to the orientation variable θ, which are denoted α_1 and ϕ_1, respectively:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\alpha_1\\ \phi_1\end{pmatrix} = \begin{pmatrix}-D_{\mathrm{rot}} & \frac{\mu\alpha_0}{2}\\ \frac{1}{\tau_d} & \frac{-1}{\tau_p}\end{pmatrix}\begin{pmatrix}\alpha_1\\ \phi_1\end{pmatrix}.$$

The basic theory of ordinary differential equations shows that α_1 and ϕ_1 will become large (that is, strong alignment will develop) precisely when $\frac{\mu\alpha_0}{2} > D_{\mathrm{rot}}\frac{\tau_d}{\tau_p}$, a conclusion that is confirmed when the analysis is extended to include the second Fourier modes of α and ϕ.

Conclusions and outlook

The initial phases of this work have established a relatively simple model that qualitatively captures important aspects of the collective behavior of ants and that can be studied using techniques that build on methods extensively used at WIAS. In some simplified situations, we can show that the establishment of a coordinated direction depends critically on the initial concentration of agents (all other parameters held constant).

Along with the colleagues at the FU Berlin, we aim to find improved ways of detecting trail formation in the output of numerical simulations. More importantly, we are trying to find simplified situations where we can assess the stability of a trail and identify the critical parameter values. This means moving beyond the eigenvalue analysis described above, which omits the spatial element and just considers the ability to establish a preferred direction in a small region of space.

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1.5 Hydrogels Models for Soft Biomaterials

André H. Erhardt, Dirk Peschka, Leonie Schmeller, and Barbara Wagner

Hydrogels are a material system that is omnipresent in nature. They appear in innumerable biological processes, but also in many smart soft-matter materials as well as medical applications. Hydrogels have an intriguingly complex phase behavior, as they interact with their environment. Their understanding would, on the one hand, help to solve some fundamental problems in soft matter physics and, on the other hand, form the basis for new optimized designs for the use in tissue regeneration, biodegradable implants, articular cartilage repair and replacement, and many other biomaterials. The increased interest in these materials has led to a vast number of theoretical and experimental studies aiming at understanding the principles of their dynamic behavior and pattern formation, reviewed, for example, in Michael S. Dimitriyev et al., Nano Futures, **3**:4 (2019).

A major research focus at WIAS is the development of thermodynamically consistent models for complex materials. In this article, we showcase for hydrogels the journey from a novel abstract thermodynamic description, to nonlinear coupled systems that capture the various phase transitions in hydrogels, to agent models for cell motion in these materials. We highlight how the theoretical and numerical framework that we developed for hydrogels answers some of the fundamental problems regarding the interface formation between liquids and hydrogels, how to systematically extend the system to include electrostatic interactions and mechanical properties of biological gel such as elastic strain-stiffening, both properties being fundamental in biomaterials.

In the simplest case, hydrogels are two-phase systems composed of an elastic network of polymer chains immersed in a liquid solvent. The transport of solvent into and out of the network leads to the swelling and drying of the hydrogel, thereby introducing large deformations of the polymer network. Aside from swelling and deswelling with their large volume changes, hydrogels can exhibit a volume phase transition giving rise to coexisting regions with different degrees of swelling and, hence, different levels of elastic stresses. Such volume changes, in turn, may lead to deformation of the boundary in contact with the surrounding bath as well as a host of patterns within the hydrogel. Since the kinetics of swelling and deswelling can change significantly upon the formation of internal interfaces by phase transitions, full time-dependent models that implicitly capture these interfaces were derived in [1], where phase-field theories served as a natural framework for developing kinetic models of hydrogels by accounting for the relevant thermodynamics as well as providing implicit descriptions of the evolving interfaces that form upon phase separation. Based on these ideas, we have developed our numerical approach.

Variational structure-preserving numerical discretization

Beyond the continuum-mechanical description of fluids and solids, complex material behavior arises from nonlinear material laws, from multiple scales, or from the consideration of additional physics, e.g., material flow, diffusion, phase separation, damage, chemical reactions, charge and heat transport. The complex dynamics in the volume and at the surface of such materials can usually be described by scalar order parameters. For these physical theories, energetic variational principles are important mathematical structures that ensure the validity of the laws of thermodynamics.

One often considers gradient systems, i.e., triples $(\mathcal{Q}, \mathcal{F}, K)$, such that the trajectory in a state space $q : [0, T] \to \mathcal{Q}$ with free energy $\mathcal{F} : \mathcal{Q} \to \mathbb{R}$ is determined by the evolution law $\partial_t q = -K(q)\mathrm{D}\mathcal{F}(q)$ formulated using a positive geometric operator $K(q) : \mathcal{Q}^* \to \mathcal{Q}$. We propose an extension of this structure by $(\mathcal{Q}, \mathcal{F}, (M, A, \mathcal{U}, S))$ that generates a saddle-point problem, where we seek chemical potentials $\eta : [0, T] \to \mathcal{U}$ and states $q : [0, T] \to \mathcal{Q}$ such that

$$\begin{aligned} A(q)\eta + M(q)\partial_t q &= 0 \\ M(q)^*\eta - S(q)\partial_t q &= \mathrm{D}\mathcal{F}(q) \end{aligned} \qquad \text{in} \quad \mathcal{U}^* \times \mathcal{Q}^*,$$

where dissipative processes are encoded in separate spaces $\mathcal{Q}$, $\mathcal{U}$. Instead of a single K, one now uses two positive operators $A(q) : \mathcal{U} \to \mathcal{U}^*$ and $S(q) : \mathcal{Q} \to \mathcal{Q}^*$ that contain irreversible processes; see [3]. The spaces $\mathcal{Q}$ and $\mathcal{U}$ are connected by the representation $M(q) : \mathcal{Q} \to \mathcal{U}^*$. This formulation also implies energy decay and therefore thermodynamic consistency by construction

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}\big(q(t)\big) = -\langle A(q)\,\eta, \eta\rangle_{\mathcal{U}} - \langle S(q)\,\partial_t q, \partial_t q\rangle_{\mathcal{Q}} \le 0,$$

where $\langle\cdot,\cdot\rangle$ denotes the dual pairing. The thermodynamic consistency is essential for many complex, nonlinear coupled problems that couple mechanics, chemistry, and (inactive) biological materials. While from a formal point of view, this reformulation is equivalent to a formulation of gradient systems using quadratic dissipation potentials $R(q,\cdot) : \mathcal{Q} \to \mathbb{R} \cup \{\infty\}$, we observe several practical advantages. Firstly, the weak form of the saddle-point problem in $\mathcal{U}^* \times \mathcal{Q}^*$ allows for a direct reformulation using Galerkin methods. The decomposition into $(M, A, \mathcal{U}, S)$ allows for a finer control of the evolution systems where $R(q,\cdot)$ is singular so that $K(q)$ is not invertible, i.e., in the presence of multiple time scales or constraints in the evolution.

Various coupling mechanisms, further constraints and a variety of irreversible, but also reversible effects can be implemented by the appropriate choice of operators, functionals, and function spaces. By defining $A(q) = K(q) - J(q)$ with the symmetric Onsager operator K and the skew-symmetric Poisson operator J, damped Hamiltonian evolution can be incorporated. This connects the saddle-point structure to many recent and classical works on Hamiltonian and Onsager partial differential equation systems, e.g., fluid flows, fluid-structure interaction, nonlinear diffusion, and reactive transport [7], which are highly relevant for biological applications and complex multiphase materials. Now, we apply such a mathematical formulation to a hydrogel.

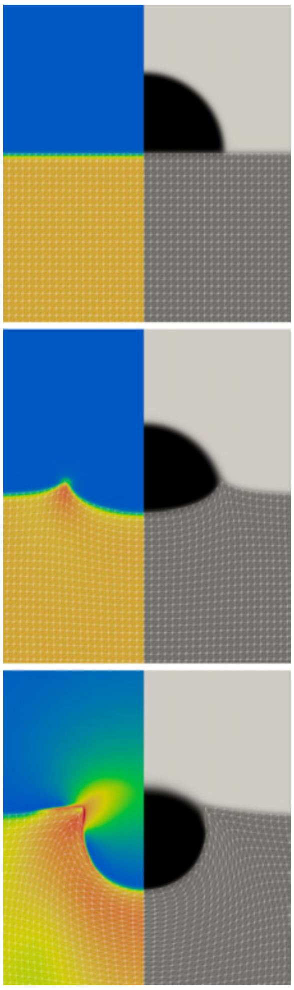

Fig. 1: *The evolution of a deforming liquid droplet on soft gel coupled to diffusion of polymer density c in the gel phase showing (left) the polymer density c and (right) a projection of the phase fields ψ_i with mesh (white)*

Some fundamental problems in soft matter physics

Within the DFG Priority Program SPP 2171 *Dynamic Wetting of Flexible, Adaptive and Switchable Surfaces* and in collaboration with experimental partners (Ralf Seemann, Experimental Physics, U Saarland), we investigated the formation, morphology, and dynamics of interfaces of liquid polymer droplets on hydrogel substrates by varying the softness (elastic modulus) of the hydrogel network.

Multiphase flow with nonlinear diffusion. Consider a multiphase flow of a liquid droplet on a hydrogel surrounded by an air phase with suitable boundary and interface conditions for a fluid-structure interaction problems with capillary surfaces. Additionally, we consider the diffusion of an concentration c inside the gel driven by entropic and mechanical forces. For any point in space $x \in \Omega \subset \mathbb{R}^d$ and time $t \in (0, T)$, the system can be modeled using phase fields $0 \leq \psi_i \leq 1$ and $\psi_i(t, x) = 1$ in the phase i and $\psi_i(t, x) = 0$ otherwise, where $i \in \{\mathrm{gel}, \mathrm{liquid}, \mathrm{air}\}$ and $\sum \psi_i = 1$. To model the additional diffusion, we introduce a polymer concentration c leading to $\boldsymbol{\psi} = (\psi_{\mathrm{gel}}, \psi_{\mathrm{liquid}}, \psi_{\mathrm{air}}, c) \in \mathbb{R}^4$. The mechanical deformation is described by $\boldsymbol{\chi}(t, x) \in \mathbb{R}^d$ for $d = 2, 3$. For $q = (\boldsymbol{\psi}, \boldsymbol{\chi})$, the free energy is composed of an elastic energy and a phase-field potential, i.e.,

$$\mathcal{F}(q) = \int_\Omega W_{\mathrm{elast}}(\boldsymbol{\psi}, \boldsymbol{F}) + W_{\mathrm{phase}}(\boldsymbol{\psi}, \boldsymbol{F}^{-T} \nabla \boldsymbol{\psi}) \,\mathrm{d}x\,,$$

with the deformation gradient $\boldsymbol{F} = \nabla \boldsymbol{\chi}$. The concentration c is characterized by the fact that it lowers the elastic modulus of the gel, and a (non-convex) mixing model must be considered for the mixing with the other phases. This is achieved by an elastic energy of the form $W_{\mathrm{elast}}(\boldsymbol{\psi}, \boldsymbol{F}) = \frac{g(\boldsymbol{\psi})}{2} \mathrm{tr}(\boldsymbol{F}^T \boldsymbol{F} - \mathbb{I})$ with elastic modulus $g(\boldsymbol{\psi}) = \psi_{\mathrm{gel}}\, g_{\mathrm{gel}}(c)$ that satisfies $g_{\mathrm{gel}}(c) > 0$ and $g'_{\mathrm{gel}}(c) \leq 0$. The phase-field energy of the system is

$$W_{\mathrm{phase}}(\boldsymbol{\psi}, \boldsymbol{F}^{-T} \nabla \boldsymbol{\psi}) = \sum_{i \in \{\mathrm{gel},\mathrm{liquid},\mathrm{air}\}} \gamma_i \left(\frac{\varepsilon}{2} |\boldsymbol{F}^{-T} \nabla \boldsymbol{\psi}_i|^2 + \frac{1}{4\varepsilon} (4\psi^2 - \psi)^2 \right) + \frac{\delta}{2} |\nabla c|^2 + G(\boldsymbol{\psi}),$$

where standard diffusion in the gel would imply $G(\boldsymbol{\psi}) = \beta^{-1} c\,(\log c - 1)$. However, to contain the polymer in the gel, we introduce a mixing term $G(\boldsymbol{\psi}) = \beta^{-1} c\,(\log c - 1) + \chi_{\mathrm{mix}}\, c\, \psi_{\mathrm{gel}}$ with the Flory–Huggins mixing parameter $\chi_{\mathrm{mix}} < 0$. The remaining part proportional to γ_i describes the energy of the interfaces between liquid, gel, and air phase, and $\delta > 0$ ensures coercivity.

The coupling via g leads to an increase of the concentration in regions with high stress, i.e., especially at the contact line; see Figure 1. This coupling of mechanics and phase fields is similar to damage models and topology optimization. Resulting phase separation phenomena were observed in soft gels in experiments. However, for theoretical predictions a better understanding of the parameters in the mixing model is required. For models with multiphase flows and diffusion, the identification of sharp interface limits is a fundamental mathematical question; cf. WIAS Preprint no. 2990.

Biological gels

Cells as well as any biological tissue are in fact not neutral hydrogels but belong to the class of polyelectrolyte gels, which consist of a network of electrostatically charged macromolecules that is swollen with an ionic fluid. These polyelectrolyte chains interact with dissolved ions in the imbibing fluid. If placed in a salt solution, chemical, electrical, and mechanical interactions occur within the gel that drive it towards an equilibrium state. Applying a stimulus, such as an electric field or a temperature change, enables the equilibrium state of the gel to be finely controlled. In [2, 5], we use non-equilibrium thermodynamics to derive a novel phase-field model for a polyelectrolyte gel that displays spontaneous formation of internal interfaces due to the onset of phase separation. In addition, we develop a thermodynamically consistent model of the surrounding ionic bath. Coupling the gel and bath models via appropriate interfacial conditions provides a means of resolving the electric double layer, the so-called *Debye layer*, and elucidating the role it plays in the gel dynamics. In addition, our model captures multi-component diffusive transport using the Stefan–Maxwell formulation to avoid anomalous diffusivities, which can arise when the diffusive flux of a species is solely driven by the gradient of its own chemical potential.

Our analysis reveals that the structure of the gel is crucially dependent on the ratio of two length scales inherent in this system: the Debye length, which is the thickness of the electric double layer, and the Kuhn length, which is proportional to the length of a segment of a single macromolecule. When the Debye length is much smaller than the Kuhn length, then the equilibrium states correspond to a gel that has a homogeneous and electrically neutral bulk with a thin electric double layer at its free surface. In our study, we show that the volume phase transition in this regime can occur via two distinct routes, either solely via the propagation of a swelling/deswelling front from the gel-bath interface or in combination with spinodal decomposition ahead of the main transition front. When the Debye and Kuhn lengths are commensurate, our model predicts a novel mode of pattern formation, resulting in stable, spatially localized structures that emanate from the electric double layer and invade the gel. In this case, the equilibrium states of the gel can be non-homogeneous and electrically charged. We show that this novel model of pattern formation arises due to the interplay between phase separation and the formation of electric double layers and can be detected through measurements of the gel size.

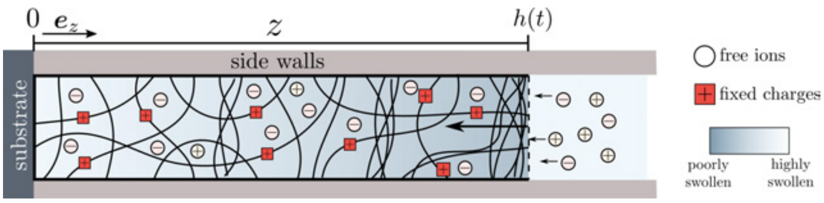

Fig. 2: *Schematic of a laterally confined polyelectrolyte gel that collapses along the z-axis only. The free interface with the bath is located at $z = h(t)$. As solvent is expelled by the gel, the free interface moves towards the left, and salt ions are absorbed/desorbed by the gel so as to maintain electro-neutrality of the gel.*

To show this in the simplest case, we consider the case of a constrained gel with monovalent fixed charges, i.e., charges of chemical valence one ($z_f = +1$), which undergoes uni-axial deformation (in the z-direction) due to the uptake or release of a monovalent ($z_\pm = \pm 1$) salt solution; see Figure 2. The gel is assumed to be attached to a substrate at $z = 0$, while the interface at $z = h(t)$ is free to move along frictionless side walls that do not influence the bulk behavior. We can reduce the corresponding governing equations to

$$\partial_t \phi_s + \partial_z(\phi_s v_n) = -\partial_z j_s, \qquad \partial_t \phi_+ + \partial_z(\phi_+ v_n) = -\partial_z j_+,$$

ϕ_s and ϕ_+ being the volume fractions of the solvent and positive mobile ions, respectively, and v_n the velocity of the network, having eliminated the volume fractions for the network and the negative mobile ions [5]. This is coupled to the constitutive laws

$$j_s = -\frac{\phi_s^2}{1-\phi_n}\partial_z \mu_s + \frac{2\phi_s}{(1-\phi_n)\mathcal{D}}\, j_+, \quad j_+ = -\frac{\mathcal{D}\phi_+\phi_-}{\phi_+ + \phi_-}\partial_z \bar{\mu} + \frac{2\phi_+\phi_-}{\phi_s(\phi_+ + \phi_-)}\, j_s,$$
$$v_n = -j_s - 2j_+, \quad \phi_n = \frac{1-\phi_s-2\phi_+}{1+\alpha_f}, \quad \phi_- = \frac{\phi_+ + (1-\phi_s-\phi_+)\alpha_f}{1+\alpha_f},$$
$$\bar{\mu} = A(\phi_s,\phi_+) + 2\omega^2\phi_s\partial_{zz}\phi_s - \omega^2\left(\partial_z\phi_s\right)^2, \quad \mu_s = B(\phi_s,\phi_+) - (1-\phi_s)\,\omega^2\partial_{zz}\phi_s - \frac{\omega^2}{2}\left(\partial_z\phi_s\right)^2,$$

where in this simple case, $A(\phi_s, \phi_+)$ and $B(\phi_s, \phi_+)$ are found as algebraic relation between ϕ_s, ϕ_+, the number of fixed charges α_f and ω being a measure for the interface thickness. Together with suitable boundary conditions, the solutions of the model show two routes to gel collapse; cf. Figure 3.

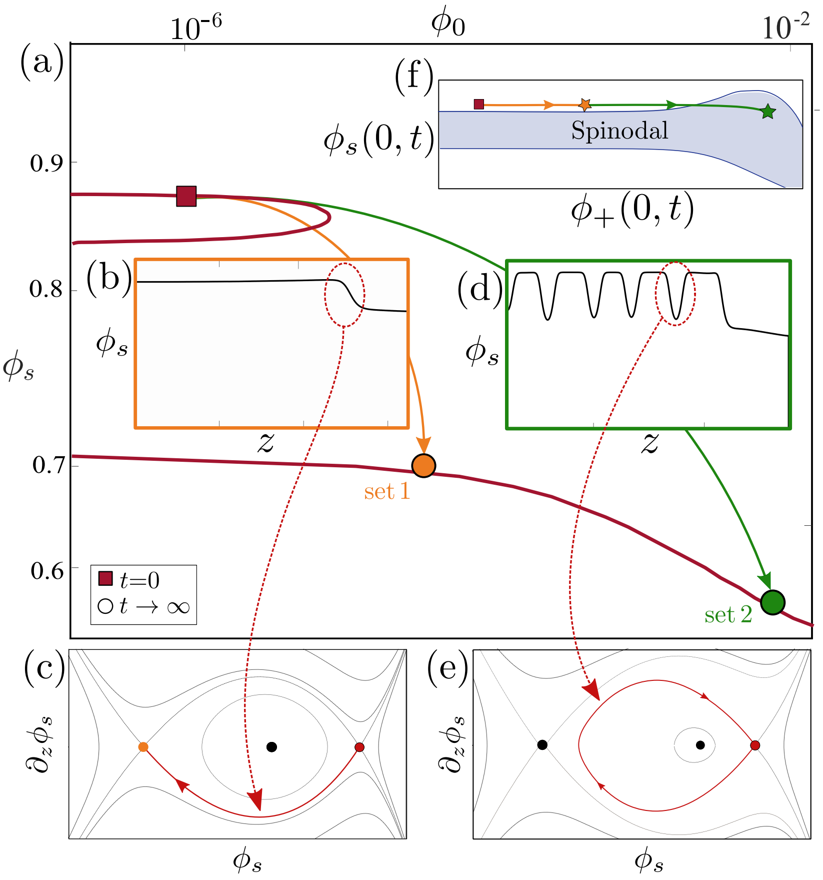

Fig. 3: *Two routes to collapse: (a) A volume phase transition is triggered by increasing the salt fraction in the bath ϕ_0 from 10^{-6} (red square) to 10^{-4} (set 1; orange circle) or 10^{-2} (set 2; green circle). (b) Set 1 leads to the first route to collapse, where a deswelling front invades the gel from the free surface. (c) A heteroclinic orbit, which provides an approximation to the propagating front. (d) The second route to collapse involves front propagation and spinodal decomposition in the bulk of the gel. (e) A two-dimensional projection of a homoclinic orbit; these orbits provide approximations of the phases that form within the bulk of the gel during the second route to collapse. (f) Evolution of the solvent and cation fraction at the substrate ($z = 0$) for parameter set 1 (orange) and set 2 (green). Stars denote the composition after the front has formed. The linearly unstable spinodal regime is shaded.*

Designing materials for biological tissue

Apart from the highly complex relation of the mechanical and elastic properties as demonstrated above even in the simplest cases, another important property of biological gels, such as fibrin or collagen gels, is their elastic tendency to strain stiffen, when forces are applied. This has to be taken into account as well when modeling the typical traction forces applied to these gels in the course of tissue remodeling. Together, with collaborators Sara Checa and Ansgar Petersen (Julius Wolff Institute, Charité) within the MATH+ Project AA1-12 * , we derived a new model for a strain-stiffening hydrogel, where the elastic part of the hydrogel is described by the strain energy density function of the incompressible Gent model

$$W_{\text{elast}}(\psi, \boldsymbol{F}) = -\frac{\mu}{2} J_m \log\left(1 - \frac{\operatorname{tr}(\boldsymbol{F}^T\boldsymbol{F} - \mathbb{I})}{J_m}\right) - \mu \log(\det(\boldsymbol{F})) + p\left(\det(\boldsymbol{F}) - (1+\psi)\right),$$

where p represents the Lagrange multiplier and $J_m = I_m - 2$, and $I_m \in \mathbb{R}$ is the limit value of the first invariant of the right Cauchy–Green deformation tensor $I_1 = \mathrm{tr}(\boldsymbol{F}^T\boldsymbol{F})$. This is coupled to an agent-based model describing the collective mechanical interactions with a strain-stiffening hydrogel.

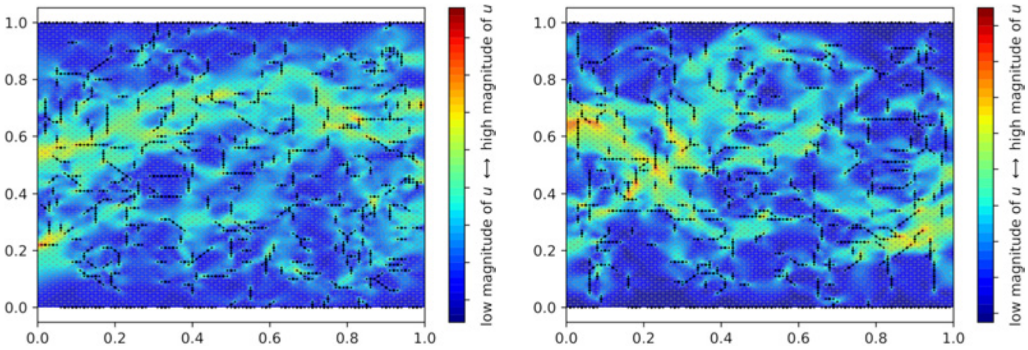

Fig. 4: *Final cell configuration and displacement field. Left: elastic material described by Neo-Hooke model. Right: elastic material described by Gent model with a limit value* I_m *of 4.*

The agent-based model (ABM) describes the collective migration of large distributions of biological cells, such as fibroblasts, on a strain-stiffening hydrogel. After initial *seeding* the cells, modeled here as dipoles, cells probe their hydrogel environment by applying a traction force, and then migrate to an empty location of the hydrogel with highest stiffness, i.e., minimal deformation. Our coupled model predicts how the cells form a pattern with a tendency to long-range alignment and quickly develop a vertical but also horizontal orientation of the dipoles; cf. Figure 4. The diagonal orientation plays only a minor role; cf. Figures 5 and 6.

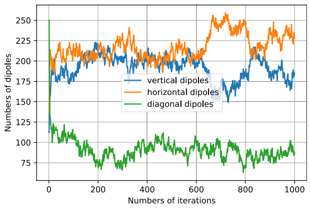

Fig. 5: *Time course of cell alignment: Neo-Hooke*

Outlook

The selection of applied projects shows the potential of the modeling framework and the numerical approach and is currently being extended to include further species; apart from electrostatic interaction, also chemical reaction and damage will need to be coupled as well as further interacting networks in order to develop more realistic models of biomaterials. On the other hand, as exciting and complex as these systems are, the rigorous mathematical theory for even the simplest models for hydrogels is still in its infancy. At WIAS, we have begun with some of the first extistence results.

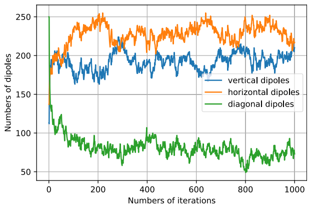

Fig. 6: *Time course of cell alignment: Gent*

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1.6 Energy-based Solution Concepts for a Geophysical Fluid Model

Thomas Eiter and Robert Lasarzik

The motion of tectonic plates, which results from convective processes within the Earth's mantle, is nowadays a widely accepted theory to explain the formation of many of the Earth's geological structures like the Himalaya mountain range in Asia or the San Andreas Fault in California, USA. These tectonic plates as a whole form the Earth's lithosphere, which consists of the Earth's crust and the uppermost part of its mantle (see Figure 1). Geophysicists at the *German Research Centre for Geosciences* in Potsdam describe this process of rock deformation as the flow of a fluid, which happens on large time scales and usually moves only several centimeters per year. Initiated from discussions within the project B01 of the Collaborative Research Center 1114: *Scaling Cascades in Complex Systems*, a group at WIAS started an analytical study of the corresponding models.

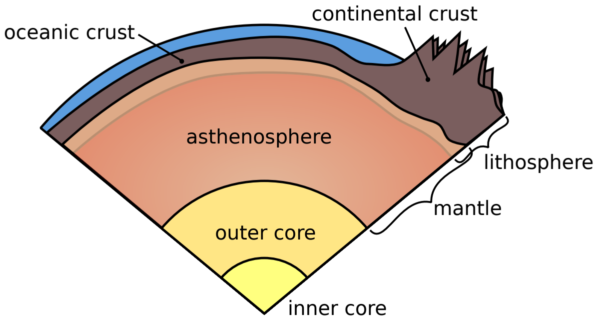

Fig. 1: *A schematic diagram of the Earth's internal structure*

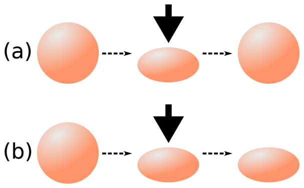

Fig. 2: *After removing forces, an elastic material returns to the original state (a), while a plastic material keeps its shape (b)*

A suitable model for such kind of geophysical flow has to take into account viscous, elastic, and plastic properties. These terms describe the resistance of the flow to deformations: viscosity in terms of deformation rates, but elasticity and plasticity in terms of the actual displacement, which differ in the property whether or not the system returns to the original state when forces are removed (see Figure 2). The plastic effects reflect the brittle nature of rocks and lead to highly nonlinear and nonsmooth terms in the corresponding partial differential equations (PDEs), so that solutions can neither be expected to be smooth nor to satisfy the equations in a pointwise sense. Therefore, a rigorous analytic investigation of the model has to overcome the limitations of classical smooth solutions and needs to be founded on generalized solution concepts. Specifying a suitable notion of generalized solutions to a nonlinear PDE can already be a nontrivial task. Besides the accessibility via mathematical tools, a good choice should also reflect physical principles like the laws of thermodynamics.

Based on these ideas, we investigated solution concepts and combined energetic considerations with a variational approach suitable for treating the nonsmooth plasticity term and for establishing existence of global-in-time solutions. However, as is also the case for much simpler fluid models, the uniqueness of solutions cannot be guaranteed. Instead, we established a *weak-strong uniqueness property* for these generalized solutions, which means that a generalized solution coincides with the (unique) smooth solution as long as the latter exists. This result is based on a *relative energy inequality*, which expresses the difference of a generalized solution to any function in terms of a *relative energy*.

In a first step, we introduced a diffusive term for the stress evolution. There are viscoelastic models where this term can be justified from physical principles, but it also improved the mathematical properties of the problem and enabled us to obtain existence of solutions in a generalized sense [1]. To also treat the case without stress diffusion, which corresponds to the scenario of the numerical investigations in [5], we introduced the notion of *energy-variational solutions* based on the aforementioned relative energy inequality. In this inequality, a passage to vanishing stress diffusion was possible, and we could show existence of energy-variational solutions in this case [2]. Additionally, we obtained a weak-strong uniqueness principle as an immediate consequence of the relative energy inequality. The idea to base a solution concept on a relative energy inequality goes back to Pierre-Louis Lions, who used a similar approach to define the so-called *dissipative solutions* to the Euler equations.

Modeling of viscoelastoplastic fluids

The fundamental equations for modeling fluid flow as a continuum are the *Navier–Stokes equations*. They describe the evolution of the *Eulerian velocity field* $\boldsymbol{v}$ that represents the velocity $\boldsymbol{v}(t,x)$ of a fluid particle at point x in space at time t in terms of two physical principles from classical mechanics: conservation of mass and balance of momentum. In particular, the latter contains the internal forces, described in terms of the *Cauchy stress tensor* $\mathbb{T}$. The physical properties represented by the model depend on the relation between the stress tensor $\mathbb{T}$ and the *strain rate* $\mathbb{D}=\frac{1}{2}(\nabla\boldsymbol{v}+\nabla\boldsymbol{v}^\top)$, which is the symmetric part of the velocity gradient and describes the relative motion between the particles. For example, if $\mathbb{T}$ is independent of the strain rate $\mathbb{D}$, then the model does not consider friction between fluid particles, and we obtain the Euler equations for a perfect fluid.

Viscoelastic fluids. The simplest models for viscoelastic rheology combine linear viscous and elastic effects. In our work, we decomposed the Cauchy stress into a radial part, governed by the pressure p, and a *deviatoric part*, which is a symmetric matrix with vanishing trace. Similarly to [5], we considered a rheology model of Jeffreys type, where the deviatoric stress consists of a linear viscous part and an additional part $\mathbb{S}$ satisfying a stress-strain relation of Maxwell type, *i.e.*, the strain rate decomposes into an elastic and a viscous contribution (see Figure 3). The elastic part is determined by the *objective stress rate* $\overset{\nabla}{\mathbb{S}}$, which is a notion of time derivative independent of the reference frame. In the literature, there are different choices for this stress rate, and we used the *Zaremba–Jaumann rate*, which is a common choice in geophysical flow models, cf. [5]. In summary, we obtain

$$\mathbb{T}=\mathbb{S}+2\mu\mathbb{D}-p\mathbb{I},\qquad \frac{1}{\eta}\overset{\nabla}{\mathbb{S}}+a\mathbb{S}=\mathbb{D}\,,\qquad \text{with}\quad \overset{\nabla}{\mathbb{S}}=\partial_t\mathbb{S}+\boldsymbol{v}\cdot\nabla\mathbb{S}+\mathbb{S}\mathbb{W}-\mathbb{W}\mathbb{S}\,, \tag{1}$$

for viscosity constants $\mu, a>0$, an elastic shear modulus $\eta>0$, and for the *spin tensor* $\mathbb{W}=\frac{1}{2}(\nabla\boldsymbol{v}-\nabla\boldsymbol{v}^\top)$, *i.e.*, the skew-symmetric part of the velocity gradient.

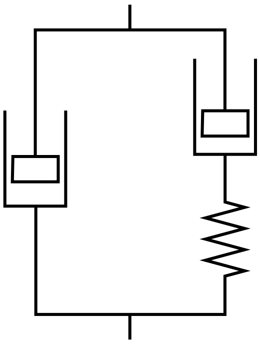

Fig. 3: *A model for Jeffreys rheology. Two linear viscous elements (dashpots) are combined with a linear elastic element (spring).*

Modeling plasticity. To model plasticity, the stress-strain relation (1) needs to be further modified. For so-called *perfect plasticity*, one fixes a *yield stress* $\sigma_{\text{yield}} > 0$, which is an upper bound for the stress magnitude, and plastic deformation sets in when this threshold is reached. We include this behavior in the previous model by replacing the evolution equation for $\mathbb{S}$ in (1) with

$$|\mathbb{S}| \leq \sigma_{\text{yield}} \quad \text{and} \quad \tfrac{1}{\eta}\overset{\nabla}{\mathbb{S}} + a\mathbb{S} + \lambda\mathbb{S} = \mathbb{D} \quad \text{for} \quad \lambda \geq 0 \quad \text{with} \quad \lambda(\sigma_{\text{yield}} - |\mathbb{S}|) = 0,$$

such that the parameter $\lambda \geq 0$ can be arbitrarily large in the case $|\mathbb{S}| = \sigma_{\text{yield}}$. This allows for arbitrarily large strain rates $\mathbb{D}$, which can be physically observed in the form of the onset of sudden motion that may result in earthquakes. In particular, this nonsmooth stress-strain relation can lead to a highly nonlinear behavior. We can abbreviate the previous relation as

$$\tfrac{1}{\eta}\overset{\nabla}{\mathbb{S}} + \partial\mathcal{P}(\mathbb{S}) \ni \mathbb{D} \quad \text{with} \quad \mathcal{P}(\mathbb{S}) = \int_\Omega \mathfrak{P}(\mathbb{S}(x))\,\mathrm{d}x, \tag{2}$$

where $\partial\mathcal{P}$ denotes the subdifferential of a convex dissipation potential $\mathcal{P}$ induced by the density $\mathfrak{P}$ given by $\mathfrak{P}(\mathbb{S}) = \frac{a}{2}|\mathbb{S}|^2$ if $|\mathbb{S}| \leq \sigma_{\text{yield}}$ and $\mathfrak{P}(\mathbb{S}) = \infty$ else (see Figure 4). For the carried-out analysis, the exact form of $\mathcal{P}$ was not relevant, and we studied a general convex, lower semicontinuous dissipation potential $\mathcal{P}\colon L^2(\Omega)^{3\times 3} \to [0,\infty]$ with $\mathcal{P}(0) = 0$.

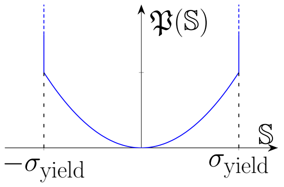

Fig. 4: *The density $\mathfrak{P}$ of the dissipation potential $\mathcal{P}$ in one dimension*

Generalized solution concepts

We consider the viscoelastoplastic fluid inside a bounded domain $\Omega \subset \mathbb{R}^3$ and in a time interval $(0,T)$ with $T > 0$. Combining the above stress-strain relation with the Navier–Stokes equations for incompressible fluids, we obtain the system

$$\rho(\partial_t \boldsymbol{v} + \boldsymbol{v}\cdot\nabla\boldsymbol{v}) = \operatorname{div}\left(\mathbb{S} + 2\mu\mathbb{D} - p\mathbb{I}\right), \qquad \operatorname{div}\boldsymbol{v} = 0, \qquad \tfrac{1}{\eta}\overset{\nabla}{\mathbb{S}} + \partial\mathcal{P}(\mathbb{S}) - \gamma\,\Delta\mathbb{S} \ni \mathbb{D} \tag{3}$$

in $\Omega \times (0,T)$ equipped with appropriate initial and boundary conditions, where $\rho > 0$ denotes the constant density. Observe that the stress-strain relation $(3)_3$ does not coincide with (2), but we introduced a term for *stress diffusion* with coefficient $\gamma > 0$. This makes the problem a fully parabolic problem, while for $\gamma = 0$, system (3) is of mixed parabolic-hyperbolic type.

The total energy of the system is given by $\mathcal{E}(\boldsymbol{v},\mathbb{S}) = \frac{\rho}{2}\|\boldsymbol{v}\|^2_{L^2(\Omega)} + \frac{1}{2\eta}\|\mathbb{S}\|^2_{L^2(\Omega)}$ and consists of the kinetic energy and the stored elastic energy. By formally multiplying $(3)_1$ and $(3)_3$ with $\boldsymbol{v}$ and $\mathbb{S}$, respectively, and integrating in space and time, we obtain the *energy-dissipation balance*

$$\mathcal{E}(\boldsymbol{v}(t),\mathbb{S}(t)) + \mu\int_0^t \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega)}\mathrm{d}s + \int_0^t\!\!\int_\Omega \partial\mathcal{P}(\mathbb{S}) : \mathbb{S}\,\mathrm{d}x\mathrm{d}s + \gamma\int_0^t \|\nabla\mathbb{S}\|^2_{L^2(\Omega)}\mathrm{d}s = \mathcal{E}(\boldsymbol{v}_0,\mathbb{S}_0), \tag{4}$$

where we used the matrix scalar product $\mathbb{A} : \mathbb{B} := \mathrm{Tr}(\mathbb{A}^\top\mathbb{B})$ and that $\operatorname{div}\boldsymbol{v} = 0$ implies the relation $\|\nabla\boldsymbol{v}\|^2_{L^2(\Omega)} = 2\|\mathbb{D}\|^2_{L^2(\Omega)}$. This shows that the total energy decreases along solutions due to the dissipative effects of the viscosity, the dissipation potential $\mathcal{P}$, and the stress diffusion. Note that (4) only holds formally since the dissipation potential may be nonsmooth, and the subdifferential $\partial\mathcal{P}$ is multi-valued in general. In this case, we can estimate the respective term in (4) by using the definition of the subdifferential

$$\mathbb{E} \in \partial\mathcal{P}(\mathbb{S}) \iff \forall \Phi \in L^2(\Omega)^{3\times 3} : \int_\Omega \mathbb{E} : (\mathbb{S}-\Phi)\,\mathrm{d}x \geq \mathcal{P}(\mathbb{S}) - \mathcal{P}(\Phi). \tag{5}$$

Finally, (4) suggests that for $\gamma > 0$, a solution $(\boldsymbol{v}, \mathbb{S})$ should be searched within the class defined by

$$(\boldsymbol{v}, \mathbb{S}) \in L^\infty(0,T; L^2(\Omega)^3 \times L^2(\Omega)^{3\times 3}) \cap L^2(0,T; H^1(\Omega)^3 \times H^1(\Omega)^{3\times 3}). \tag{6}$$

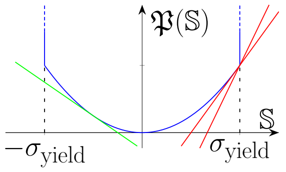

Fig. 5: *While the subdifferential is single-valued at points where $\mathcal{P}$ is smooth (green), it can be multi-valued where this is not the case (red)*

Generalized solutions. A first attempt to find a suitable notion of weak solutions is to multiply the equations $(3)_1$ and $(3)_3$ with smooth test functions and to integrate. However, for $(3)_3$, we again meet the problem that $\partial\mathcal{P}$ can be multi-valued. To circumvent this problem by means of (5), we instead formally multiply $(3)_3$ with $\mathbb{S}-\Phi$ for a test function Φ, which leads to a variational formulation. We proceed similarly for the evolution of $\boldsymbol{v}$. In summary, we call a pair $(\boldsymbol{v}, \mathbb{S})$ with (6) a *generalized solution* to (3) if it satisfies

$$\frac{\rho}{2}\|\boldsymbol{v}-\boldsymbol{\varphi}\|^2_{L^2(\Omega)}\Big|_0^t + \int_0^t\int_\Omega \Big[\rho\partial_t\boldsymbol{\varphi}\cdot(\boldsymbol{v}-\boldsymbol{\varphi}) - \rho\boldsymbol{v}\cdot\nabla\boldsymbol{v}\cdot\boldsymbol{\varphi} + (\mathbb{S}+\mu\nabla\boldsymbol{v}) : \nabla(\boldsymbol{v}-\boldsymbol{\varphi})\Big]\,\mathrm{d}x\mathrm{d}s \leq 0, \tag{7}$$

$$\frac{1}{2\eta}\|\mathbb{S}-\Phi\|^2_{L^2(\Omega)}\Big|_0^t + \int_0^t\Big[\int_\Omega \Big(\frac{1}{\eta}\overset{\nabla}{\Phi}-\mathbb{D}\Big) : (\mathbb{S}-\Phi) + \gamma\,\nabla\mathbb{S} : \nabla(\mathbb{S}-\Phi)\,\mathrm{d}x + \mathcal{P}(\mathbb{S})-\mathcal{P}(\Phi)\Big]\,\mathrm{d}s \leq 0 \tag{8}$$

for a.a. $t \in (0,T)$ and all suitable test functions $(\boldsymbol{\varphi}, \Phi)$. Note that the nonlinear terms are hidden in the Zaremba–Jaumann rate $\overset{\nabla}{\Phi} : \mathbb{S}$ (see $(1)_3$). In particular, choosing both test functions equal to 0, we obtain separate energy inequalities for the kinetic and the elastic energy. Summing up and applying (5), these resemble (4) with an inequality. This energy estimate serves as an *a priori* bound in our analysis. In [1], we showed existence of generalized solutions to (3) for $\gamma > 0$ by regularization of the dissipation potential $\mathcal{P}$. This makes it possible to work with a weak formulation and to show existence via a Galerkin approximation. As usual, this approach only yields weak convergence of an approximating sequence, but to pass to the limit in the nonlinear terms in (8), the strong convergence with respect to $\mathbb{S}$ is necessary. Within the function class from (6), this follows from the famous Aubin–Lions lemma, which explains the necessity of stress diffusion, that is, of the assumption $\gamma > 0$.

Relative energy inequality. We further derived an inequality for the *relative energy* $\mathcal{R}(\boldsymbol{v}, \mathbb{S} \mid \boldsymbol{\varphi}, \Phi) = \mathcal{E}(\boldsymbol{v}-\boldsymbol{\varphi}, \mathbb{S}-\Phi)$, which provides an energy-based way to measure distances. From (7), (8), and Gronwall's inequality, one concludes that the generalized solution satisfies the *relative energy inequality*

$$\begin{aligned}&\mathcal{R}(\boldsymbol{v}(t), \mathbb{S}(t) \mid \boldsymbol{\varphi}(t), \Phi(t)) - \mathcal{R}(\boldsymbol{v}_0, \mathbb{S}_0 \mid \boldsymbol{\varphi}(0), \Phi(0))\mathrm{e}^{\int_0^t \mathcal{K}(\boldsymbol{\varphi},\Phi)\,\mathrm{d}s}\\ &+ \int_0^t \Big(\mathcal{W}^{(\mathcal{K})}(\boldsymbol{v}-\boldsymbol{\varphi}, \mathbb{S}-\Phi \mid \boldsymbol{\varphi}, \Phi) + \mathcal{P}(\mathbb{S})-\mathcal{P}(\Phi) + \Big\langle \mathcal{A}(\boldsymbol{\varphi}, \Phi), \begin{pmatrix}\boldsymbol{v}-\boldsymbol{\varphi}\\ \mathbb{S}-\Phi\end{pmatrix}\Big\rangle\Big)\mathrm{e}^{\int_s^t \mathcal{K}(\boldsymbol{\varphi},\Phi)\,\mathrm{d}\tau}\,\mathrm{d}s \leq 0\end{aligned} \tag{9}$$

for a.e. $t \in (0,T)$ and all sufficiently regular $(\boldsymbol{\varphi}, \Phi)$; see [2]. The weight $\mathcal{K} \geq 0$ determines the regularity of test functions $(\boldsymbol{\varphi}, \Phi)$, the function $\mathcal{W}^{(\mathcal{K})}$ denotes the relative dissipation-like quantity

$$\begin{aligned} \mathcal{W}^{(\mathcal{K})}(\tilde{\boldsymbol{v}}, \tilde{\mathbb{S}} | \boldsymbol{\varphi}, \Phi) &:= \mathcal{K}(\boldsymbol{\varphi}, \Phi)\, \mathcal{E}(\tilde{\boldsymbol{v}}, \tilde{\mathbb{S}}) \\ &+ \int_\Omega \mu |\nabla \tilde{\boldsymbol{v}}|^2 + \gamma |\nabla \tilde{\mathbb{S}}|^2 - \rho \tilde{\boldsymbol{v}} \cdot \nabla \tilde{\boldsymbol{v}} \cdot \boldsymbol{\varphi} + \tfrac{1}{\eta} (\tilde{\boldsymbol{v}} \otimes \tilde{\mathbb{S}}) : \nabla \Phi - \tfrac{1}{\eta} (\tilde{\mathbb{S}} (\nabla \tilde{\boldsymbol{v}} - \nabla \tilde{\boldsymbol{v}}^\top)) : \Phi \,\mathrm{d}x, \end{aligned} \tag{10}$$

and $\mathcal{A} = (\mathcal{A}_1, \mathcal{A}_2)$ is the system operator defined in such a way that a smooth pair $(\boldsymbol{\varphi}, \Phi)$ satisfies (3) if and only if $\mathcal{A}_1(\boldsymbol{\varphi}, \Phi) = 0$ and $\mathcal{A}_2(\boldsymbol{\varphi}, \Phi) \in \partial \mathcal{P}(\Phi)$ in $(0,T)$. In particular, if we choose $\mathcal{K}$ such that $\mathcal{W}^{(\mathcal{K})}$ is nonnegative, e.g., $\mathcal{K}(\boldsymbol{\varphi}, \Phi) = C \big(\|\boldsymbol{\varphi}\|^s_{L^r(\Omega)} + \|\Phi\|^q_{L^p(\Omega)} + \|\Phi\|^2_{L^p(\Omega)} \big)$ for a certain constant $C > 0$ and suitable parameters p, q, r, s, then for any sufficiently regular solution $(\boldsymbol{\varphi}, \Phi)$, the inequality (9) reduces to $\mathcal{R}(\boldsymbol{v}(t), \mathbb{S}(t) \mid \boldsymbol{\varphi}(t), \Phi(t)) \leq \mathcal{R}(\boldsymbol{v}_0, \mathbb{S}_0 \mid \boldsymbol{\varphi}(0), \Phi(0)) \mathrm{e}^{\int_0^t \mathcal{K}(\boldsymbol{\varphi}, \Phi)\,\mathrm{d}s}$. When the initial values of $(\boldsymbol{v}, \mathbb{S})$ and $(\boldsymbol{\varphi}, \Phi)$ coincide, we thus conclude $\boldsymbol{v} = \boldsymbol{\varphi}$ and $\mathbb{S} = \Phi$. This shows that generalized solutions satisfy the weak-strong uniqueness principle.

Energy-variational solutions. The notion of energy-variational solutions is based on the relative energy inequality (9). As explained above, stress diffusion was necessary to show existence of generalized solutions in the sense of (7), (8), since weak convergence in the function class (6) was sufficient to perform the limit in the nonlinear terms. Without stress diffusion, we lose control of $\nabla \mathbb{S}$, so that a passage to the limit in (8) is not possible for $\gamma = 0$, so that the above notion of generalized solution seems not suitable in this case. Instead, we proposed a different solution concept and called a pair $(\boldsymbol{v}, \mathbb{S})$ an *energy-variational solution* for the *regularity weight* $\mathcal{K}$ if it satisfies the relative energy inequality (9) for all test functions $(\boldsymbol{\varphi}, \Phi)$ in a suitable class. If we take

$$\mathcal{K}(\boldsymbol{\varphi}, \Phi) = C \big(\|\Phi\|_{L^\infty(\Omega)} + \|\nabla \Phi\|_{L^3(\Omega)} \big) \tag{11}$$

for a suitable constant $C > 0$ such that $\mathbb{S}$ appears in the function $\mathcal{W}^{(\mathcal{K})}$ in (10) in a convex way, then weak convergence is sufficient to pass to the limit $\gamma \to 0$ in (9). In this way, we showed existence of energy-variational solutions in the case $\gamma = 0$. Since the relative energy inequality (9) holds by definition, nonnegativity of $\mathcal{W}^{(\mathcal{K})}$ implies a weak-strong uniqueness principle for energy-variational solutions as above. This can not be deduced for $\mathcal{K}$ as in (11), but for

$$\mathcal{K}(\boldsymbol{\varphi}, \Phi) = C \big(\|\boldsymbol{\varphi}\|^s_{L^r(\Omega)} + \|\Phi\|^2_{L^\infty(\Omega)} + \|\nabla \Phi\|^2_{L^3(\Omega)} \big) \tag{12}$$

for sufficiently large $C > 0$ and suitable parameters r, s. Due to monotonicity properties with respect to the regularity weight, a weak-strong uniqueness principle also follows for energy-variational solutions with the weight $\mathcal{K}$ as in (11).

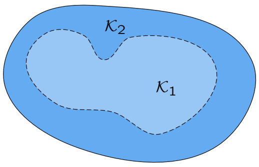

Fig. 6: *The set of energy-variational solutions depends on the regularity weight $\mathcal{K}$. If $\mathcal{K}_1 \leq \mathcal{K}_2$, every energy-variational solution for $\mathcal{K}_1$ is an energy-variational solution for $\mathcal{K}_2$.*

Conclusions and outlook

We studied a model that describes the deformation of rocks in the lithosphere as the flow of a fluid with viscous, elastic, and plastic properties. Since solutions are not smooth in general, we proposed a generalized solution concept based on a variational formulation that takes into account the energy of the system. In this framework, we could only show an existence result after introducing stress diffusion. To omit this term, we introduced the notion of energy-variational solution, where a passage to the limit of vanishing stress diffusion was possible. This solution concept is based on a relative energy inequality, which also ensures a weak-strong uniqueness principle for energy-variational solutions.

Since the concept of energy-variational solutions is rather new, an extension to other systems might also be of interest, which was done for a general class of hyperbolic conservation laws in the recent preprint [3]. Although energy-variational solutions are not unique in general, a suitable choice of the regularity weight may lead to a convex structure of the set of solutions, which may allow to choose a unique physically relevant solution by a minimization procedure. For example, this idea was successfully realized for simpler fluid models in [4].

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[2] T. Eiter, K. Hopf, R. Lasarzik, *Weak-strong uniqueness and energy-variational solutions for a class of viscoelastoplastic fluid models*, Adv. Nonlinear Anal., **12** (2023), pp. 20220274/1–20220274/31.

[3] T. Eiter, R. Lasarzik, *Existence of energy-variational solutions to hyperbolic conservation laws*, WIAS Preprint no. 2974, 2022.

[4] R. Lasarzik, *Maximally dissipative solutions for incompressible fluid dynamics*, Z. Angew. Math. Phys., **73** (2022), pp. 1/1–1/21.

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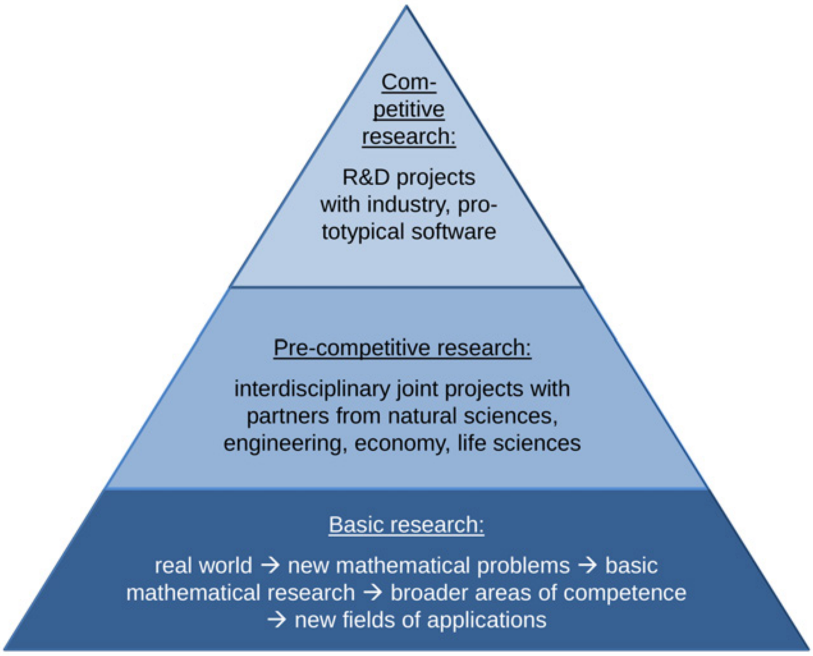
2 WIAS in 2022

- Profile
- Structure and Scientific Organization
- Activities in Equal Opportunities and Work-Life Issues
- 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 *Common Administration of FVB* is in charge of its administrative business. The official German name of the institute is *Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e. V.*



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

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

The Weierstrass Institute is dedicated to university education on all levels, ranging from the teaching of numerous classes at the 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 the international collaboration in applied mathematics by organizing workshops and running guest programs. The institute is embedded in a dense network of scientific partners. In particular, it maintains various connections with Leibniz institutes and actively takes part in the forming and development of strategic networks in its fields. Thus, the WIAS coordinates the **Leibniz Research Network “Mathematical Modeling and Simulation (MMS)”** connecting 36 partners from all sections of the Leibniz Association. Modern methods of MMS are imperative for progress in science and technology in many research areas. The activities of the network are supported by a grant from the Strategic Fund of the Leibniz Association. After the Leibniz MMS Days as the central annual meeting of the network had to be postponed at short notice due to the pandemic in March 2020, this could be caught up from April 25 to 27, 2022, at the Potsdam Institute for Climate Impact Research (PIK). The meeting marked a successful relaunch of scientific face-to-face workshops, which are fundamentally important for this network structure, and was attended by 55 scientists from 20 institutions.

The **Mathematical Research Data Initiative (MaRDI)** , funded for five years since Oct. 1, 2021, (http://www.mardi4nfdi.de/) is currently in its second year and has been actively working to develop services for the community. MaRDI has successfully launched the initial version of the Portal https://portal.mardi4nfdi.de and will be integrating, e.g., the AlgoData-knowledge graph on algorithms (https://algodata.mardi4nfdi.de) and MaRDMO, tools that will assist researchers in their research data management (RDM) planning. Additional services developed within the consortia will be integrated into the MaRDI Portal making it a central one-stop point of access. Additionally, MaRDI is currently working on publishing a white paper on RDM, for grant proposals and research projects that researchers could use when writing proposals or creating data management plans for their project, supplementing the existing DFG checklists. As a part of the general outreach program, a 4-issue Newsletter focusing on each of the F.A.I.R principles has been published (https://www.mardi4nfdi.de/community/newsletter; subscribe), breaking down what this means for researchers and mathematical data. In addition, workshops and mini-symposia in the areas of discrete mathematics, scientific computing, and computer algebra have been organized. WIAS is operating the MaRDI coordination office and has three positions in the consortium working on workflows and software in statistics as well as for neuroscientific data and on mathematical models formulated for partial differential equations.

How WIAS is handling its own research data is one focus of the new **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 since November 2022 Chair of the center. The structure of MATH+ integrates and merges the Research Center Matheon, which was funded from 2002 to 2014 by the DFG and subsequently by the Einstein Center for Mathematics ECMath, the Berlin Mathematical School (BMS), and others.

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

2.2 Structure and Scientific Organization

2.2.1 Structure

In 2022, WIAS was organized into the following divisions for fulfilling its mission: Eight research groups, two Leibniz groups, two Weierstrass groups, and one Focus Platform[1] form the scientific body of the institute. In their mission, they are supported by the departments for technical and administrative services.

The Secretariat of the International Mathematical Union (IMU, see page 62), hosted by WIAS, is a supportive institution for the international mathematical community. Moreover, WIAS hosts the German Mathematics Association DMV and the Society of Didactics of Mathematics GDM.

Research Groups:

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

Flexible Research Platform:

LG NUMSEMIC. Numerical Methods for Innovative Semiconductor Devices
LG DYCOMNET. Probabilistic Methods for Dynamic Communication Networks
WG BIP. Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes
WG DOC. Data-driven Optimization and Control
FP 1. Quantitative Analysis of Stochastic and Rough Systems

The organization chart on page 50 gives an overview of the organizational structure of WIAS in 2022.

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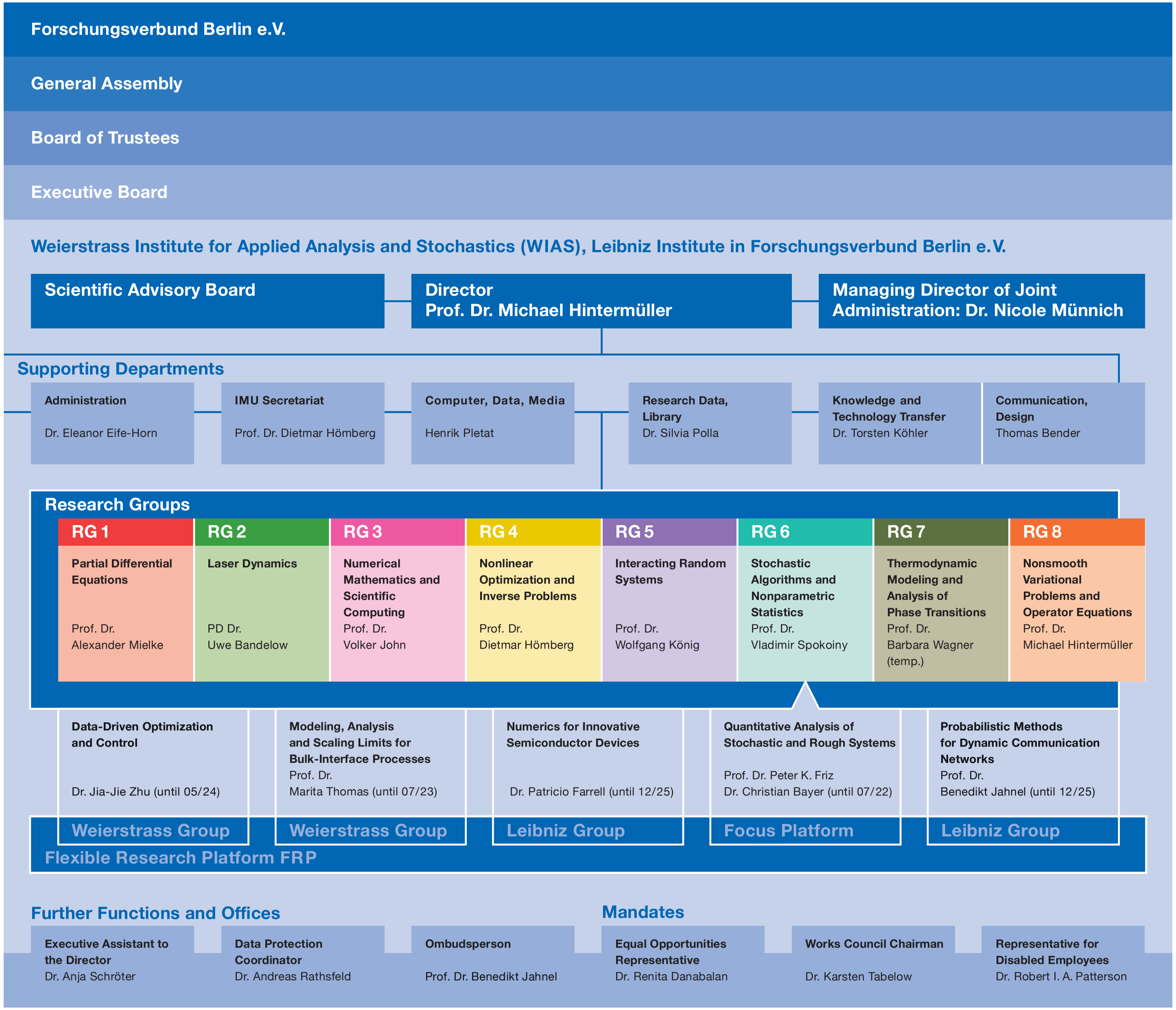
[1] In the following, the terms "research group" will often be abbreviated by "RG," "Leibniz group" by "LG," Weierstrass group by "WG," and Focus Platform by "FP."



Forschungsverbund Berlin e.V.

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RG 2
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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

Data-Driven Optimization and Control
Dr. Jia-Jie Zhu (until 05/24)
Weierstrass Group

Modeling, Analysis and Scaling Limits for Bulk-Interface Processes
Prof. Dr.
Marita Thomas (until 07/23)
Weierstrass Group

Numerics for Innovative Semiconductor Devices
Dr. Patricio Farrell (until 12/25)
Leibniz Group

Quantitative Analysis of Stochastic and Rough Systems
Prof. Dr. Peter K. Friz
Dr. Christian Bayer (until 07/22)
Focus Platform

Probabilistic Methods for Dynamic Communication Networks
Prof. Dr.
Benedikt Jahnel (until 12/25)
Leibniz Group

Flexible Research Platform FRP

Further Functions and Offices

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Dr. Anja Schröter

Data Protection Coordinator
Dr. Andreas Rathsfeld

Ombudsperson
Prof. Dr. Benedikt Jahnel

Mandates

Equal Opportunities Representative
Dr. Renita Danabalan

Works Council Chairman
Dr. Karsten Tabelow

Representative for Disabled Employees
Dr. Robert I. A. Patterson

2.2.2 Main Application Areas

The research at WIAS focused in 2022 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

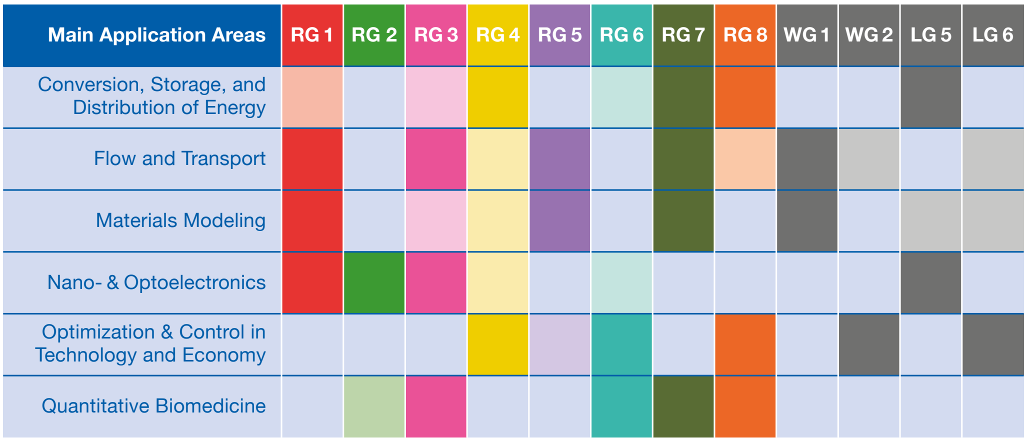
- **Conversion, Storage, and Distribution of Energy**
- **Flow and Transport**
- **Materials Modeling**
- **Nano- and Optoelectronics**
- **Optimization and Control in Technology and Economy**
- **Quantitative Biomedicine**

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

2.2.3 Contributions of the Groups

The eight Research Groups, the Leibniz 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 2022 in the interdisciplinary solution process described above (dark color: over 20% of the group's working time, light color: up to 20% of the group's working time, blue: no contribution).



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

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

In the following, special research topics are listed that were addressed in 2022 within the general framework of the main application areas.

Conversion, Storage and Distribution of Energy

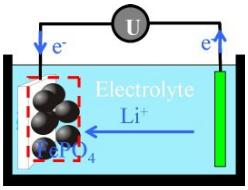


Fig. 1: *Sketch of a lithium-ion battery (LiFePO4)*

This main application area takes account of an economic use of energetic resources based on mathematical modeling and optimization. With regard to future developments, sustainability and aspects of electro-mobility play a major role. Lithium-ion batteries belong to the key technologies for storing renewable energy, for which mathematical models are developed in RG 7. Modern mathematical methods such as homogenization techniques enable a sound description of porous battery electrodes. With this, some key aspects are the prediction of the cell voltage, the incorporation of ageing phenomena, and validation with experimental data. RG 3 and RG 7 cooperate in modeling the transport processes and their evaluation by simulations. Furthermore, RG 4 and RG 8 investigate aspects of uncertainty in energy management via stochastic optimization or uncertainty quantification. Here, the emphasis is put on gas networks and renewable energies with uncertain parameters given, e.g., by demand, precipitation, or technical coefficients. In this context, new perspectives in modeling and analyzing equilibria in energy markets with random parameters and when coupling markets with the underlying physical or continuum mechanical properties of the energy carrier in a power grid open up.

Core areas:

- Light-emitting diodes based on organic semiconductors (OLEDs; in RG 1 and RG 3)
- Modeling of experimental electrochemical cells for the investigation of catalytic reaction kinetics (in RG 3)
- Lithium-ion batteries (in RG 3 and RG 7)
- Modeling and analysis of coupled electrochemical processes (fuel cells, batteries, hydrogen storage, soot; in RG 3 and RG 7)
- Nonlinear chance constraints in problems of gas transportation (in RG 4)
- Parameter identification, sensor localization, and quantification of uncertainties in PDE systems (in RG 8)
- Modeling and simulation of charge transport in perovskite solar cells (in LG NUMSEMIC)
- Modeling and optimization of weakly coupled minigrids under uncertainty (in RG 4)

Flow and Transport

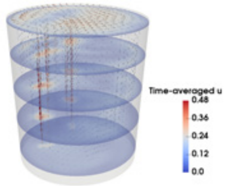


Fig. 2: *Time-averaged turbulent flow through a ladle*

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

Core areas:

- Thermodynamic models and numerical methods for electrochemical systems (in RG 1, RG 3, and RG 7)
- Development and analysis of physically consistent discretizations (in RG 3 and LG NUMSEMIC)
- Modeling and numerical methods for particle systems (in RG 1, RG 5, and WG DOC)
- Modeling of nanostructures of thin films (in RG 7)
- Computational hemodynamics (in RG 3 and RG 8)
- Scientific software platforms `ParMooN` and `pdelib` (in RG 3)
- Description of random message trajectories in spatial telecommunication models (in LG DYCOMNET)
- Thermomechanical modeling, analysis, and simulation of multiphase flows (with free boundaries; in RG 7 and WG BIP)
- Theoretical analysis of intermittent mass flow through random media (in RG 5)
- Gradient flow and optimal transport applications to machine learning and data-driven optimization (in WG DOC)
- Analysis, simulation, and optimal control of nonlinear electrokinetics in anisotropic microfluids (in RG 4)

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.

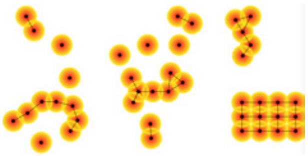


Fig. 3: *A realization of a many-body system showing a small crystal in the lower right corner*

Core areas:

- Homogenization and localization in random media (in RG 1, RG 5, and LG DYCOMNET)
- Phase transitions in interacting many-particle systems of condensation, crystallization and gelation type (in RG 1, RG 5, and LG DYCOMNET)
- Asymptotic analysis of nano- and micro-structured interfaces, including their interaction with volume effects (in RG 7 and WG BIP)
- Dynamical processes in nonhomogeneous media (in WG BIP, RG 1, RG 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 7 and WG BIP)

- Thermodynamically consistent electrochemical models of lithium-ion batteries, fuel cells, and solid oxide electrolytes (in RG 3 and RG 7)
- Stochastic and thermomechanical modeling of phase transitions (in RG 4, RG 5, and LG DYCOMNET)
- Hysteresis effects, e.g., in electro/magneto-mechanical components, elastoplasticity, lithium batteries (in RG 1, RG 7, and WG BIP)
- Modeling of elastoplastic and phase-separating materials including damage and fracture processes (in RG 1, RG 7, and WG BIP)
- Derivation and analysis of local and nonlocal phase field models and their sharp-interface limits (in RG 7 and WG BIP)
- Modeling and simulation of electronic properties of perovskites (in LG NUMSEMIC)

Nano- and Optoelectronics

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

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

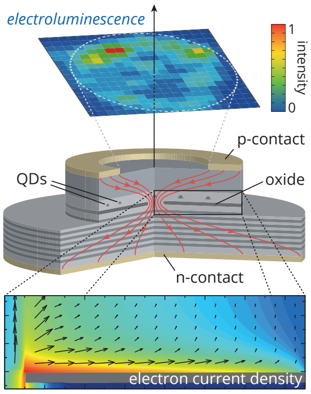


Fig. 4: *Simulated spreading of injection current density in a quantum-dot-based single photon emitter with Al-oxide aperture. An improved design was proposed on that base in:* M. Kantner, U. Bandelow, T. Koprucki, J.-H. Schulze, A. Strittmatter, H.-J. Wünsche, *Efficient current injection into single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

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 and RG 2)

- Laser structures and their dynamics (high-power lasers, single-photon emitters, quantum dots; in RG 1, RG 2, and RG 3)
- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in RG 2)
- Photovoltaics, OLED lighting, and organic transistors (in RG 1 and RG 3)
- Electronic properties of nanostructures such as nanowires (in RG 1 and LG NUMSEMIC)

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.

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.

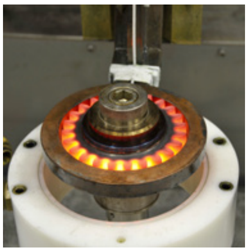


Fig. 5: *Induction heat treatment of a gear*

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.

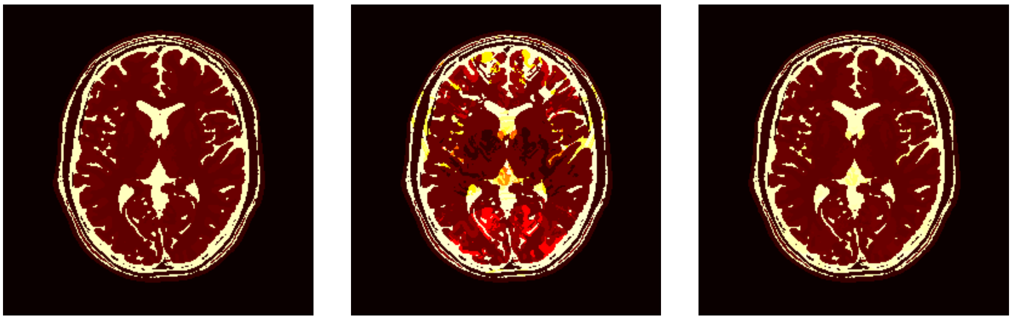


Fig. 6: *Quantitative MRI: Estimation of the T_2 relaxation times of matter leading to characterization of different types of tissue. (1) Ground truth, (2) State-of-the-art dictionary-based method (improved variant of Magnetic Resonance Fingerprinting MRF), (3) Integrated physics-based approach, where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

Core areas:

- Numerical methods for biofluids and biological tissues (in RG 3 and RG 8)
- Image processing (in RG 6 and RG 8)
- Modeling of high-resolution magnetic resonance experiments (in RG 6)
- Free boundary models for actin filament networks (in RG 7)
- Modeling of a nanopore for the analysis of DNA-type macromolecules (in RG 7)
- (Bio-)physics-based quantitative imaging (in RG 6 and RG 8)

2.3 Activities in Equal Opportunities and Work-Life Issues

WIAS is committed to an equal opportunities policy that aims at increasing the number of women among the scientific staff and especially in leading positions. This aim is to be achieved both by creating a family-friendly environment and by the equal opportunities officers' involvement in staffing procedures.

In accordance with a decision of the WIAS scientific management, one of its members is appointed to take charge of equal opportunities issues always for the period of one year. Alexander Mielke, head of Research Group 1 *Partial Differential Equations*, was designated as the person in charge in 2022. Andrea Eismann as the Equal Opportunities Officer and Jutta Lohse as her deputy spent again much time reading applications and participating in job interviews to ensure that in the case of equal qualifications and suitability, persons of the underrepresented gender be given preferential consideration.

In January, the Central Equal Opportunities Officer of FVB invited women scientists to an online screening of the documentary film “Picture a Scientist” by Ian Cheney and Sharon Shattuck, followed by a discussion. In May, biannual womens’ meetings were reinstated at the institute. In June, WIAS became an Institutional Member of the European Women in Mathematics. In September, Renita Danabalan was elected the new Equal Opportunities Officer and Andrea Eismann her deputy. On October 5–7, the “Junior Female Researchers in Probability” Workshop took place in Berlin, co-organized—jointly with other organizers of the International Research Training Group IRTG 2544 *Stochastic Analysis in Interaction*—by Alexandra Quitmann of WIAS RG 5. In the Director’s Meetings, measures to promote female postdocs are discussed. A program shall be started in 2023.

In 2022, five new female master’s degree candidates were recruited as student assistants at WIAS in the WIAS Female Master Students Program. Katharina Hopf participated in the Leibniz Mentoring Program 2021/2022 that supports highly qualified female post-doctorate researchers on their path to obtaining a professorship or other leading positions.

audit berufundfamilie. Since 2013, WIAS has been certified and re-certified (optimization phase and consolidation phase) as a family-friendly employer by the *audit berufundfamilie*. This certificate documents the institute’s dedication to a sustainable family- and life-phase-conscious personnel policy. In the second half of 2022, much work was done for the re-audit (dialog phase). A report and a self-assessment had to be prepared, using also the results of an employee survey that took place in Spring 2022. On the so-called *Dialog Day* on Nov. 11, a dialog on quality and development took place in four discussion rounds with different representatives of human resources, the management, and the different organizational groups, on the implementation of the audit and their satisfaction with that process, as well as on topics like stress, communication, and mobile work, followed by an evaluation by the auditor. On the basis of the results, a plan of action was written and sent in January 2023 to the auditor. A decision on the re-certification is expected for March, 2023.

Although not all measures envisaged in the “Objective agreement for confirmation of the certificate for the *audit berufundfamilie* 2020–2023” could be implemented due to COVID-19, our already high standards of family-friendliness established in the “Company agreement regarding the compatibility of career and family” were further improved and consolidated. Employees can, for instance, make use of the services offered by the family service *benefit@work* at no charge. Many employees work from home.

The *work and family* team monitoring and supporting the implementation of family-friendly policies at WIAS comprised in 2022 Olaf Klein (project head of the *audit berufundfamilie*), Alexander Mielke (management), Jutta Lohse, Veronica Bove, and Pia Pfau, who will head the project from 2023.

In 2022, the team informed the staff regularly about relevant issues and events (announcements and offers of webinars, online talks, and online events on, e.g., holiday programs for children, speaking with children on war – dealing with fear, confidence in times of crisis, time to just breathe, nonviolent communication, care for family members, etc.; distribution of information material related to these topics). In May, a talk on Unconscious Bias was organized.

Zertifikat seit 2013
audit berufundfamilie
www.berufundfamilie.de

The Christmas party for the children of the collaborators could again take place in situ on Dec. 19. Sixteen children and their parents enjoyed the visit of Father Christmas in our new meeting area in the library.

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 2022, having raised a total of 4.43 million euros, from which 49 additional researchers [2] (plus 10 outside WIAS; Dec. 31, 2022) were financed. In total in 2022, 29.8 percent of the total budget of WIAS and 45.37 percent[2] of its scientific staff originated from grants.

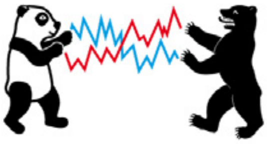
For a detailed account of projects funded by third parties, the reader is referred to the appendix, Section A.2 Grants below on pages 129ff.

2.5 Participation in Structured Graduation Programs

Graduate School *Berlin Mathematical School (BMS)*

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

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



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

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

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

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

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

2.6 Scientific Software

Scientific software is a tool to evaluate models and algorithms investigated at WIAS. Moreover, software helps to transfer research results to other scientific fields, to industry, and to the general public. The underlying problems often pose very specific and advanced requirements, which cannot be satisfied by standard software that is widely available; hence, the development of algorithms and scientific software belongs to the scientific tasks of WIAS. As a consequence, WIAS is working on the implementation of rules of good scientific practice in the realm of software development. Software-based publications in specific journals and as WIAS Technical Reports are encouraged. The production, dissemination, and sale of software is not part of the core duties of WIAS. Nevertheless, several codes developed at WIAS are distributed outside of WIAS and have earned a good reputation. See page 188ff. for a list of software packages that WIAS makes available. Licensing models depend on the specifics of the corresponding projects. Codes are offered under open source and proprietary licenses as well as combinations thereof.

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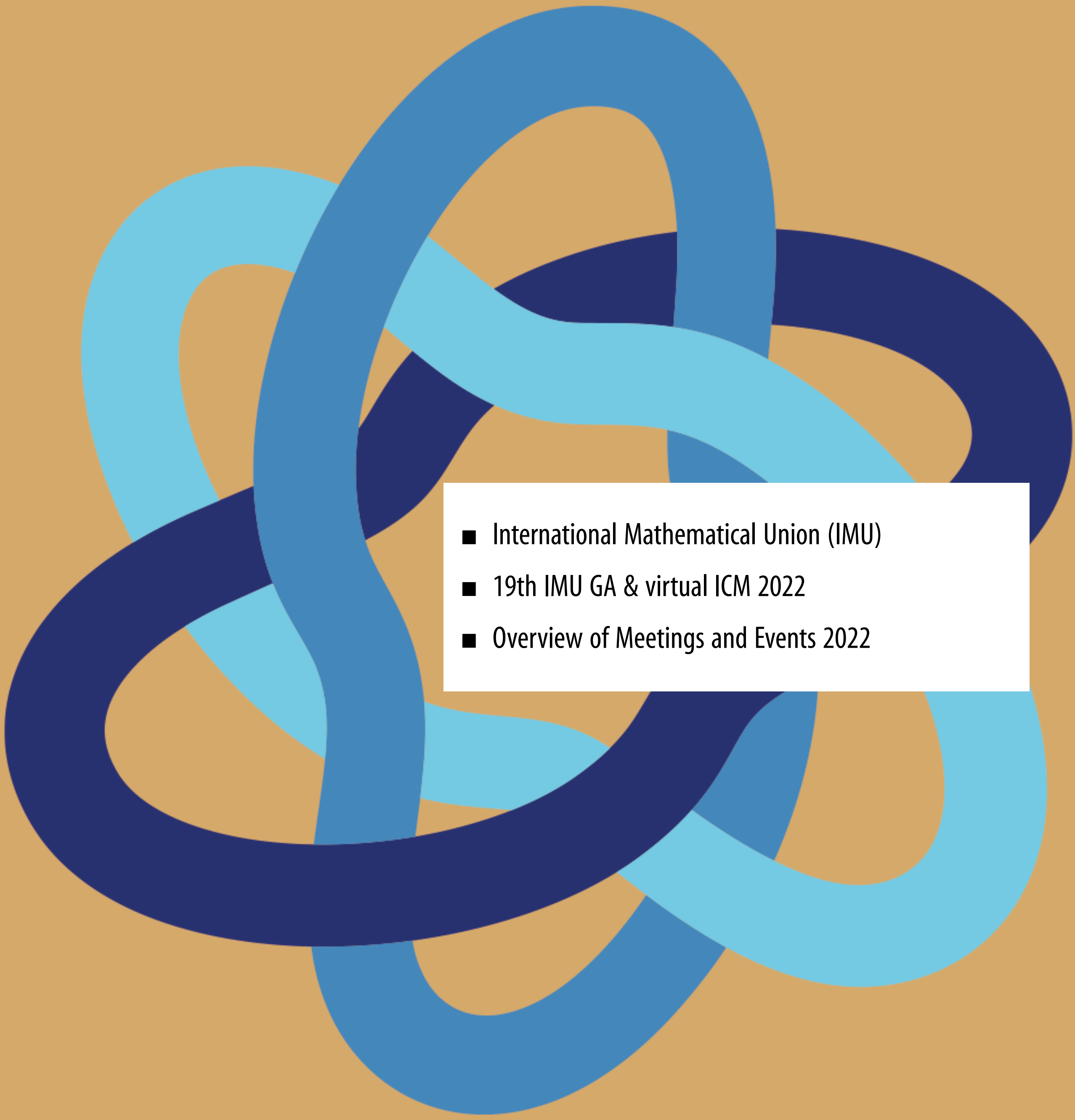
[2] Including scholarship holders.

3 IMU@WIAS



- International Mathematical Union (IMU)
- 19th IMU GA & virtual ICM 2022
- Overview of Meetings and Events 2022

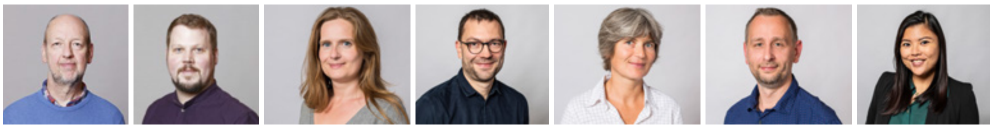
3.1 International Mathematical Union (IMU)

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

The collaboration between WIAS and the IMU was installed via a Memorandum of Understanding (2010) and a Cooperation Agreement (2013) that covered an initial period of ten years. After a positive evaluation of the work of the IMU Secretariat during the period 2011–2018, the IMU General Assembly 2018 passed a resolution to enter into a new and unlimited Cooperation Agreement, which was signed immediately after the General Assembly.

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

Staff members



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

Scott Jung, *Manager of the IMU Secretariat*. S. Jung's responsibilities include heading and supervising the administrative operations of the Secretariat and actively participating in the implementation of the decisions and duties of the EC and the IMU General Assembly, which is done in close cooperation with 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 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 promoting the work of both commissions, managing their web presence – including public relations and communications – and handling grant applications and support programs.

Mariusz Szmerlo, *IMU Accountant*. M. Szmerlo is, under the supervision of the IMU Treasurer, in charge of executing the financial decisions of the IMU, which includes budget management of the IMU Secretariat, application for and supervision of third-party funds, handling membership dues, all financial aspects of grants, and administering expense reimbursements.

Birgit Seeliger, *IMU Archivist*. B. Seeliger is responsible for the IMU Archive and in charge of preserving and making paper documents, photos, pictures, and IMU artifacts accessible, as well as supporting the decision process concerning the electronic archiving of IMU documentation. She also provided additional administrative support to CWM in 2022.

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

Vanessa Chung, *Project Assistant*. V. Chung joined the IMU Secretariat in January 2021. Her primary task is to support the administrative work of the IMU Secretariat, in particular, to assist in the organizational handling of CDC programs and general IMU activities.

The IMU Secretary General

Helge Holden (Professor at the Norwegian University of Science and Technology (NTNU), Trondheim) was IMU Secretary General from 2015 until 2022. He maintained regular contact with the IMU Secretariat via electronic communication, and frequently visited the office.

Helge Holden's second and final term as IMU Secretary General ended in December 2022. The new IMU Secretary General for the coming term (2023–2026) will be Christoph Sorger, Professor of Mathematics at Université de Nantes, France.

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

3.2 19th IMU GA & virtual ICM 2022

Carlos E. Kenig, IMU President (2019–2022), Helge Holden, IMU Secretary General (2015–2022)

2022 was always going to be a momentous and challenging year for the IMU, with the Union's 19th General Assembly (GA) and the next instance of its quadrennial congress – the International Congress of Mathematicians (ICM) – due to take place. However, world events unfolded in a manner that could not be anticipated at the start of the year and in ways that profoundly impacted the IMU's plans. The EC had its scheduled annual meeting on February 24–27, 2022. Due to the pandemic, the meeting was again held virtually. The planning for the GA and ICM 2022 were already high on the agenda. The 18th IMU GA in 2018 had decided to award ICM 2022 and the 19th IMU GA to Russia with Saint Petersburg as the venue. However, with the unprovoked and aggressive Russian invasion of Ukraine on February 24, it was clear that the IMU could not proceed with the GA and the ICM as planned. We seriously studied the options of what to do instead and ultimately decided to take over the organization of a virtual ICM – with free participation for all – and an in-person GA. At that point, there were no additional financial or human resources available to us, and we only had four months to plan and execute our decisions.

19th IMU General Assembly in Helsinki

Let us start with the GA, which is a rather intense two-day business meeting with 200+ participants. Here elections are carried out, budgets decided, and the venue for the next ICM is selected, in addition to many other decisions that set the direction of the IMU for the coming four years. It is important for the legitimacy of the decisions that are taken that as many of our members as possible are present. Following the EC's decision to relocate the GA, we received several generous offers from our member states to host the meeting, and we also solicited a number of offers ourselves. After carefully reviewing several options, we accepted the generous offer from the Council of Finnish Academies to host the GA in Helsinki, Finland. With its historical and important position between East and West, we found Helsinki to be the ideal venue.

The 19th IMU GA took place on July 3–4. Just as in 2018, the IMU offered to cover travel expenses for one delegate from each Adhering Organization and hotel accommodation for all participants at the GA. There were around 165 participants present in Helsinki, with a further 30 participants joining the meeting remotely. The fact that air traffic, in particular in Europe, continues to be difficult in the post-pandemic period, and that several participants unfortunately tested positive right before they were due to travel, made the number of remote participants higher than anticipated in the weeks before the GA. For the first time in the history of the GA, all votes were carried out using a fully electronic system, and this turned out to be a great success.

Many important decisions were made at the GA, and we will report on a few key ones here. The GA decided to emphasize the IMU's commitment to freedom of science by including a new article in the IMU Statutes. Specifically, the Article

The Union adheres to the International Science Council's principle of embodying the free and responsible practice of science, freedom of movement, association, expression and communication for scientists, as well as equitable opportunities for access to science, its production and benefits, access to data, information and research material; and actively upholds this principle, by opposing any discrimination on the basis of such factors as ethnic origin, religion, citizenship, language, political or other opinion, gender, gender identity and sexual orientation, disability or age.

was added to the IMU Statutes.

Fig. 1: *19th IMU General Assembly group photo*

The new IMU President and Secretary General will be Hiraku Nakajima (Japan) and Christoph Sorger (France), respectively. Their four-year term will commence on January 1, 2023.

The GA passed a resolution expressing support for all mathematicians affected by the war in Ukraine, and in particular the IMU calls upon its members and other scientific organizations to do everything they can to assist our Ukrainian colleagues in these difficult times.

Some of the IMU's Adhering Organizations face temporary adverse circumstances that result in problems paying their IMU membership dues. The GA decided to establish a "reserve fund", based on earmarked donations to assist members in financial difficulties. The EC will administer this fund and consider requests for assistance from members on a case-by-case basis.

It is the prerogative of the GA to decide the location of the next ICM, and the GA voted in favor of the bid from the USA, with ICM 2026 to be held in Philadelphia on July 22–29, 2026, preceded by the 20th IMU GA in New York City on July 19–20, 2026.

IMU Award Ceremony

The unique circumstances in which we found ourselves in 2022 also occasioned a rather unique event. On July 5, the day after the GA, we held the first ever IMU Award Ceremony, hosted in the Aula of Aalto University in Helsinki. We were honored that Mr. Sauli Niinistö, the President of Finland, opened the ceremony. Fortunately, all four Fields Medalists – Hugo Duminil-Copin, June Huh, James Maynard, and Maryna Viazovska, the inaugural IMU Abacus Medalist Mark Braverman, as well as the recipient of the Leelavati Prize, Nikolai Andreev, were able to be present in Helsinki. The recipients of the Chern Medal and the Gauss Prize, Barry Mazur and Elliott H. Lieb respectively, participated in the ceremony remotely.

***Fig. 2:** The 2022 Fields Medalists at the IMU Award Ceremony in the Aula of Aalto University. Photo: Jussi Rekiaro*

For each winner, the audience heard the brief citation of the prize committee and a laudatio by an expert in the field, and also watched the superb videos made by the Simons Foundation. The fully packed Aula enjoyed a delightful award ceremony in an electric atmosphere.

The virtual ICM 2022

Let us now turn to the ICM. Following the EC's decision to switch to a virtual ICM, we started right away to re-establish contact with all speakers, re-inviting those that had declined the first invitation, and collecting titles and abstracts for their talks. At the same time, we investigated various options regarding a suitable platform. Ultimately we accepted an offer from the K.I.T. Group, a subsidiary of the Messe Berlin GmbH group of companies, which is based in Berlin. We decided to organize the program according to Central European Summer Time (CEST). Knowing that this could potentially be problematic for speakers located in completely different time zones, each speaker was given the choice between giving a live talk or submitting a prerecorded one. Happily about 2/3 of the speakers agreed to give a live talk. To develop the platform for the virtual ICM was no small task, and we are immensely grateful to the Heidelberg Laureate Forum Foundation (HLFF) for their generous financial support. In addition, the ICM Satellite Coordination Group, led by Alexei Borodin, Martin Hairer, and Terence Tao, worked independently of the IMU to organize various overlay events. We are also grateful to this group for their efforts.

On July 6, we took advantage of the fact that the Fields Medalists and the IMU Abacus Medalist were all present in Helsinki, and arranged for them all to give their plenary ICM prize lectures in front of a live audience in the Auditorium of Aalto University. This was a great success, with outstanding lectures delivered by the laureates. Both the IMU Award Ceremony and the ICM 2022 prize lectures are available on the IMU YouTube channel .

Over July 7–14 we had a fully virtual ICM for the first time in IMU history. In the lead up to the ICM, we worked closely with the K.I.T. Group to develop a platform that would not only deliver the lectures, but also allowed for a Q&A [Questions and Answers] with the speakers. However, in the last few days before the virtual ICM launched, the K.I.T. Group encountered serious technical problems, which necessitated the restructuring of the format for the virtual ICM at very short notice. This was an exceptionally stressful period for all involved. To cut a long story short, we ended up with a simplified platform that posted all talks on the IMU YouTube channel but eliminated the possibility of a Q&A with the lecturers. This was of course disappointing, but the upside was that, in this format, no registration was necessary, and thus the ICM was truly open to all.

Fig. 3: *virtual ICM 2022 banner*

We remained in Helsinki after the in-person events there for the duration of the virtual ICM, so as to have the opportunity to attend as many lectures as possible. We were very impressed by how the invited speakers handled the new format. Many lectures were given in person in front of a local live audience, and we felt that the speakers had gone the extra mile to make their lectures as engaging and accessible as possible. The experience we all gained in giving video lectures over the two years of the pandemic was certainly evident.

With all lectures now published on the IMU YouTube channel, it pleases us to see that many are taking the opportunity to watch them after they were given at the ICM. We hope that this will continue to serve as a repository of the most exciting and cutting-edge work currently being undertaken in mathematics, and one which is freely and openly accessible to the world. We are also certain that this feature of recording and publishing all ICM lectures on the IMU YouTube channel will become a part of future ICMs.

We would like to warmly thank all the speakers and panelists of the virtual ICM for their great effort in providing excellent talks and panel discussions under very challenging circumstances.

The successful outcome and delivery of the GA and ICM in 2022 are the consequence of a concerted effort by many colleagues. It had to be carried out under very difficult and constrained financial circumstances, and put a severe strain on IMU personnel. In addition to HLFF, we are immensely grateful to the London Mathematical Society, the Mathematical Society of Japan, NTNU, CDC, ICMI, and the Friends of the International Mathematical Union for their generous financial support. We are equally very thankful to all the self-less volunteers who did a wonderful job in developing the outstanding scientific organization of the Congress. We are especially thankful to EC members Nalini Joshi and Paolo Piccione, and to Martin Hairer, chair of the ICM 2022 Program Committee, for their very valuable help in the preparation of the virtual ICM. The IMU is also extremely grateful to the IMU staff at the Secretariat in Berlin for their remarkable efforts in dealing with the many administrative and logistical challenges that arose in 2022.

The successful outcome would not have been possible without the support we received from the community – indeed it was not clear what the right decision would be when we had to make it in the latter part of February 2022, nor could we foresee how things would turn out given that we only had four months to deliver these events. We are glad that we were able to organize an in-person GA and a full-scale virtual ICM at short notice – although we would not volunteer to do so again another time under similar constraints!

3.3 Overview of Meetings and Events 2022

Meeting of the IMU Executive Committee, February 24–27, 2022. The fourth annual meeting of the 2019–2022 IMU EC was held virtually. Hosted online by the IMU Secretariat.

Participants: Carlos E. Kenig, Helge Holden, Nalini Joshi, Loyiso G. Nongxa, Luigi Ambrosio, Andrei Okounkov, Paolo Piccione, R.T. Ramadas, Gang Tian, Günter M. Ziegler, Shigefumi Mori, Hiraku Nakajima, Christoph Sorger, Dietmar Hömberg, Valeria Simoncini, Scott Jung. Guests invited for particular agenda items: Stanislav Smirnov.

Meeting of the IMU Executive Committee, July 2, 2022. As is customary, the IMU EC met the day before the IMU GA to discuss various aspects of the meeting and assign responsibilities. Hosted at the Marina Congress Center, Helsinki, Finland.

Participants: Carlos E. Kenig, Helge Holden, Nalini Joshi, Loyiso G. Nongxa, Paolo Piccione, R.T. Ramadas, Gang Tian, Günter M. Ziegler, Shigefumi Mori, Hiraku Nakajima, Christoph Sorger, Dietmar Hömberg, Scott Jung.

ICMI Executive Committee Meeting: June 28–30, 2022. The first in-person meeting of the 2021–2024 ICMI EC took place in June 2022. Due to the COVID-19 pandemic, all previous meetings had been virtual. Hosted at the IMU Secretariat.

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

"Mathematics Unites". The International Day of Mathematics (IDM), March 14, 2022. "Mathematics Unites" was the theme for the IDM in 2022. The celebrations involved 1,961 events worldwide, with virtual celebrations also held in several languages, notably in Arabic, English, French, Portuguese, and Spanish. The theme for IDM 2023 will be "Mathematics for Everyone".

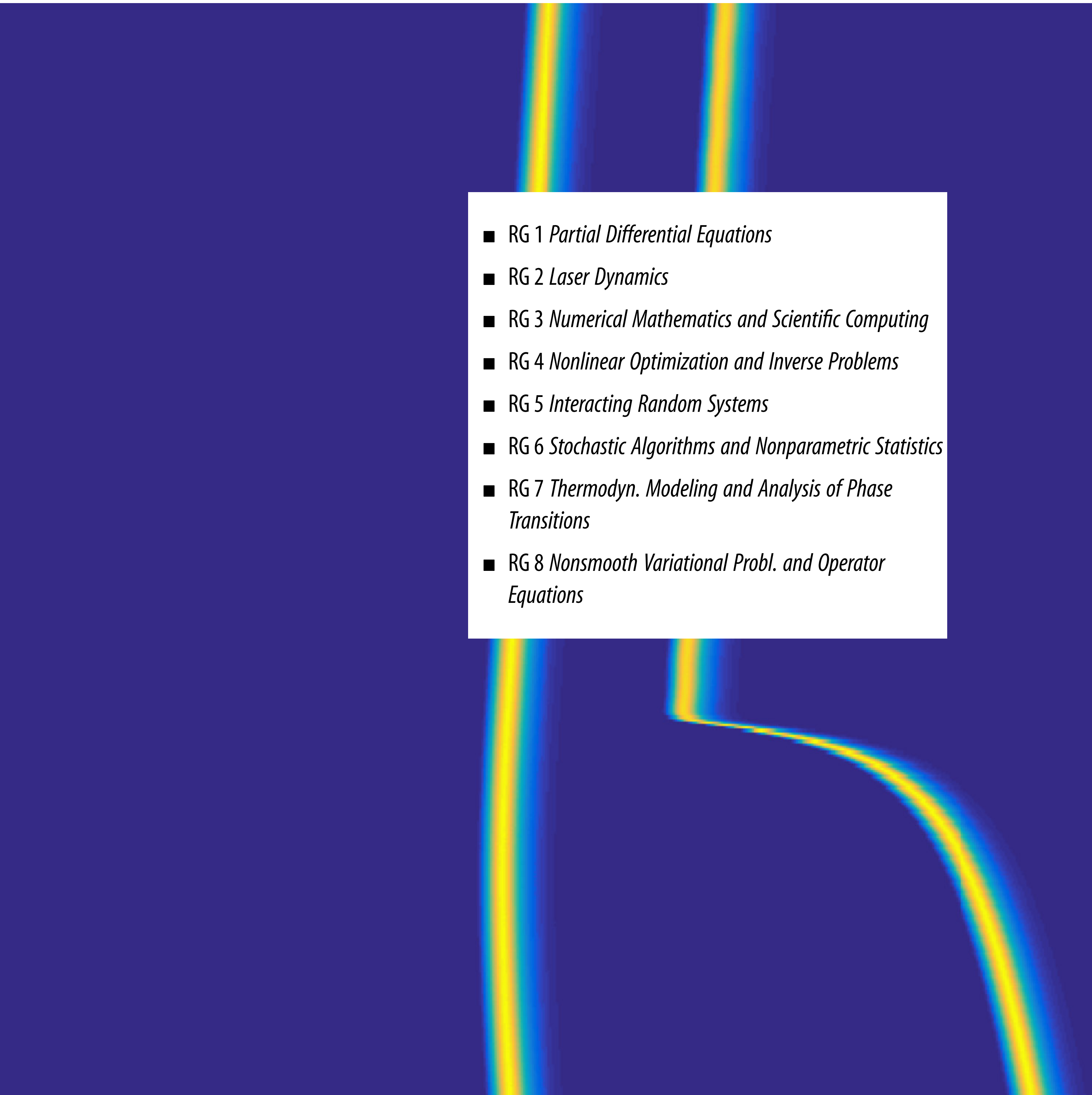
19th IMU General Assembly | IMU Award Ceremony 2022, Helsinki, Finland, July 3–5, 2022.

International Congress of Mathematicians 2022, virtual, July 6–14, 2022.

AK Archive Berlin-Brandenburg Regionaltreffen. A meeting of Leibniz Association archivists from Berlin-Brandenburg was hosted at the IMU Secretariat on December 6, 2022. The meeting was coordinated by IMU Archivist B. Seeliger, and the primary topic of discussion was email archiving.

Guests at the Secretariat. Incoming IMU Secretary General Christoph Sorger visited the IMU Secretariat between October 10–14, 2022, to begin the handover and transition process ahead of his assuming office in 2023.

4 Research Groups' Essentials



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

4.1 Research Group 1 "Partial Differential Equations"

Head:	Prof. Dr. Alexander Mielke
Deputy Head:	Dr. Matthias Liero
Team:	Dr. Pierre-Étienne Druet Dr. Thomas Eiter Priv.-Doz. Dr. Annegret Glitzky Dr. Martin Heida Dr. Katharina Hopf Dr. Michael Kniely (long-term guest) Dr. Thomas Koprucki Dr. Anieza Maltsi Dr. Oliver Marquardt Arbi Moses Badlyan Michael O'Donovan Willem van Oosterhout Dr. Petr Pelech Dr. Joachim Rehberg Stefanie Schindler Priv.-Doz. Dr. Burkhard Schmidt Leon Schütz Magdalena Sliwinska (WIAS Female Master Students Program) Dr. Artur Stephan Dr. Petr Vágner
Secretary:	Andrea Eismann
Nonresident Member:	Prof. Dr. Jürgen Sprekels

The Research Group RG 1 *Partial Differential Equations* continued its scientific work on the mathematical analysis of partial differential equations (PDEs) and their usage for modeling in sciences and engineering. The mathematical theory is developed in close connection with relevant problems in applications. These problems include multiscale and multiphysics problems in optoelectronic semiconductor devices, reaction-diffusion equations (also including temperature coupling), and nonlinear material models with internal variables. The mathematical methods belong to pure functional analysis, mathematical physics, pure and applied analysis, calculus of variations, as well as numerical analysis. Special emphasis is set on qualitative methods for Hamiltonian, gradient, or consistently coupled systems, and on multiscale methods for deriving effective large-scale models from models on smaller scales and stochastic particle systems. Existence, uniqueness, and regularity for initial and boundary value problems in nonsmooth domains and with nonsmooth coefficients are also central topics. The qualitative study of PDEs provides a deeper understanding of the underlying processes and is decisive for the construction of efficient numerical and optimization algorithms.

Fig. 1: *Michael Kniely, long-term visitor of RG 1*

Michael Kniely has been a visiting scientist within RG 1 since March 2022. During his two-year stay, which is financed by an Erwin Schrödinger Fellowship of the Austrian Science Fund (FWF), he has been collaborating with members of RG 1 on electro-energy-reaction-diffusion systems.

Five minisymposia at the "SIAM Conference on Analysis of Partial Differential Equations (PD22)," March 14–18, 2022, were co-organized by Thomas Eiter, Martin Heida, Matthias Liero, Alexander Mielke, and Artur Stephan.

From March 21 to April 11, 2022, Oliver Marquardt held a tutorial on the calculation of electronic properties of semiconductor heterostructures using the open-source SPHInX software library, which is in part maintained by WIAS. The objective was to enable scientists from different backgrounds who work in the field of semiconductor nano-structures to independently perform standard simulations by using the generalized $\mathbf{k}\cdot\mathbf{p}$ module of the SPHInX library.

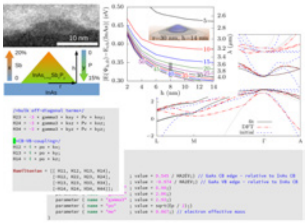


Fig. 2: *Calculating electronic properties of semiconductor hetero-structures with the SPHInX package*

On June 20 and 21, 2022, the online event “Young Researchers’ Forum on Mathematical Fluid Mechanics” organized by Thomas Eiter together with Ryosuke Nakasato and Keiiche Watanabe (both from Waseda University, Tokyo) took place. In order to enhance the exchange between early-career scientists, there were plenary talks and discussion forums as well as short talks in which Ph.D. students presented their research topics.

Karen M. Gambaryan from Yerevan State University, Armenia, visited WIAS in July 2022 within the framework of a long-established collaboration with Oliver Marquardt. The purpose of both his visit in Berlin and the following visit of Oliver Marquardt at Yerevan State University from September 24 to October 22, 2022, was to research novel graded-composition quantum dot molecules by combining experiments and simulations.

In autumn 2022, Matthias Liero co-organized together with members of RG 3, RG 7, and WG BIP the international workshop “MathBio22 – Mathematical Models for Biological Multiscale Systems,” which featured nine invited and 15 contributed talks. Mathematical methods were identified and discussed that bridge the gap in scale and complexity between microscopic descriptions of biological and biophysical systems with corresponding PDE descriptions. The focus of the workshop was on the multiscale nature innate to biological processes connecting interacting biomolecules with complex systems such as cells, tissue, and organs to elucidate macroscopic phenomena.

Anieza Maltsi successfully defended her Ph.D. thesis “A mathematical study of the Darwin–Howie–Whelan equations for Transmission Electron Microscopy” at Humboldt-Universität zu Berlin in November 2022. Two members of RG 1 completed their habilitations at the Technische Universität Berlin and the Humboldt-Universität zu Berlin, respectively. Martin Heida defended his habilitation thesis “Geometric and Measure Theoretic Aspects of Stochastic Homogenization” in February 2022. Matthias Liero’s thesis “Mathematical Analysis of Charge and Heat Flow in Organic Semiconductor Devices", defended in July 2022, discusses mathematical models describing the electrothermal behavior of organic semiconductor devices.

Fig. 3: *Ph.D. defense of Anieza Maltsi*

The annual meeting of the Mathematical Research Data Initiative (MaRDI) took place in November 2022 in hybrid form. The different task areas within the consortium gave overviews on their work, and keynote talks by Martin Grötschel (Berlin-Brandenburgische Akademie der Wissenschaften) and Cord Wiljes (Directorate of Nationale Forschungsdateninfrastruktur – NFDI) highlighted the importance of research data management and informed about activities within NFDI.

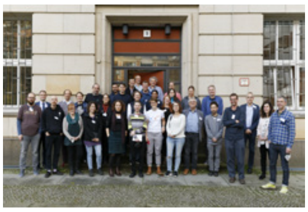


Fig. 4: *MaRDI Annual Workshop 2022*

Alexander Mielke, Head of RG 1, was awarded the “MATH+ Distinguished Fellowship” for his outstanding contributions to the mathematical sciences. Thomas Eiter was chosen to give the 2022 Junior Richard-von-Mises Lecture titled “On time-periodic viscous flow around a moving body.”

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 WG BIP *Modeling, Analysis and Scaling Limits for Bulk-Interface Processes* and was driven by a subproject of the Collaborative Research Center CRC 1114 *Scaling Cascades in Complex Systems*, where RG 1 participates in the project B09 "Materials with discontinuities on many scales," and subprojects in the Priority Programme SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*, namely, the projects "Analysis of thermomechanical models with internal variables" and "Fractal and stochastic homogenization using variational techniques." 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+.

Stochastic homogenization. In the field of stochastic homogenization, recent work on infinite range jump processes was continued. Recent results for regular grids, i.e., $\mathbb{Z}^d$, were extended in the WIAS Preprint no. 2931 to infinite range jump processes on a random subset of $\mathbb{Z}^d$ and to arbitrary point processes in $\mathbb{R}^d$. The main achievements in this work are new Poincaré-type inequalities and compactness results, which are needed for the derivation of effective, homogenized equations in such geometric settings.

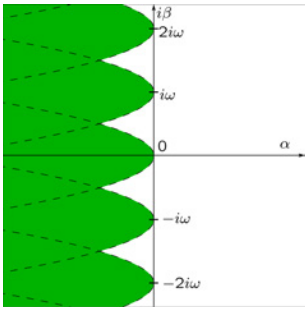


Fig. 5: *For translating and rotating bodies, the essential spectrum of the linearized operator consists of infinitely many parabolas*

Time-periodic flow past a moving body. A classical problem of fluid dynamics is the viscous flow past a translating and rotating obstacle, for example, a propeller in the whole space. If the translational velocity passes a certain threshold, the steady motion becomes unstable, and the flow starts to oscillate. To investigate these time-periodic solutions mathematically, one cannot work in classical Sobolev spaces, since the functional framework has to reflect the spatial decay of solutions in the underlying unbounded domain. In the recent publications Eiter, J. Math. Fluid Mech., 2022, and [1], novel results in this direction were established: The linearized problem was studied based on the corresponding resolvent problem. In the case without translation, uniform resolvent estimates were derived, which were sufficient to show existence of solutions to the linearized time-periodic problem. If the obstacle performs a translation, then the spectral properties become more involved (see Figure 5), and the uniformity of the resolvent estimates requires additional restrictions. Therefore, the existence of time-periodic solutions merely follows under a compatibility condition that seems to be necessary [1]. In the recent WIAS Preprint no. 2942, a general approach to maximal L^p-regularity for time-periodic problems was established, which lead to an existence result for the flow around an oscillating body in a bounded fluid container. An extension to the setting of an unbounded domain, where pointwise decay properties have to be included, is currently under preparation.

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.

Hellinger–Kantorovich gradient flows and geodesic curves. The Hellinger–Kantorovich distance on the space of nonnegative measures was introduced some years ago in a cooperation between Giuseppe Savaré (Milan) and RG 1 to describe the interaction of optimal transport and optimal creation and destruction of mass. It can be viewed as an infimal convolution of the famous Kantorovich–Wasserstein and the Hellinger distance. Due to its interesting structural properties, it has gained a lot of attention in the recent years. In the preprint [2], fine regularity properties of solutions of the underlying extremal problem and associated geodesic curves were established. More precisely, these regularity properties concern the differentiability of optimal Hellinger–Kantorovich potentials in the dual formulation of the distance and of the forward and backward solutions to the associated Hamilton–Jacobi equation. It was shown that on the contact set, where forward and backward solutions agree, delicate first- and second-order super-differentiability properties are satisfied that can be used to establish regularity properties of geodesic curves with respect to the Hellinger–Kantorovich distance. The latter is necessary to characterize convexity properties of functionals on the space of nonnegative measures along such curves and is therefore directly related to the theory of metric gradient flows, which was investigated in the WIAS Preprint no. 2973.

Figure 6 shows the forward and backward solutions of the Hamilton–Jacobi equation with initial data that are optimal for the Hellinger–Kantorovich distance between two Dirac measures.

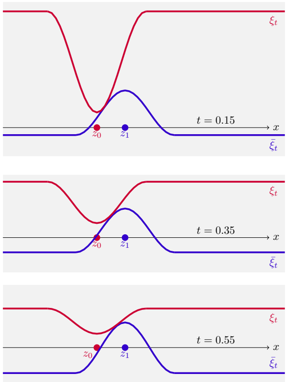


Fig. 6: *Forward (red) and backward (blue) solution of the Hamilton–Jacobi equation at different times*

Stability in entropic cross-diffusion. In physics, chemistry, and biology, cross-diffusion equations describe the temporal evolution of the densities or mass fractions of a multicomponent system. Novel stability estimates for cross-diffusion equations were derived based on an underlying entropic structure [3]. The estimates involve the Bregman distance associated with the entropy function to measure the distance between a weak and a strong solution and, hence, imply the weak-strong uniqueness property. Model-specific adjustments of the Bregman distance were necessary when handling non-isothermal chemical reaction-diffusion processes in order to deal with renormalized solutions. A key advantage of the entropic approach is the robustness of the technique, which allows treating models of multiple components with different mechanical properties and strong cross-effects. The method was adapted in a recent joint work with Martin Burger (Erlangen) (Hopf & Burger, Nonlinear Anal., 2022) to multi-species diffusion with volume constraint.

Semiconductor and optoelectronic devices

In this field, the group benefits from a strong cooperation with RG 2 *Laser Dynamics*, RG 3 *Numerical Mathematics and Scientific Computing*, and LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*. In the Berlin Mathematics Research Center MATH+, the group participated in the projects AA2-10 “Electro-mechanical coupling for semiconductor devices” (with LG NUMSEMIC and Barbara Zwicknagl from Humboldt-Universität zu Berlin) and IN-7 “Electronic properties of gate-confined quantum dots in Si-Ge hetero-structures for qubit generation” together with Torsten Boeck from the Leibniz-Institut für Kristallzüchtung (IKZ) and Oliver Brandt from the Paul-Drude-Institut für Festkörperelektronik (PDI).

In 2022, work in the UVSimTec project started. This project, funded in the framework of the Leibniz competition, is a collaboration with the Ferdinand-Braun-Institut (FBH), the Leibniz-Institut für Kristallzüchtung (IKZ), the Research Group “Experimental Nanophysics and Photonics” at the Technische Universität Berlin, and the Institute for Optoelectronics at the Friedrich-Alexander-Universität Erlangen-Nürnberg.

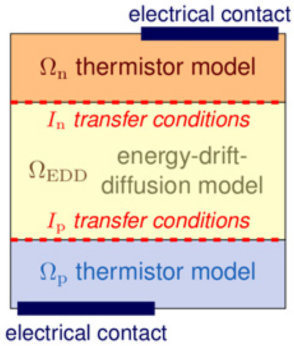


Fig. 7: *Sketch of domain geometry for coarse-grained electrothermal model*

Coarse-grained electrothermal models for organic devices. For the efficient and accurate description of electrothermal feedback in organic semiconductor devices, a coarse-grained model was derived that combines stationary energy-drift-diffusion equations in a subdomain Ω_{EDD} with thermistor-type equations in electron and hole transport layers Ω_{n} and Ω_{p} of organic devices and suitable transmission conditions; see Figure 7. The transmission conditions at I_{n} and I_{p} reflect the normal flux conservation and force local charge neutrality evaluated at the present temperature distribution.

Using regularization arguments and Schauder’s fixed point theorem, the existence of weak solutions was demonstrated. After studying first the situation for classical inorganic semiconductor devices with Boltzmann statistics, these techniques were extended by taking into account the statistical relation given by the Gauss–Fermi integral and mobility functions depending on the temperature, charge-carrier density, and field strength, which is required for a proper description of organic devices; see [4]. For boundary data compatible with thermodynamic equilibrium additionally uniqueness could be verified. Moreover, bounds and higher integrability properties for the electrostatic potential and the quasi-Fermi potentials as well as the temperature were established.

Symmetries in transmission electron microscopy imaging. The main goal of transmission electron microscopy (TEM) is to extract information on the specimen from the generated TEM images. This is particularly used for detecting shapes, sizes, and composition of inclusions in crystalline materials, like quantum wells and quantum dots, which are commonly used as optically active regions in nanophotonic devices. However, there is no direct way to infer the geometric properties of the inclusion from the image, due to the highly nonlinear behavior of the dynamic diffraction. Hence, a commonly taken approach is to simulate the imaging process with inclusions described by parametrized data. Then, the comparison with experimental pictures can be used to fit the chosen parameters and deduce the desired data of the experimental inclusions.

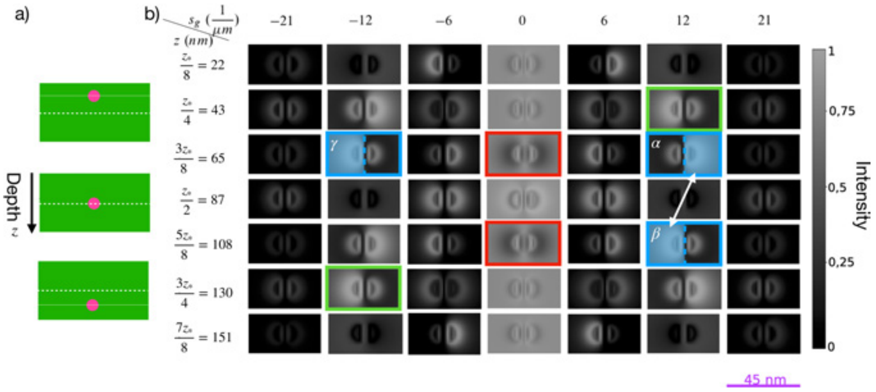


Fig. 8: *Series of TEM images for a spherical quantum dot, showing different kinds of symmetries between images*

An important feature in this process are symmetries that may occur in the imaging for two reasons; first, the inclusions may have certain symmetries and, second, the TEM images may display symmetries that are related, but not identical. The latter arise from the fact that the experimental setup may have its own intrinsic symmetry properties. For the imaging process, it was mathematically proven in [5] that the intensities are invariant under specific transformations. This is done by analyzing the Darwin–Howie–Whelan equations, which are derived from the Schrödinger equation and describe the propagation of the electron wave through the sample. A combination of the proven invariances with specific properties of the strain profile can then explain symmetries observed in TEM images. This approach was applied to study symmetries in TEM images provided by partners from the Institute of Optics and Atomic Physics at the Technische Universität Berlin using selected examples in the field of semiconductor nanostructures such as quantum wells and quantum dots.

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4.2 Research Group 2 "Laser Dynamics"

Head:	Priv.-Doz. Dr. Uwe Bandelow
Deputy Head:	Dr. Matthias Wolfrum
Team:	Dr. Shalva Amiranashvili Dr. Oleksandr Burylko Lasse Ermoneit Alexander Gerdes Katharina Joachimsmeyer (WIAS Female Master Students Programme) Dr. Markus Kantner Lutz Mertensкötter Dr. Alexander Pimenov Dr. Mindaugas Radziunas Fenja Severing (WIAS Female Master Students Programme) Mina Stöhr Dr. Andrei G. Vladimirov
Secretary:	Laura Smain, Veronica Bove

The research of this group is devoted to the study of mathematical problems that appear in nonlinear optics, optoelectronics, and quantum devices. The research activities include mathematical modeling, theoretical investigation of fundamental physical effects, implementation of numerical methods, efficient modeling and simulation of complex devices, and the development of related mathematical theory, mostly in the field of *dynamical systems*. The research is mainly devoted to the application-oriented research topics *dynamics of semiconductor lasers* and *pulses in nonlinear optical media* and contributes to the WIAS core-expertise in *modeling and simulation of semiconductor devices*. Recently, the group has intensified its efforts in the area of modeling and simulation of semiconductor devices for quantum technologies in a cross-group activity together with RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, and LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*.

In 2022, external funding was received within the DFG Collaborative Research Center (CRC) 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*, subproject A3 "Self-organization and control in coupled networks and time-delayed systems," and from the Cluster of Excellence MATH+, project AA2-13 "Data-driven stochastic modeling of semiconductor lasers" together with Technische Universität (TU) Berlin and Ferdinand Braun Institute (FBH) Berlin. The project *Hybrid Chip-scale Frequency Combs Combining III–V Quantum-Dash Mode-Locked Lasers and High-Q Silicon-Nitride Microresonators* (HybridComb) supported by the German Research Foundation (DFG) jointly with the Agence Nationale de la Recherche (ANR, France) has started in May 2022. This is a joint project with Karlsruhe Institute of Technology, Physics Institute in Nice, Telecom SudParis, and Centre for Nanosciences and Nanotechnologies at the University of Paris-Saclay. Also in 2022, the project *UV Lasers: From Modeling and Simulation to Technology* (UVSimTec, Leibniz competition "Collaborative Excellence") has started, which is a joint project together with RG 1, RG 3, TU Berlin, Universität Erlangen-Nürnberg, Leibniz-Institute for Crystal Growth (IKZ), and FBH. Moreover, in 2022 we sold a license for our software `BALaser` to an industry partner.

Further funding was granted for new projects starting in 2023: The three-year project *Excellence in Photonic Crystal Surface Emitting Lasers* (PCSELence) was acquired in the Leibniz competition "Collaborative Excellence" together with RG 3 and LG NUMSEMIC. The project partners are the FBH (coordinating partner) and the group of Prof. S. Noda from Kyoto University (associated partner). The new MATH+ project AA2-17 "Coherent transport of semiconductor spin-qubits: Modeling, simulation and optimal control" is devoted to simulation of a quantum bus for qubit transfer in SiGe semiconductor quantum processors, see Figure 1. The project is a joint activity together with RG 1 and TU Berlin. Collaboration partners are RWTH Aachen, JARA-FIT Institute for Quantum Information, IKZ and TU Munich.

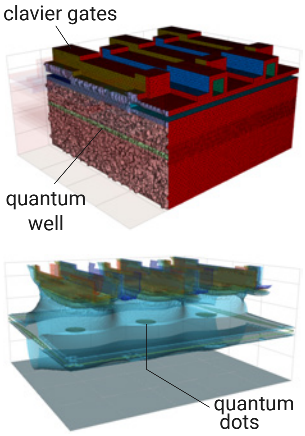

Fig. 1: *Simulation of a quantum bus (with RG 3) where qubits are stored in gate-defined quantum dots*

The cooperation with Russia within the framework of the DFG-RSF (Russian Science Foundation) projects "Underlying nonlinear science of hybrid SOA-fiber laser systems with feedback" and "Collective dynamics of heterogeneous networks of active elements" was suspended as a reaction to the Russian invasion in Ukraine. Since November the group has been hosting Dr. O. Burylko (Institute of Mathematics of the National Academy of Sciences of Ukraine), who received a special MATH+ fellowship for mathematicians from Ukraine. An onsite international workshop "Nonlinear Waves and Turbulence in Photonics" with 18 invited talks was organized to strengthen the cooperation between scientists engaged in nonlinear optics. It was followed by an online meeting, "Minisymposium for Young Researchers," targeted at Ph.D. students. Moreover, the group participates in organizing and performing joint research projects within the Leibniz Research Network "Mathematical Modeling and Simulation (MMS)."

Dynamics of semiconductor lasers

Steady states in dynamical semiconductor laser models. We developed and utilized numerical algorithms for computing stable and unstable steady states in dynamic semiconductor laser models defined by nonlinear ordinary differential equations (ODEs), delay-differential equations (DDEs), or time-dependent partial differential equations (PDEs) with one space dimension. We calculated and analyzed the steady states in order to improve, jointly with our collaboration partner FBH, specific laser emission properties, such as, e.g., the linewidth of the laser. The algorithms are based on semi-analytic techniques for calculating the instantaneous optical modes and Newton–Raphson iterations for the resulting algebraic system of equations. Our results [1] were reported also in an invited talk at the conference "Numerical Simulation of Optoelectronic Devices 2022." Numerical algorithms were included in the software kit `LDSL-tool`.

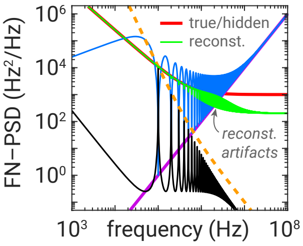

Fig. 2: *Reconstruction of the FN–PSD from DSH data using a Wiener filter*

Accurate estimation of laser linewidth. A new research topic are narrow-linewidth lasers and the related issue of (non-Markovian) noise in semiconductor lasers. Narrow-linewidth lasers are key components for many quantum technologies (*e.g.*, optical atomic clocks, matter-wave interferometers, ion-trap quantum computers). The spectral linewidth of a laser is obtained by measuring the laser's frequency noise power spectral density (FN–PSD). The standard method is the delayed self-heterodyne (DSH) beat note technique, where considerable post-processing is required to remove the footprint of the experimental setup in order to derive the FN–PSD of the free-running laser. The traditional approach, however, disregards the detector noise and thereby induces unphysical artifacts in the reconstructed FN–PSD. We developed an improved post-processing routine based on a parametric Wiener filter [2], which is free of reconstruction artifacts, provided that a good estimate of the signal-to-noise ratio is supplied; see Figure 2. In our method, artifacts are deliberately suppressed to minimize the consistency error. Thereby it yields an accurate estimate of the linewidth even in the case of strong measurement noise, where the intrinsic linewidth plateau is not visible using the traditional approach.

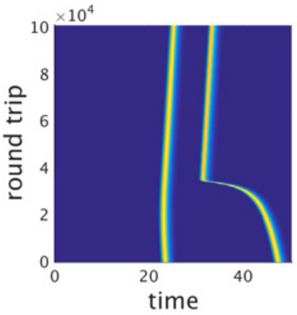

Fig. 3: *Temporal soliton bound state formation in a nonlinear mirror mode-locked laser*

Dynamics of nonlinear mirror mode-locked lasers. Interaction equations governing the slow time evolution of the coordinates and phases of weakly interacting temporal cavity solitons in a delay differential equation model of a nonlinear mirror mode-locked laser were derived in [3]. It was shown that in the case of long-range interaction due to gain depletion and slow recovery apart from the usual repulsion leading to harmonic mode-locking regimes, an attractive interaction is also possible. This attraction can lead to a formation of incoherent weakly oscillating soliton bound states with the soliton phase difference growing monotonously in time; see Figure 3. Unlike the non-local one, local interaction via electric field envelope tails depends strongly on the soliton phase difference and can result in anti-phase or in-phase stationary or breathing harmonic mode-locking regimes. The phase plane of the interaction equation is shown in Figure 4, where the red (blue) limit cycle corresponds to a stable (unstable) breathing soliton bound state.

Pulses in nonlinear optical media

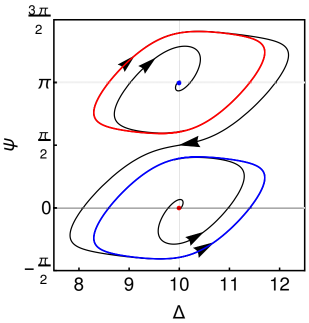

Fig. 4: *Phase plane of the soliton interaction equations. Δ is the soliton separation, and ψ is their phase difference.*

New theory of four-wave mixing interactions. Propagation of optical pulses in guided systems is typically considered in a narrow moving computational domain, by assuming unidirectionality, expanding the dispersion relation, using complex envelopes with only positive frequencies, and solving the evolution problem by employing the space variable instead of time. At least some of these assumptions are not suitable for extreme pulses, which require a more accurate description. Therefore, the fundamental problem of the nonlinear wave propagation and modulation instability was studied using full Maxwell equations, full dispersion law and all possible four-wave mixing processes for all possible frequencies. One result was an accurate proof that negative-frequency waves cannot be excited in such a way. Another one: We demonstrated excitation of backward waves, which looks similar to the Brillouin scattering and yet takes place without necessity of material waves [4]. These results were also presented in a Scientific Highlights article on page 10.

Temporal cavity solitons in a Kerr resonator with two filters. A mathematical model of a Kerr cavity with two Lorentzian spectral filters having different central frequencies was developed in the form of a second-order delay-differential equation. It was shown that the dispersion introduced by the filters can lead to modulational instability and appearance of stable temporal cavity solitons even when the intracavity material dispersion is negligible. It was demonstrated that in a certain limit the model equation can be reduced to the famous Lugiato–Lefever equation with additional diffusion term. The modeling approach developed is also suitable for the analysis of more complex systems with two spectral filters, such as Mamyshev oscillators.

Theory of dynamical systems

The mathematical research on dynamical systems provides the theoretical background for the applied topics in optoelectronics and nonlinear optics of this group. Ongoing work within the CRC 910 is related to temporal dissipative solitons in delay-differential equations and collective dynamics in large coupled systems. In a cooperation with the Leibniz-Institut für Neurobiologie (LIN), which was initiated within the Leibniz Research Network "Mathematical Modeling and Simulation (MMS)," we investigated the adaptation of event-related fields in the auditory cortex based on a dynamical oscillators network model [5]. The model describes excitatory and inhibitory interactions of cell populations, with the excitatory connections modulated by short-term synaptic depression. Using time-scale separation methods, it was possible to analyze and understand the experimentally measured event-related fields and their adaptation as a superposition of the network modes with the adapted connectivity.

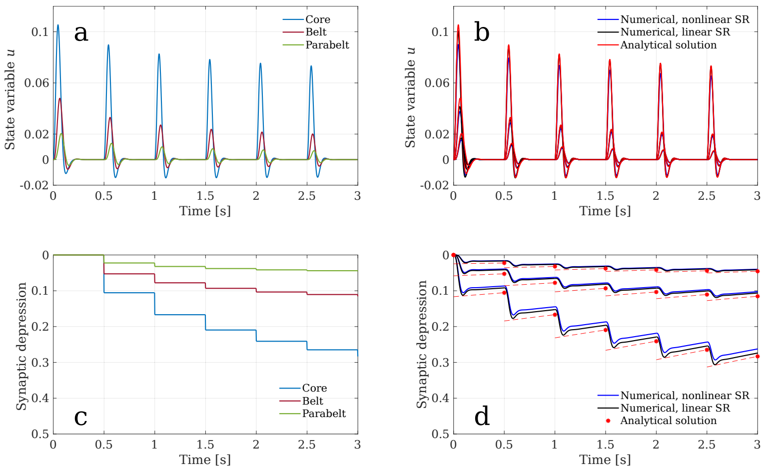

Fig. 5: *Dynamics of the audio cortex under periodic stimulation: adaptation of the event-related fields by short-term synaptic depression; for details, see [5]*

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4.3 Research Group 3 “Numerical Mathematics and Scientific Computing”

Head:	Prof. Dr. Volker John
Deputy Head:	Dr. Jürgen Fuhrmann
Team:	Dr. Naveed Ahmed Maryam Asadi (WIAS Female Master Students Program) Camilla Belponer Priv.-Doz. Dr. Alfonso Caiazzo Dr. Medine Demir Priv.-Doz. Dr. Wolfgang Dreyer (long-term guest) Derk Frerichs-Mihov Dr. Felipe Galarce Marín Mihaela Karcheva (Apprentice) Sarah Katz Dr. Zahra Lakdawala Xu Li (scholarship holder) Leo Markmann (Apprentice) Cristina Melnic (WIAS Female Master Students Program) Dr. Christian Merdon Dr. Baptiste Moreau Dr. Ondřej Pártl Daniel Runge Dr. Holger Stephan Timo Streckenbach Dr. Ulrich Wilbrandt Marwa Zainelabdeen (WIAS Female Master Students Program)
Secretary:	Marion Lawrenz

RG 3 studies the development of numerical methods, their numerical analysis, and it works at implementing software for the numerical solution of partial differential equations (PDEs). Many of the research topics have been inspired by problems from applications in fields like computational biomedicine (see the Scientific Highlights article by Alfonso Caiazzo on page 15), numerical methods for charge transport (in cooperation with LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*), and computational fluid dynamics (CFD). The international standing of the group in CFD has been highlighted by the success of the workshop “Numerical Methods and Analysis in CFD” in July 2022, which was organized jointly by Carsten Carstensen (Humboldt-Universität zu Berlin), Volker John, and Stefan Sauter (ETH Zürich). Presentations at the workshop included the first of the three topics detailed below.

Divergence-free discretizations in CFD

In the previous year, RG 3 was involved in the development of novel divergence-free schemes for the discretization of the incompressible Navier–Stokes equations in continuation of its research on pressure-robustness in computational fluid dynamics.

In cooperation with collaborators from the Shandong University, a novel family of schemes was suggested that are based on the classical Scott–Vogelius finite element methods. These methods usually only work on special meshes, e.g., barycentrically refined ones, that ensure inf-sup stability and therefore unique solvability of the problem. The novel approach in [4] enriches the velocity space not by higher-order bubbles as in previous classical approaches, but employs some additional equal-order Raviart–Thomas functions. They are chosen in such a way that the method is guaranteed to be inf-sup stable on arbitrary shape-regular simplicial meshes and yields a divergence-free solution. This solution consists of a pressure-robust, optimally converging H^1-conforming part and a small $H(\mathrm{div})$-conforming part that can be included to have a fully divergence-free velocity field, e.g., for use in flow-transport coupled problems that appear in several projects. In two space dimensions and for a quadratic velocity ansatz space, the novel approach adds two additional Raviart–Thomas bubbles on each triangle, which is the same number that is used by, e.g., the classical P2-bubble element. However, besides the lower polynomial degree of the enrichment functions and the exact preservation of the divergence constraint, one remarkable feature of the new approach is the possibility of an algebraic reduction step that reduces the numerical costs to compute the discrete solution essentially to that of a $P_k \times P_0$ system. That means that all higher-order pressure degrees of freedom and all enrichment degrees of freedom are removed from the linear system and can be obtained afterwards by a low-cost post-processing [4].

The approach was also successfully extended to time-dependent Navier–Stokes flows where the additional difficulty of discretizing the convection term appears. Here, two possible discretizations were suggested and analyzed. One employs the upwinding known from discontinuous Galerkin (DG) methods, and the other one only involves volume integrals. Both of them preserve the skew symmetry that is essential for conservation of energy, linear momentum, and angular momentum. Moreover, the scheme was proven to be convection robust without compromising any beneficial properties from the Stokes case, in particular, the possibility of the reduction step. The efficiency and accuracy of the novel schemes was showcased in the challenging Kelvin–Helmholtz instability benchmark problem [1], see Figure 1 for some snapshots. An implementation of the novel schemes is also available in the Julia package `GradientRobustMultiPhysics.jl` [5].

Collaborations and research on these novel schemes will continue, possibly regarding preconditioners and linear solvers, as well as their application to related nonlinear problems.

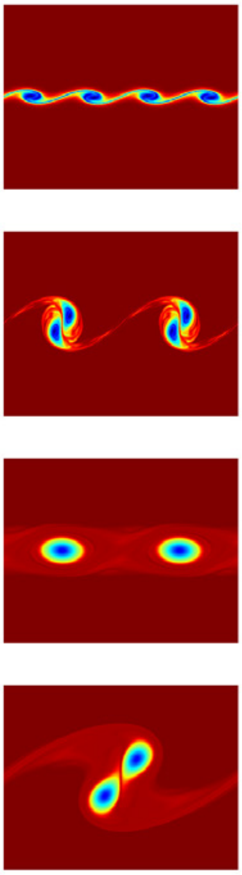

Fig. 1: *Snapshots of the Kelvin–Helmholtz instability problem at times* $T = 10, 34, 200, 272$

On deploying deep learning techniques in CFD

In recent decades, deep neural networks, a form of deep learning, have seen a steep increase in interest, see Figure 2 for a representation. Even though that these techniques were invented as early as in the 1960s, they seem to be realizing their potential only in recent years. Last year, RG 3 started to find ways to exploit this potential in CFD as well. Convection-diffusion-reaction equations are basic models that describe the transport of a scalar quantity, e.g., heat, mass, or species concentration, within a flowing medium. These equations are used to study a wide range of problems in fields such as fluid dynamics, heat transfer, mass transfer, chemical engineering, and biology. In the convection-dominated case, the convection is much stronger than the diffusion and, hence, the transport of the quantity of interest is primarily due to the motion of the fluid. It is well known that many classical numerical methods struggle to approximate the solution accurately in the

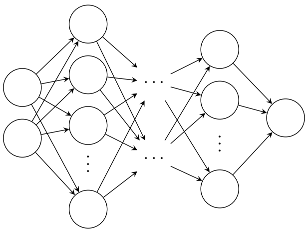

Fig. 2: *Representation of a deep neural network with two inputs and one output*

convection-dominated regime on feasible grids. The convection-dominated situation can be seen as a multiscale problem, where the layers are the small scales that cannot be resolved. Numerical solutions are often polluted by unphysical values such as negative concentrations or concentrations larger than 100%, so-called *spurious oscillations*. This is also the case for DG methods; see, e.g., Figure 3 for a discrete discontinuous P_1 solution to a classical benchmark problem proposed by Hughes, Mallet, and Mizukami. Due to the boundary conditions of the problem, its solution takes values in $[0, 1]$ and is characterized by being 0 in one part and 1 in the other part of the domain, except for a steep gradient that connects these two regions; see also [2] for a concrete definition.

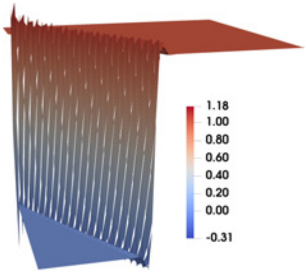

Fig. 3: *The discrete solution of a benchmark problem, which should lie in* $[0, 1]$*, obtained with linear DG finite elements exhibits large spurious oscillations*

Slope limiters are a known way to significantly reduce unphysical values in a post-processing step. First, based on local features of the solutions, they try to identify regions where unphysical values occur, and second, the solution is locally replaced in the spotted regions. Since it is well known that deep neural networks are universal function approximators; in [2], it was investigated how to use deep neural networks to mark the regions that are polluted by spurious oscillations. To this end, various configurations of multilayer perceptron models, a special type of neural networks, were implemented in TensorFlow, a widely used open-source framework for deep learning. After they have been trained with data, which came from the P_1 discrete solution to the above-mentioned benchmark problem, the best model was identified and afterwards applied to higher-order discrete solutions. To archive this, a way was found how to couple TensorFlow to the in-house research software `ParMooN` in the sense that trained networks can be loaded and used. It was observed that it is still capable to identify reasonable regions and produce solutions with significantly less spurious oscillations even though it was not trained with such data; see Figure 4. Usually, the quality was comparable to the classical post-processing methods. Afterwards, this network was applied to another benchmark problem with similar features of the solution. It was still able to obtain reasonable solutions with measurable less unphysical values, but the classical methods have produced slightly better results [2]. One reason certainly is that the networks have been trained with data from classical methods. In the future, paths to generate training data independent of classical methods have to be identified. Furthermore, other types of deep neural networks might be investigated.

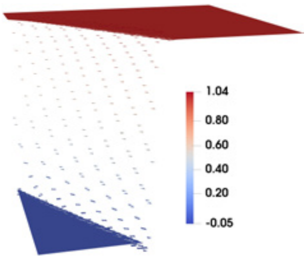

Fig. 4: *The discrete solution of Figure 3 post-processed with the best neural network of [2] shows significantly less spurious oscillations*

Another inspiring idea are so-called *physics-informed neural networks* (PINNs), which are a way of deploying deep neural networks directly as numerical approximations of the solution of PDEs. In the future, RG 3 will explore the capabilities but also the limitations of PINNs as well as further applications of deep neural networks in CFD simulations.

`PDELib.jl` – a Julia-based framework for the solution of partial differential equations

The programming language Julia has been developed with a focus on applications in data science and scientific computing. It combines efficiency, high abstraction level, and a rather simple syntax. Julia comes along with a growing package ecosystem and a best-in-class package manager that supports reproducible research and a rapid pace of cooperative package development. Tools, e.g., for the solution of systems of ordinary differential equations, optimization, and bifurcation analysis, neural networks are readily available from the Julia ecosystem and can be readily integrated into project code, without the need for own implementations or maintenance of a complicated build system.

Leveraging the experience gained with the development of the PDE solver toolbox `pdelib`, which was realized in a combination of C++ and Python, similar core functionalities for the solution of PDEs have been implemented in Julia. This effort resulted in a number of related Julia packages that are subsumed under the label `PDELib.jl`. Functionalities include grid generation and grid management, visualization for functions on grids, and efficient sparse matrix assembly. Based on this foundation, the package `VoronoiFVM.jl` [3] implements the Voronoi box-based finite volume method for nonlinear systems of PDEs on one-, two-, and three-dimensional simplicial meshes. The availability of forward-mode automatic differentiation in Julia removes the burden of the implementation of derivatives of complicated nonlinear functions from the shoulder of the users of the package. A similar approach was taken in the finite element package `GradientRobustMultiPhysics.jl` [5] already mentioned. All packages were registered under open source licenses in the Julia General Registry and are thus available to the Julia community.

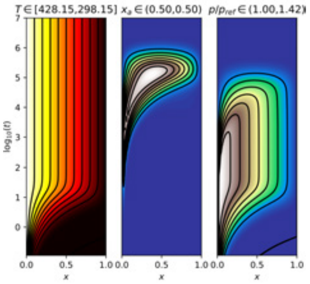

Fig. 5: *Time evolution of temperature, molar fraction, and pressure in a nonisothermal dusty gas model [7, 3]*

The packages `VoronoiFVM.jl` and `GradientRobustMultiPhysics.jl` provide core functionalities to several research projects realized within the group and in cooperation with other WIAS research groups: semiconductor device simulation with LG NUMSEMIC, RG 1 *Partial Differential Equations*, and RG 2 *Laser Dynamics*, ion channel modeling with RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*. These packages are used as well for the simulation of solid oxide cells with University of Chemistry and Technology Prague [6] and for multiscale modeling of heterogeneous catalysis with Fritz Haber Institute Berlin.

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4.4 Research Group 4 “Nonlinear Optimization and Inverse Problems”

Head:	Prof. Dr. Dietmar Hömberg
Deputy Head:	Priv.-Doz. Dr. René Henrion
Team:	Vitalii Aksenov Dr. Ingo Bremer Moritz Ebeling-Rump Priv.-Doz. Dr. Martin Eigel Robert Gruhlke Hanyue Gu (WIAS Female Master Students Program) Dr. Holger Heitsch Dr. Robert Lasarzik Nina Kliche Okunowa Toluwani (WIAS Female Master Students Program) Sophie Luisa Plato Dr. Andreas Rathsfeld Janina Schütte David Sommer
Secretary:	Anke Giese

The research group investigates optimization and inverse problems occurring in current engineering and economic applications. A specific focus of research in optimization and optimal control is the investigation of special structures resulting from the presence of uncertain and nonsmooth data. Our work is related to the main application areas 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 2022 are detailed.

Stochastic and nonsmooth optimization

The research on stochastic and nonsmooth optimization is associated with projects within the programs DFG Transregio (TRR) 154, Berlin Mathematics Research Center MATH+, and Gaspard

Monge Program for Optimization (PGMO) funded by Fondation Mathématique Jacques Hadamard. A major achievement in 2022 was the successful application for the third and last funding period (2022–2026) of TRR154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks*. The funding of the running PGMO project (together wih Hasnaa Zidani, Rouen) could be renewed as well for another year, and a second PGMO project was set up for one year (together with Tatiana González Grandón, Flensburg, and Didier Aussel, Perpignan). Within MATH+, one project expired (together with Caren Tischendorf, Berlin) and work on a new one was started within RG 4.

Regarding TRR 154, work turned about four topics: time-dependent probabilistic capacity maximization in gas networks; two- and multistage chance constraints [4]; probabilistic turnpike phenomenon in a discrete-time problem of optimal control (see Figure 1, left); necessary and sufficient optimality conditions in a (static) partial differential equations (PDE)-constrained optimization problem subject to uniform (with respect to the domain) probabilistic state constraints. The latter research is a joint activity with RG 8 and builds a bridge to the first PGMO project where time dependence is added and some probabilistic end-point constraint (with respect to time) considered instead. Future research will be devoted to the algorithmic solution of these problems and will heavily rely on ideas developed in [1].

The aim of the newly started MATH+ project is to model, analyze, and algorithmically solve the optimal dispatch and design of minigrids with uncertain parameters (demand, energy provided by renewables). This topic is also related with the second PGMO project, which, however, looks at the problem from an operations research perspective with additional economic aspects (tariffs), but with a simplistic battery model. The MATH+ project, in contrast, aims at incorporating an appropriate differential equation for battery (un-)/loading and aging under random parameters (e.g., load) such that inequality constraints (e.g., demand satisfaction) can be guaranteed with a given, sufficiently high probability. In a first step, a simple optimal control problem for the temperature management of a battery is analyzed, where the ambient temperature is considered to be random (see Figure 1, right) and the battery temperature has to be kept in a certain range with given probability.

Besides the project-driven research, the earlier initiated cooperation with Abderrahim Jourani (Dijon) and Boris Mordukhovich (Detroit) on the optimal control of polyhedral sweeping processes and with Kawtar El Karfi and Driss Mentagui (Kenitra, Morocco) on an agricultural investment problem with uncertain parameters led to joint publications.

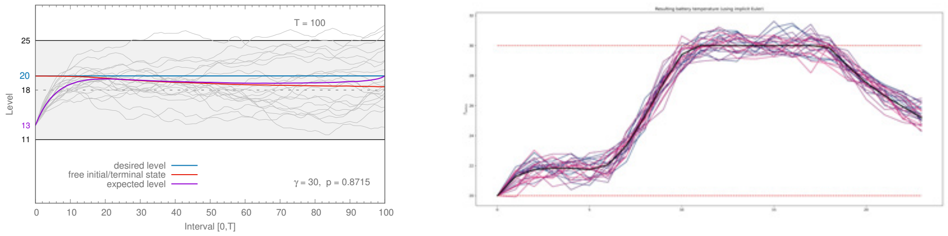


Fig. 1: *Left: Turnpike phenomenon in reservoir management with random inflow and controlled release. Right: Scenarios for battery temperature in an optimal control problem under random ambient temperature.*

Inverse problems for stochastic data and reconstruction of stochastic surfaces

Interacting particle systems for Bayesian inference. Ensemble methods such as the *ensemble Kalman sampler* or *affine invariant Langevin dynamics* have become popular approaches for the solution of Bayesian inference problems. Under adequate assumptions on the underlying ergodic stochastic process, particles initially sampled from some simple distribution are transported to an invariant measure according to the posterior measure. Since the computation is expensive when many interacting particles are transported, a new approach with a dampened Langevin dynamic was devised in [2] that reduces the number of calls of the underlying model significantly, for which two key ideas are responsible as shown in Figure 2. First, different sample enrichment strategies were examined. These allow to start with a small set of particles that gets enlarged after longer simulation intervals. Second, a homotopy approach was introduced by which the transport to highly nonlinear and multimodal distributions becomes feasible. In numerical experiments, it was shown that the developed method improves on the current state-of-the-art and is capable to treat even challenging distributions.

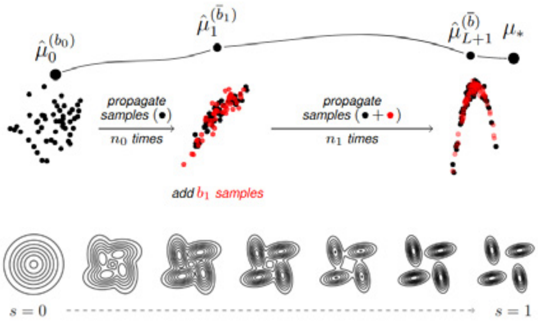


Fig. 2: *Top: Particle transport to the invariant measure and enrichment. Bottom: Homotopy approach interpolating between a simple Gaussian and a multimodal distribution (left to right).*

Multilevel neural networks for adaptive finite element simulations. Neural networks (NN) have become an indispensable tool in many scientific areas and engineering due to the large expressivity of their compositional representation. In addition to pattern matching tasks, they become increasingly important in the area of scientific machine learning for the simulation of complex physical models. When solving PDEs, it can be observed that the accuracy of the classical approaches has not been reached yet, which can, in particular, be attributed to large parameter architectures that are not adapted to the problem structure and are difficult to train. As a remedy, a new architecture was developed that mimics well-known multigrid finite element solvers. This allows to exploit the multiscale structure by generating fewer training data on finer levels of a grid hierarchy, hence reducing the training complexity and leading to better approximations. Moreover, this is the basis for the derivation of an error estimation procedure that will result in an even more data-efficient adaptive approach.

Polymorphic uncertainties and low-rank Gaussian processes. The description of uncertainties commonly is carried out in a probabilistic context. However, a popular application in engineering is the introduction of expert knowledge in terms of fuzzy logic. In collaboration with engineering partners from the Technische Universität Berlin, an elasticity model problem on a fuzzy perforated domain was examined. Stress peaks in the material over time lead to fatigue and eventually structural failure. A new domain decomposition approach with local surrogate responses was devised. For this, an alternating Schwarz method was combined with local NN predictions, leading to an efficient numerical approach for the considered high-dimensional models.

Another compression technique than NNs was used in the context of Gaussian process (GP) regression. For this class of high-dimensional problems, where the amount of sampling data determines the polynomial complexity, low-rank hierarchical tensors were used for efficient kernel learning. The central idea was to compose a low-rank function with a GP covariance function, leading to an increased expressivity when compared to NN architectures.

Scatterometry with rough surfaces. Roughness effects for the scattering of waves by non-perfect planar surfaces are not negligible. The rigorous solution of, e.g., the Dirichlet problem for the Helmholtz equation is to be modified in order to account for the finite cross section of beams. Using this, the density function of the reflected intensity can be approximated by that of periodic or biperiodic surfaces. Corresponding formulas for the far-field pattern are derived in [7], and necessary assumptions for their validity are fixed.

Optimal control of multifield and multiscale problems

One main focus of this year's research effort was the analysis of a coupled nonlinear system of partial differential equations, modeling the spatial-temporal interaction of a predator-prey pair. Introducing a generalized solution concept based on a weak formulation for the prey and an energy- and entropy-like inequality for the predator, we were able to prove the existence of these generalized solutions in all space dimensions, where the existence of weak solutions, yet unknown, seems to be out of reach. These generalized solutions fulfill the weak-strong uniqueness property that we proved with the aid of a relative energy inequality, which was a novel approach in the realm of PDEs for biological applications.

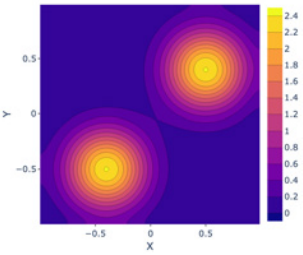


Fig. 3: Prey density at some time $t > 0$

This predator-prey model was of particular interest to us, due to its relevance in biological pest control, where predators that actively hunt the present pest are especially convenient. Numerical simulations, which we performed, indeed suggested that the considered model captures the hunting behavior of the predator, which can, for example, be seen in Figure 3 and Figure 4, where it is visible that predators have accumulated where prey is plenty. In future, we hope to collaborate with Hawassa University in Ethiopia and industrial partners in the production of ornamental plants, like the rose grower Afriflora, on including an optimal control strategy into the model to improve the effectiveness of biological pest control.

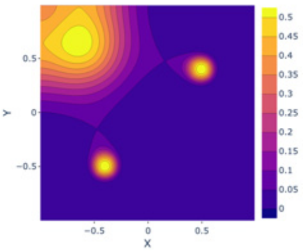
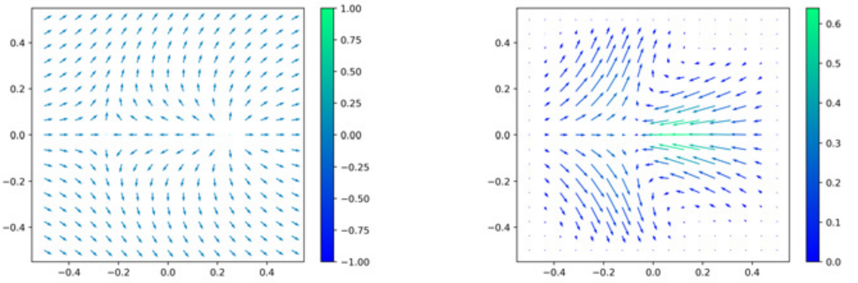


Fig. 4: Predator density at some time $t > 0$

In a different project in cooperation with RG 1, we investigated multidimensional hyperbolic conservation laws. These PDE systems are omnipresent in models of continuum physics. Important examples are the incompressible and compressible Euler equations for gas dynamics. In [3], we provided a novel analytical framework, called *energy-variational solutions*, for such systems. This framework provides a rich variational structure for evolutionary PDEs and implies several nice properties for the solutions, e.g., solutions are known to exist and coincide with strong solutions. As long as such solutions exist, they form a semi-flow, i.e., restrictions and concatenations of solutions of smaller and larger time intervals, respectively, are known to be solutions again. Furthermore, the solution set is known to be convex and weakly-star closed. These properties pave the way for an application of techniques from optimal control in order to select a suitable physically relevant solution by maximizing the dissipation rate and using set-valued continuity properties. The solvability concept of energy-variational solutions heavily depends on the choice of the regularity weight $\mathcal{K}$, which has to be chosen for the considered PDE system. For a certain choice, the equivalence of energy-variational and dissipative weak solutions was shown to hold for the incompressible and compressible Euler system. For dissipative weak solutions, the equations are fulfilled in a distributional sense up to a defect measure, which is an auxiliary variable for the system. One advantage of energy-variational solutions is that the auxiliary variable to quantify the energy defect is only one-dimensional in contrast to the measure-valued defect for dissipative weak solutions.

An additional advantage of energy-variational solutions was explored in [6], where the numerical approximation of the Ericksen–Leslie equations, a model for anisotropic fluids, was considered. There, it was proven that solutions to a fully discrete, implementable, and structure-inheriting finite-element scheme converge to an energy-variational solution in the limit of vanishing discretization for a particular regularity weight $\mathcal{K}$. Moreover, the algorithm was implemented and tested on different benchmarks in the field of anisotropic fluids (see Figure 5).



(a) Initial value for the anisotropy in the fluid (b) Velocity field after a short time $t > 0$

***Fig. 5:** The given initial value for the anisotropy with zero initial velocity induces a velocity after a short period of time*

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4.5 Research Group 5 “Interacting Random Systems”

Head:	Prof. Dr. Wolfgang König
Deputy Head:	Dr. Robert Patterson
Team:	Anne Flöge (WIAS Female Master Students Program) Dr. Tejas Iyer Julian Kern Heide Langhammer Dr. Elena Magnanini Alexandra Quitmann Dr. Michiel Renger Helia Shafigh Dr. Huanyu Yang Dr. Alexander Zass Dr. Willem van Zuijlen
Secretary:	Christina van de Sand

The activities of the Research Group RG 5 *Interacting Random Systems* during 2022 dealt primarily with collections of entities distributed in space and undergoing random interactions or events. 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. This can include changes in the observable properties of materials or the emergence of patterns. The applications and motivations for the research can generally be found in topics arising in the natural sciences.

After the rapid development of the group in 2021, the last year has seen more continuity enabling intensive work on projects within the German Science Foundation Priority Program *Random Geometric Systems (SPP 2265)*. In collaboration with WG BIP *Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes* and Freie Universität Berlin, the group secured funding in the third phase of the German Science Foundation Collaborative Research Center *Scaling Cascades in Complex Systems (CRC 1114)* building on hard work during 2021.

Two new Ph.D. students joined the group during 2022, and one long-term member of the group left on reaching the end of his contract. It is expected that the group composition will remain stable next year as we apply for a second phase of the *SPP 2265* coordinated by the group leader.

Physical travel to exchange and discuss ideas with other scientists was possible on a much greater scale in 2022 than in the immediately preceding years. This was very welcome since although online and hybrid formats have established themselves as methods for the presentation of results, video conferencing is not a good substitute for informal and exploratory scientific discussions in person. The group was very pleased to host the First Annual Conference of the *SPP 2265* in Berlin. The conference took place in Berlin and was the first time members of the *SPP 2265* had met on a large scale since its inception. One member of the RG 5 was part of the organizing committee for the hybrid workshop “Junior Female Researchers in Probability.” In collaboration with the LG DYCOMNET *Probabilistic Methods for Dynamic Communication Networks*, a conference on “Random Point Processes in Statistical Physics” was organized.

Three topics of significant progress in the research of the RG 5 in the area of interacting spatial particle systems are discussed briefly below. Further topics studied in the group during 2022 include large deviations and variational representations of the limiting dynamics for interacting particle systems of chemical reaction type, regularity structures for random materials and trail formation in agent-based models.

In teaching, the head of RG 5, supported by group members, supervised many bachelor's and master's theses at Technische Universität Berlin on various topics, many of which arose out of research in the group. A small number of theses were supervised independently by experienced post-doctoral members of the group. Two group members gave lecture courses at Freie Universität Berlin.

Condensation phenomena of Bose–Einstein type

In 1925, Albert Einstein conjectured the existence of a new kind of state of matter in a symmetrized particle ensemble. He was extending an idea of Satyendra Nath Bose, and the conjectured new state of matter became known as Bose–Einstein condensate (BEC). In such a condensate, a positive fraction of the gas particles at extremely low temperature remain in the same quantum mechanical state. Searching for mathematical understanding of this, which remains a prominent open problem, is one focus of the work of RG 5.

In one of its projects on this topic, the group considers a canonic free bosonic many-body system (ideal gas) with N particles at finite inverse temperature $\beta > 0$ in the thermodynamic limit, i.e., in a large box Λ_N in $\mathbb{R}^d$ of volume N/ρ, where $\rho > 0$ is the fixed particle density. The Hamiltonian is given by $\mathcal{H}_N^{(\Lambda)} = -\frac{1}{2}\sum_{i=1}^N \Delta_i^{(\Lambda)}$, where $\Delta^{(\Lambda)}$ is the Laplace operator in Λ.

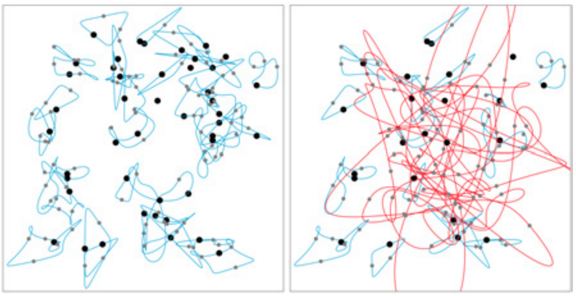

Fig. 1: *Depiction of two ensembles of Brownian loops. On the left, the particle density is low, and no long loop appears, while on the right, there is a very long loop (red).*

The main object of study in an ongoing project is the one-particle reduced density operator with kernel $\gamma_N^{(\Lambda)}(x,y)$, the partial trace of the symmetrized (i.e., projected on permutation-invariant wave functions) operator

$$\frac{1}{Z_N^{(\Lambda)}(\beta)} \mathrm{e}^{-\beta \mathcal{H}_N^{(\Lambda)}}.$$

It is known (see, e.g., [4]) that BEC corresponds to *off-diagonal long-range order* (ODLRO), that is, to the fact that the largest eigenvalue of this operator is of order N. A rigorous proof that such a phenomenon does occur seems to be missing in the literature much to our surprise (the result is often cited). We employ the Feynman–Kac formula to express $\gamma_N^{(\Lambda)}$ in terms of Brownian loops (see Figure 1) and are proving ODLRO for large particle densities ρ, for three types of boundary conditions: empty (the loops are allowed to exit the box), periodic (the box is a torus), and zero (the loops stay inside the box).

RG 5 also worked in 2022 on a partially interacting version of the Bose gas, where any two particles inside a loop are subject to a repellence. Here, we derived a large-deviation principle for the joint statistics of all the loop lengths and a criterion for the existence of the BEC phase transition. The occurrence of this is proved using lace expansions, but only in dimensions $d \geq 5$. This restriction is only due to the proof technique; actually, the phase transition is conjectured to occur in dimensions ≥ 2 for this model (not only ≥ 3, as in the free Bose gas!). The main value of our analysis is the insight that all the Brownian loops with that interaction behave like the well-known self-repellent random walk.

Spatial coagulation and gelation

A coagulation process describes the behavior of a particle system where pairs of particles merge as time passes. These models have a wide range of applications that is thoroughly described in [1]. It was observed that a certain kind of phase transition could happen, depending on the coagulation kernel, leading to a phenomenon called *gelation*, which we can interpret as the creation, in finite time, of at least one cluster containing a positive fraction of the entire mass in the system.

In collaboration with Luisa Andreis (Università degli Studi di Milano), we are investigating a model of coagulation for spatially distributed particles. More precisely, each coagulation event occurs after an exponential waiting time whose average duration is $1/K$, where K is the *coagulation kernel* and depends both on the masses and the positions of the particles involved in the coagulation. Both particles involved in a coagulation disappear and are replaced by a single new particle located at a position that can be random (e.g., one of the positions of the two, according to some probability) or deterministic (e.g., the center of mass).

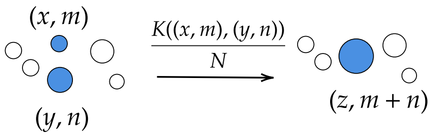

Fig. 2: *Two particles with masses m and n merge to form a new particle of mass $m+n$ at position z. The scaling factor N denotes the total mass of particles in the system.*

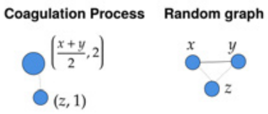

Fig. 3: *In order to have coupling, the merging event must occur before the appearance of an edge between x and z, or between y and z.*

We study a spatial version of the Marcus–Lushnikov process, the classic coalescent process that captures the cluster dynamics (without merger history). Starting from the generator of the process, we provide conditions on the kernel under which gelation occurs. In some special cases, the coagulation process can be coupled with an inhomogeneous random graph as illustrated in Figure 3. Our research in this direction is discussed further in the next section. In particular, our research identifies an upper bound for the gelation time in terms of the critical parameter that determines the appearance of a giant component in the inhomogeneous random graph.

An important part of our analysis is the characterization of the limiting behavior of the coagulating particle systems with a nonlinear kinetic equation — a spatial version of the Flory equation. This is a system of differential equations that describes the evolution in time of the particle density as a function of size and position. The approach taken in our work is an extension to the non-spatial setting developed in [2]. The derivation of nonlinear kinetic equations in order to summarize the behavior of large and complex systems of interacting particles or even agents is one of the key skills that has been developed at the WIAS over many years.

Spatial coagulation and random graphs

In this project, we employed an explicit large-deviation analysis to study in great detail a simplified version of a coagulation process: a process of growing random graphs where coagulation events are represented by adding an edge. The connection between random graphs and coagulation in settings where particles have no spatial location is something we have exploited in the past. We have now extended this connection to include simplified models for the coagulation of particles with individual positions; the crucial step in this direction was to examine the so-called *inhomogeneous random graph*.

The idea is that we view the initial particles (monomers) as vertices on a graph, and approximate the merging of two particles in a coagulation event by drawing an edge on the graph (which one can think of as a physical bond between two monomers). The size of a coagulated particle is now represented by the size of a connected component in the graph, which will contain many monomers/vertices. Our first results about this model can be found in [3].

We derived a large-deviations principle for the empirical measures that register the spatial composition and sizes of both the microscopic and macroscopic components. The emergence of macroscopic components (or coagulated particles), whose size is proportional to the total mass in the system, is an intriguing phenomenon also known as *gelation* and has important consequences for the properties of the system.

Our large-deviations result provides much more understanding of gelation than was previously available. We fully describe the parameter regime in which gelation is typical and also provide explicit formulas for the exponential decay rate of the probability of observing untypical gelation. In an indirect way, our results even capture the possibility of having mesoscopic clusters. We are now extending this novel large-deviations approach to more general spatial coagulation processes of the type described in the previous section.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

Head:	Prof. Dr. Vladimir Spokoiny
Deputy Head:	Priv.-Doz. Dr. John Schoenmakers
Team:	Dr. Christian Bayer Franz Besold Simon Breneis Dr. Oleg Butkovsky Dr. Pavel Dvurechensky Dr. Alexey Kroshnin Dr. Vaios Laschos Luca Pelizzari Dr. William Salkeld Dr. Alexandra Suvorikova Dr. Karsten Tabelow Dr. Nikolas Esteban Tapia Muñoz Dr. Yannic Vargas
Secretary:	Christine Schneider
Nonresident Member:	Prof. Dr. Peter Friz

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

Members of the research group participated in the DFG Collaborative Research Center SFB 1294 *Data Assimilation*, the *Berlin Center for Machine Learning*, the DFG International Research Training Group IRTG 1792 *High Dimensional Non Stationary Time Series*, the DFG International Research Training Group IRTG 2544 *Stochastic Analysis in Interaction*, the DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*, and the Cluster of Excellence *Berlin Mathematics Research Center MATH*$^+$.

Statistical data analysis

The focus within the project area *Statistical data analysis* is on methods that automatically adapt to unknown structures using some weak qualitative assumptions. *Statistical inference* helps to address an important question of reliability of the statistical decision, and it is nowadays an unavoidable element of any statistical analysis. The research includes, e. g., frequentist and Bayesian methods for dimension reduction and manifold learning, change-point detection, regularization and estimation in inverse problems, model selection, feature identification, inference for random networks and complex statistical objects using optimal transport and Wasserstein barycenter. Research within this subarea covered both theoretical and applied statistical problems.

Highlights 2022:

- The article "Generalized self-concordant analysis of Frank–Wolfe algorithms" by Pavel Dvurechensky (RG 6), Kamil Safin, Shimrit Shtern, and Mathias Staudigl was published in Math. Programm.
- The article "An accelerated method for derivative-free smooth stochastic convex optimization" by Eduard Gorbunov, Pavel Dvurechensky (RG 6), and Alexander Gasnikov was published in SIAM J. Optim.
- The paper "Decentralized local stochastic extra-gradient for variational inequalities" by Alexandr Beznosikov, Pavel Dvurechensky (RG 6), Anastasia Koloskova, Valentin Samokhin, Sebastian U. Stich, and Alexander Gasnikov was presented at the 36th Conference on Neural Information Processing Systems (NeurIPS 2022).
- The paper "Clipped stochastic methods for variational inequalities with heavy-tailed noise" by Eduard Gorbunov, Marina Danilova, David Dobre, Pavel Dvurechensky (RG 6), Alexander Gasnikov, and Gauthier Gidel was presented at the 36th Conference on Neural Information Processing Systems (NeurIPS 2022).
- The paper "The power of first-order smooth optimization for black-box non-smooth problems" by Alexander Gasnikov, Anton Novitskii, Vasili Novitskii, Farshed Abdukhakimov, Dmitry Kamzolov, Alexandr Beznosikov, Martin Takac, Pavel Dvurechensky (RG 6), and Bin Gu was presented at the 38th International Conference on Machine Learning (ICML 2022).
- The new *MATH*$^+$ project AA4-13 "Equilibria for distributed multi-modal energy systems under uncertainty" (PIs: Michael Hintermüller (RG 8), Caroline Geiersbach (RG 8), Pavel Dvurechensky (RG 6), Aswin Kannan (Humboldt-Universität zu Berlin)) was approved to be funded.

In 2022, the members of the group made some significant contributions to statistical literature.

A new manifold learning method is proposed and studied in Puchkin & Spokoiny (arXiv:1906.05014; appeared in *J. Mach. Learn. Res.*, 2022). The results claim that the method of structural adaptation yields rate optimal manifold recovery with the accuracy corresponding to the intrinsic manifold dimension in place of the dimension of the ambient space. The general results from Spokoiny (arXiv:2201.06327, 2022) offer a unified statistical approach to a broad class of models called *stochastically linear smooth (SLS)*. The results extend and drastically improve the previous results from Spokoiny and Panov (arXiv:1910.06028, to appear in *Bernoulli*) and provide accurate finite sample bounds on the error of penalized maximum likelihood estimation and accuracy of Gaussian approximation of the posterior distribution.

We continued the research started by Kroshnin, Spokoiny, and Suvorikova in WIAS Preprint no. 2788 (Ann. Appl. Probab. 2021) and investigated the properties of non-asymptotic confidence balls in the Bures–Wasserstein space; see Kroshnin, Spokoiny, and Suvorikova (arXiv:2111.12612, 2021). This technique appears to be helpful for the solution of real-world problems. It provides a potential tool for analyzing three-dimensional genome folding described via Hi-C matrices. The Hi-C matrix can be considered as the adjacency matrix of a graph. Each node is a genomic region, and each edge represents the spatial adjacency of two regions. The goal is to find a proper description of Hi-C space and analyze the resulting structure. For example, we are interested in recovering the "most typical" Hi-C matrix in the observed sample. Figure 1 illustrates the idea. It depicts three-dimensional multidimensional scaling (MDS) projections of the barycenters of Hi-C matrices progressing through the cell cycle and the corresponding confidence balls. The color represents the hour of the progression. Red is a non-synchronized state, i.e., the barycenter of cells whose developmental stage is not known.

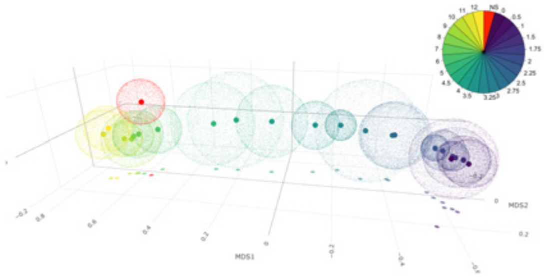

Fig. 1: The gradual transition of the barycenters of the cells from 0 to 12 hours can be observed in the three-dimensional space

Within the MATH+ project EF3-8 "Analysis of brain signals by Bayesian optimal transport" (jointly with Technische Universität Berlin), we considered the population Wasserstein barycenter problem from the perspective of the Bayesian approach. Based on the formulation of the Wasserstein barycenter problem as an optimization problem, we construct a quasi-log likelihood and use it to construct a Laplace approximation for the corresponding posterior distribution. The latter is used to propose concentration results that depend on the effective dimension of the problem. Preliminary numerical results illustrate the effectiveness of a two-sample test procedure based on these theoretical results. In the broader sense, this approach is planned to be applied to general optimization problems, mimicking gradient- and Hessian-free second-order optimization procedures.

Motivated by statistical inverse problems that lead to optimization problems with singular loss functions, such as covariance matrix estimation or Poisson inverse problem, we proposed new stepsizes and a new analysis for the classical Frank–Wolfe algorithm in a non-classical setting of a generalized self-concordant function minimization. A classical sublinear rate was obtained, and a generalization for minimization on polytopes with a linear convergence rate was proposed. The result was published in the Mathematical Programming journal.

An important part of the research in the group is dedicated to distributed optimization algorithms motivated by large-scale empirical risk minimization problems. In this setting, the data in the statistical inverse problem is distributed among a network of agents/nodes/devices, and the goal is for the whole system to solve the problem by communicating information between the nodes. In the centralized approach, one of the nodes is chosen to be central and can communicate with all the other nodes. In the decentralized setting, the network is a connected graph, and only local communication is allowed between the nodes sharing an edge. In 2022, we moved further in this direction and considered distributed stochastic variational inequalities and games. We developed a unifying distributed framework for such problems that includes as special cases settings like centralized, decentralized, and even settings with time-varying computational networks. The paper containing a theoretical analysis and promising numerical experiments, including the training of generative adversarial networks, was published in the proceedings of the Conference on Neural Information Processing Systems 2022.

The research group contributes to the WIAS main application area Quantitative Biomedicine, especially for (quantitative) imaging problems and in neuroscientific applications. There, focus is on bridging the scales between microscopic tissue properties and the mesoscopic resolution in magnetic resonance (MR) Imaging data. In particular, we performed a detailed analysis of the estimation bias in AxiSymmetric Diffusion Kurtosis Imaging and developed a tailored bias correction method (Oeschger et al., Magn. Reson. Med., 2022). Together with RG 3, RG 6 worked on the MATH$^+$ project EF3-11 "Quantitative tissue pressure imaging via PDE-informed assimilation of MR data" and developed a displacement and pressure reconstruction method from magnetic resonance elastography images and applied it in a silico brain model (WIAS Preprint no. 2933), see also the Scientific Highlights article "Biophysics-based modeling and simulation in medical imaging" on page 15.

In March 2022, the task area "Statistics and Machine Learning" within the Mathematical Research Data Initiative (MaRDI) (`http://www.mardi4nfdi.de/`) held a meeting at Technische Universität München to further shape their role within the consortium. The annual MaRDI meeting took place in November 2022 at WIAS in hybrid form. There, the different task areas gave a progress report, and within several bar camps, next steps for the development of the mathematical contributions to the German National Research Data Infrastructure NFDI were identified.

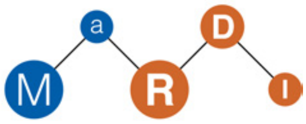

Fig. 2: *The Mathematical Research Data Initiative will contribute to build the NFDI for mathematics*

Stochastic modeling, optimization, and algorithms

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

Highlights 2022:

- A MATH$^+$ Distinguished Fellowship was awarded to Peter K. Friz.
- The article "Well-posedness of stochastic heat equation with distributional drift and skew stochastic heat equation" by Siva Athreya, Oleg Butkovsky, Khoa Lê, and Leonid Mytnik was accepted in Commun. Pure Appl. Math.
- The article "Optimal stopping with signatures" by Christian Bayer, Paul Hager, Sebastian Riedel, and John G. M. Schoenmakers was accepted in Ann. Appl. Probab.
- The *MATH*$^+$ project AA4-9 "Volatile electricity markets and battery storage: A model-based approach for optimal control" (PIs: Christian Bayer, Dörte Kreher (Humboldt-Universität zu Berlin), Manuel Landstorfer) started.
- The article "Reconstructing volatility: Pricing of index options under rough volatility" by Peter K. Friz and Thomas Wagenhofer (TU Berlin) was accepted in Math. Finance.
- The article "Rough semimartingales and p-variation estimates for martingale transforms" by Peter K. Friz and Pavel Zorin–Kranich was accepted in Ann. Appl. Probab.

The research on nonlinear Markov or McKean–Vlasov (MV) processes, which are stochastic processes related to nonlinear Fokker–Planck equations whose dynamics at a certain time depend on the present distribution of the process at that time, was continued. Such processes arise in various applications, for example, lithium battery modeling, population dynamics, neuroscience, and financial mathematics. The study of singular McKean–Vlasov equations that turn up in the smile calibration problem for plain vanilla options, for instance, was continued in the year under report, and culminated in WIAS Preprint no. 2921. In such equations, the dependence on the distribution involves the conditional expectation of some component with respect to another one. This dependence is of singular nature such that established numerical particle methods fail to work. As a way out, the singular MV stochastic differential equation (SDE) was regularized by replacing the conditional expectation by a functional that depends on the unknown distribution in a Lipschitz continuous way and approximates the conditional expectation arbitrarily close. This led to a particle method where the approximate conditional expectation is obtained via cross-sectional ridge regression in a *reproducing kernel Hilbert space*.

Dual methods in optimal stopping and control are important to assess the quality of certain stopping or control policies for certain decision problems arising in energy markets. Rather than maximizing over a family of stopping times or adaptive controls like in the primal approach, in the dual approach one minimizes, over a set of martingales, a certain dual representation that corresponds to the stopping or control problem under consideration. As a rule, such minimizing martingales are not unique. Moreover, they may be only *weakly optimal* in the sense that they minimize the dual representation, but tend to induce high variance. In contrast, there may exist more preferable martingales, so-called *strongly* or *surely* optimal ones, which give rise to an (upper) estimation with vanishing variance. In [2], a randomized empirical dual optimization procedure was presented that sorts out such undesirable *weak* martingales, and which can be implemented as a *linear program*.

In the area of optimal control, a regression-based primal-dual martingale approach for solving finite time-horizon *Markov decision processes* with general state and action space was developed in WIAS Preprint no. 2957. As a result, this method allows for the construction of tight upper and lower biased approximations of the value functions and provides tight approximations to the optimal policy. In particular, we prove tight error bounds for the estimated duality gap featuring polynomial dependence on the time horizon and sublinear dependence on the cardinality/dimension of the possibly infinite state and action space.

The work on numerical quadrature methods for solutions of stochastic differential equations based on numerical smoothing of discontinuous target functionals was continued. These methods exhibit considerably faster convergence speeds to the true expectation especially for financial options (with nonsmooth payoffs) or calculations of probabilities of events or even densities. Additionally, optimal damping regimes for Fourier pricing of European options in multidimensional markets were developed. Damping is required in order to enforce integrability of the Fourier transforms of payoff-functions, a necessary requirement for fast Fourier pricing method. However, while admissible ranges of damping parameters are widely reported in the literature, optimal choices within these ranges are essentially neglected. Numerical experiments supported by theory presented in WIAS Preprint no. 2968 show that the choice of damping parameters has a significant impact on the accuracy of the pricing routine. In addition, well-performing yet simple rules for the choice of damping parameters are given.

Focus Platform *Quantitative Analysis of Rough and Stochastic Systems*

The investigation of rough volatility models continued. The numerical counterpart of previous theoretical investigation (published in Ann. Appl. Probab.) is now published in [4]; implied volatility expansions also led to a fundamental work on our understanding of cumulants in generic stochastic models [5]. We also pioneered a new connection between stochastic and rough analysis (Peter K. Friz, Pavel Zorin-Kranich, Ann. Appl. Probab. accepted).

The development of efficient Markovian approximations to rough volatility models was continued. Based on earlier results published in [1], efficient numerical simulation methods for the rough Heston model are developed. 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.

More progress in the weak error analysis of Euler-type approximations of rough stochastic volatility models was made. A first rigorous analysis was published in Bayer, Fukasawa, Nakahara, "On the weak convergence rate in the discretization of rough volatility models," SIAM J. Financial Math., 13(2), 2022. In a later breakthrough, weak rate $\min(1/2 + 3H, 1)$ was proved for a large class of payoff functions.

The work on the log-ordinary differential equation (ODE) method for solving controlled differential equations driven by (deterministic) rough paths was continued. An algorithm allowing adaptive control of the time-steps as well as the local degree of the method was developed and tested in numerous numerical examples, including examples from machine learning.

Research focused on signature methods and rough paths on an abstract level. As an example, iterated-integrals signatures were shown to encode geometric invariants (Joscha Diehl, Rosa Preiß, Michael Ruddy, Nikolas Tapia, "The moving frame method for iterated-integrals: Orthogonal invariants," Found. Comput. Math., 2022) and distributional properties of paths (Paul Hager, Peter K. Friz, Nikolas Tapia, "Unified signature cumulants and generalized Magnus expansions," Forum Math. Sigma 10, 2022, no. e42), the latter via their cumulants. An extension of the iterated-sums signatures to time series with values in general semirings was introduced in Joscha Diehl, Kurusch Ebrahimi-Fard, Nikolas Tapia, "Tropical time series, iterated-sums signatures and quasi-symmetric functions," SIAM J. Appl. Algebra Geom. 6, 2022, no. 4, pp. 563–599, in order to understand invariants to operations other than time warping, useful in different applied contexts.

At the theoretical level, continuation of previous work led to the study of geometric features of the space of controlled paths associated with branched rough paths (Mazyar Ghani Varzaneh, Sebastian Riedel, Alexander Schmeding, Nikolas Tapia, "The geometry of controlled rough paths," 2022, arXiv:2203.05946). Finally, related algebraic techniques were applied to understanding moment-cumulant relations in the framework of non-commutative probability as natural operations on power series (Kurusch Ebrahimi-Fard, Frédéric Patras, Nikolas Tapia, Lorenzo Zambotti, "Shifted substitution in non-commutative multivariate power series with a view toward free probability," 2022, arXiv:2204.01445).

Another important area of research was regularization by noise. While this phenomenon is quite well understood in the case of Brownian forcing, much less is known if the forcing is non-Markovian (for example, fractional Brownian) or infinite dimensional (for example, space-time white noise). This happens not because regularization by noise is specific to the Brownian case, but rather because there are very few tools available to study this problem in other setups for infinite-dimensional or non-Markovian stochastic systems. Strong existence and uniqueness for stochastic partial differential equations (SPDEs) with distributional drift were established, in particular, for the skew stochastic heat equation. Rates of convergence of the Euler scheme for SDEs with irregular drift driven by Levy noise were additionally studied. Work in progress is to get well-posedness for SDEs driven by fractional Brownian motion under optimal conditions.

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4.7 Research Group 7 “Thermodynamic Modeling and Analysis of Phase Transitions”

Head (acting):	Prof. Dr. Barbara Wagner
Deputy Head (acting):	Priv.-Doz. Dr. Olaf Klein
Team:	Dr. André H. Erhardt Christine Keller Dr. Manuel Landstorfer Alexander Marx Dr. Rüdiger Müller Dr. Mudassar Razzaq Leonie Schmeller Alireza Selahi
Secretary:	Ina Hohn

Research Group 7 conducts research on multiscale modeling, analysis, and numerical simulation of complex materials. The main expertise are the thermodynamically consistent modeling, systematic asymptotic methods, in particular, for singularly perturbed problems, rigorous analysis of the derived models, and analysis of hysteresis properties. Application areas focus on fundamental processes that drive micro- and nano-structuring of multi-phase 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, and polyelectrolyte gels, as well as material models of electrochemistry such as for lithium-ion batteries and electro-catalytic applications, and models for magnetorestrictive materials. For the corresponding, typically, free boundary problems of systems of coupled partial differential equations the research group develops mathematical theory and numerical algorithms.

Multiphase flow problems in soft and living materials

Dewetting dynamics and morphology of liquid polymers on hydrogels. In the tandem project “Dynamic wetting and dewetting of viscous liquid droplets/films on viscoelastic substrates” (PIs: Barbara Wagner (RG 7), Ralf Seemann (Saarbrücken)) within the DFG Priority Programme SPP 2171 *Dynamic Wetting of Flexible, Adaptive and Switchable Surfaces*, and in close collaboration with Dirk Peschka (WG BIP) we also set up a new weak formulation and a corresponding new numerical algorithm for a hydrogel model that we previously developed. This was extended to a system that couples a liquid poymer layer with the hydrogel to model the dewetting process of a liquid layer from possibly soft phase-separation substrates and, together with the group of Ralf Seemann, we address fundamental open questions regarding morphology and dynamics of a liquid layer on soft gels.

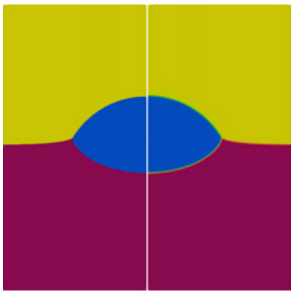

Fig. 1: *Sharp interface vs. diffuse interface for mobility* $m(\varepsilon) = \varepsilon^{5/2}$

Sharp-interface limit. A natural question that arises in the context of phase-field models is about the sharp-interface limit $q_\varepsilon \to q_0$, as the interface width tends to zero, i.e. $\varepsilon \to 0$. The models that we consider are (extended) gradient structures in the sense of $(\mathcal{Q}, \mathcal{F}, (M, A, \mathcal{U}, S))$. In our work [4], we perform a systematic investigation of an appropriate choice of Cahn-Hilliard mobility m in the dual dissipation $\langle A(q)\eta, \eta\rangle = \int m(\varepsilon)\nabla\eta \cdot \nabla\eta \,\mathrm{d}x$. In particular, our benchmark system is a three-phase model, so we find suitable scaling rules for the mobility that allows the limit transition to the intended sharp-interface limit even in the case of moving contact lines, as opposed to pure interface problems. We consider Cahn–Hilliard mobilities of the form $m(\varepsilon) = m_0\varepsilon^\alpha$, $0 \leq \alpha \leq \infty$. Abels et al. give an upper bound on the Cahn–Hilliard mobility (Math. Models Methods Appl. Sci., 2012), and Schaubeck 2014 and Abels 2022 give a lower bound in the case of interfaces. We show numerical convergence of the phase-field model against the desired sharp-interface limit for $\alpha \in (\underline{\alpha}, \bar{\alpha})$, using space-time norms and estimating the numerical discretization errors in both models. In particular, for the system with moving contact line, the value $\alpha_{\text{opt}} = 2$ seems optimal, and the comparison is shown in Figure 1. The free energy for the phase-field model is of the form

$$\mathcal{F}_\varepsilon(q_\varepsilon) = \int_\Omega W_{\text{elast}}(\boldsymbol{F}, \psi) + W^\varepsilon_{\text{phase}}(\psi, \boldsymbol{F}^{-T}\nabla\psi)\mathrm{d}x\,,$$

and the limiting energy reads

$$\mathcal{F}_0(q_0) = \sum_{i\in\{s,\ell,a\}} \int_{\Omega_i} W^i_{\text{elast}}(\boldsymbol{F})\mathrm{d}x + \sum_{ij\in\{s\ell,sa,\ell a\}} \int_{\Gamma_{ij}} \gamma_{ij}|\mathrm{cof}(\boldsymbol{F})\cdot\boldsymbol{\nu}|\,\mathrm{d}s\,,$$

with surface tensions γ_{ij}, outer normal $\boldsymbol{\nu}$, and the index ε and 0 denote the phase-field and sharp-interface contributions, respectively.

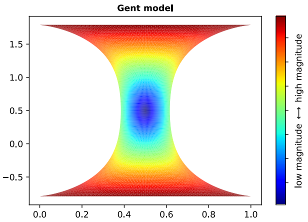

Fig. 2: *Deformation of a two-dimensional sheet during elastic stretch in vertical direction, leaving the side boundaries free*

Current research focuses on the avoidance of possible limitation due to locking by choosing incompressible models with suitable inf-sup stable finite elements. Additionally, by choosing degenerate state-dependent mobilities $m = m(\varepsilon, \psi)$ and techniques as in Dziwnik et al., Nonlinearity, 2017, one should be able to increase the region of validity compared to $m = m(\varepsilon)$.

Mathematical modeling of cellular self-organization on stimuli-responsive extracellular matrix (ECM). Initiated by the interdisciplinary project (MATH+ AA1-12) headed by Sara Checa and Ansgar Petersen (both at Charité), Barbara Wagner, and André H. Erhardt (both RG 7), we developed a model for a strain-stiffening hydrogel (cf. Figure 4) that has the mechanical response typical for fibrin gel, used by our experimental partner. This was coupled to an agent-based model for the collective movement of cells while they excert a traction force on the hydrogel. We extended two-dimensional numerical code for the hydrogel to three space dimensions in order to resolve mechanical response of a thin hydrogel sheet to applied traction forces by a collection of cells. The numerical simulations for different initial cell configurations resolve the long-time mechanically driven cellular organization. Extensions beyond the purly mechanical aspects include electrostatic effects such as developed polyelectrolyte gels interacting with a surrounding ionic bath [2, 5].

Poroelastic mechanics of articular cartilage. Initiated and financially supported through a seed grant by the UK Regenerative Medicine Platform "Acellular/Smart Materials-3D Architecture" (MR/R015651/1), an interdisciplinary team of biomedical engineers at the Imperial College London, University of Delaware, and Oslo University, and applied mathematicians at the University of Nottingham, University of Oxford, University of Bristol, and the Weierstrass Institute (Barbara Wagner) developed a design approach for engineered poroelastic materials that approximates the native performance of articular cartilage. The design approach is based on a fiber-reinforced hydrated network and establishes a design strategy by quantifying the poroelastic response using mixture theory to model the material system. The study lays the foundation for developing scaffold systems and designing poroelastic cartilage implants and has been awarded with a patent. The work has now been submitted for publication [1].

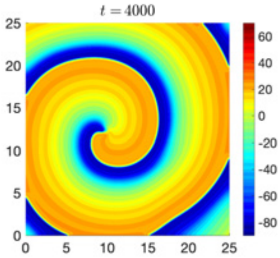

Fig. 3: Spiral wave

Mathematical models of cardiac dynamics and its analysis. The mathematical investigation of complex dynamics in cardiology is becoming increasingly important for the study of cardiac arrhythmia such as early afterdepolarizations (EADs). In this line of research, André H. Erhardt (RG 7) and Susanne Solem (Norwegian University of Life Science) analyzed the dynamics of an established cardiac cell model and the corresponding underlying mechanism by means of bifurcation analysis [6]. Furthermore, self-organizing electrophysiological patterns occurring in the heart like spiral waves, cf. Figure 3, and fibrillation, cf. Figure 4, were numerically investigated. The synchronization of cardiac cells and the potential spreading of cardiac arrhythmias to the tissue were studied, and it is shown that bifurcations associated with EADs are also linked to wave break-up leading to cardiac death at the tissue level.

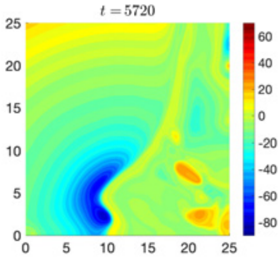

Fig. 4: Fibrillation

Mathematical models and theory of electrochemical processes

Within RG 7, the whole spectrum of modern mathematical modeling and simulation of various electrochemical systems is carried out. Based on non-equilibrium thermodynamics and its coupling to electrodynamics, we perform model development, numerical implementations and simulations, as well as post-processing and model validation of fundamental electroyltes, electrode-electrolyte interfaces, and electrochemical reactions. These results are used to model lithium-ion batteries[7], multi-material electrocatalysis, and bio-electrochemical systems, such as ion channels, on the basis of third-party funded research projects. Mathematical techniques, such as asymptotic expansions, (periodic) homogenization theory, and inverse problems, as well as numerical methods, such as finite volume schemes, are important tools for RG 7 and are continously further developed in cooperation with RG 1, RG 3, and RG 4.

MATH+ AA2-6: “Modeling and simulation of multi-material electrocatalysis (MultECat).” This project, headed by Manuel Landstorfer (RG 7) and Jürgen Fuhrmann (RG 3) with Rüdiger Müller (RG 7) as PostDoc working on the project, aims at continuum models for electrocatalysis at multi-material electrodes on a $nm - \mu m$ scale. The modeled processes couple reactions on catalytic interfaces, reactant transport in electrolytes, and charge transport in catalyst substrates. The project terminated by the end of 2022, and Rüdiger Müller left the institute.

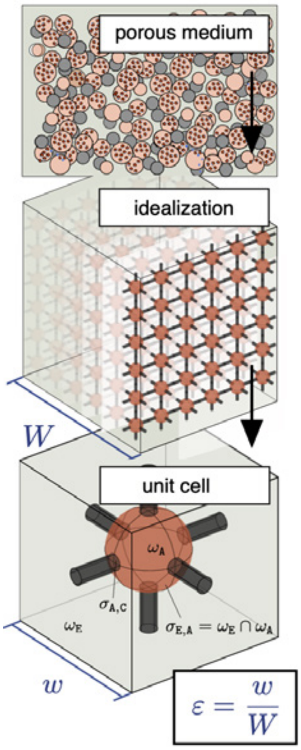

Fig. 5: Sketch of the periodic homogenization technique

The project analyzed the impact of non-constant dielectric susceptibility on the boundary layer as the environment of electrocatalytic reactions. It was found that the dielectric saturation due to strong electric fields considerably narrows the boundary layers and thereby further increases the local electric field strength. Moreover, by a combination of field strength dependence of χ and concentration-dependent dielectric decrement, the concentration profiles of the ions in the boundary layer can become non-monotonous.

To analyze dependence of electrocatalytic reactions on the crystallographic orientation of surfaces, formal asymptotic methods are employed, especially analyzing the quasi-electrostatic limit and the quasi-magnetostatic limit of Maxwell equations [9].

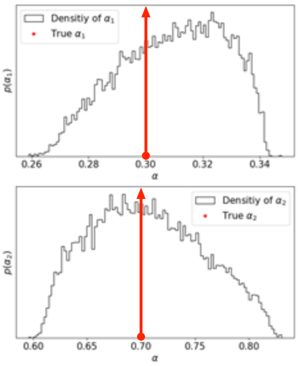

Fig. 6: *Posterior density of the polynomial coefficients*

MATH+ AA4-8: "Recovery of battery ageing dynamics with multiple timescales" is headed by Martin Eigel of RG 4, Martin Heida of RG 1, and Manuel Landstorfer of RG 7, with Alireza Selahi of RG 7 working as Ph.D. student on the project. The project aims at developing a data-driven methodology to recover the dynamics of battery ageing on the basis of a parametrized mathematical model and experimental data. We succeeded in determining the evolution of certain parameters (such as the diffusion coefficient in the active phase of a battery) of the model as a function of the cycling number. These parameters satisfy an evolution equation in the form of an ordinary differential equation, the right-hand side of which was determined leveraging methods of Bayesian inverse problems (see Figure 6), given numerically generated data of the charge-discharge cycle of a lithium-ion battery (LIB). The right-hand side is assumed to be of polynomial structure.

Furthermore, we generalized the modeling framework of a porous LIB, proposed in [7], to account for various particle radii, especially radius distribution functions, in a periodic unit cell. For an N-particle electrode unit cell, the resulting $N+3$ partial differential equations (PDEs) are self-consistently built in a MATLAB/COMSOL environment and numerically solved to allow for transient charge and discharge simulations. We currently investigate many particle effects, e.g., if smaller or larger particles are deliathiated first upon discharging, and extend the model towards degradation effects.

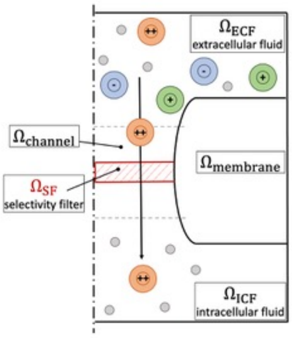

Fig. 7: *Sketch of the extracellular and intracellular fluid connected by a channel with a selecitivity filter*

MATH+ 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 Ph.D. student, the project aims to develop a PDE-based model framework to predict current-voltage relations of calcium-ion channels in biological applications. Key feature of this modeling procedure is the ability to vary salt concentrations, applied voltages, and channel elasticity to support the interpretion of measured results.

Julia-based simulations were performed to study the ion activities in the channel and to calculate current-voltage characteristics. Our model describes the evolution of salt concentrations as well as the electric potential. The ion channel itself is treated as a geometric domain with permanent surface charge.

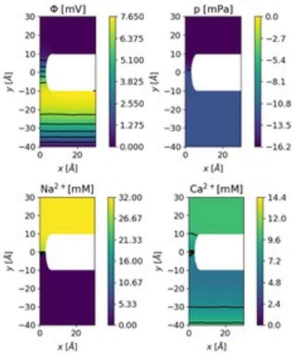

Fig. 8: *Simulation results for a calcium (Ca^{2+})-selective ion channel: electric potential (top left), pressure (top right), sodium (bottom left), and calcium (bottom right)*

As illustrated in Figure 7, an ion channel is essentially composed of different phases, i.e., in addition to the pore itself, the electrolyte, and the cell membrane, there is a special region within the channel called the *selectivity filter*. This area ensures that only a certain type of ions can enter the intracellular region. We introduced an additional embedded domain with Neumann interface conditions to simulate this behavior. In calcium-selective ion channels, for example, calcium can preferentially pass through the filter region, as demonstrated in Figure 8.

Hysteresis, electromagnetic-mechanical components, and uncertainty quantification

The investigations on uncertainty quantification for models involving hysteresis operators were continued. Using experimental data for Terfenol-D, provided by Carmine S. Clemente and Daniele Davino (Benevento, Italy), appropriate values for the parameters in a model following Sec. 5.1 of Davino–Krejčí–Visone (2013) were computed. Information on the uncertainty of these parameters was determined by using the software package UQLab (Marelli–Sudret (2014), https://www.uqlab.com/) to perform Markov chain Monte Carlo computations to get samples representing some posterior density. A scatter plot involving c_1 and c_2 as in Davino–Krejčí–Visone (2013), a further parameter for some output shift, and the variance σ^2 of the noise is shown in Figure 9.

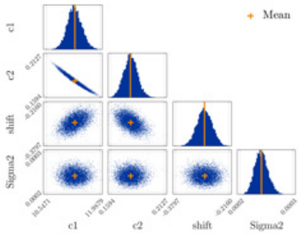

Fig. 9: *. Scatter plot showing the samples representing the posterior density for c_1, c_2, $shift$, and σ^2*

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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 Jo Andrea Brüggemann Sarah Essadi Dr. Denis Korolev Dr. Jonathan Leake (BMS Dirichlet Postdoc) Dr. Kostas Papafitsoros Clemens Sirotenko Steven-Marian Stengl Mike Theiß Sophie Gehricke (WIAS Female Master Students Program)
Guests:	Prof. Dr. Martin Brokate Prof. Dr. Juan Carlos De los Reyes Jonas Holley Dr. Olivier Huber
Secretary:	Pia Pfau

The research expertise of the group lies in the area of optimization associated to nonsmooth energies in infinite-dimensional spaces as well as to partial differential equations (PDEs) with nonsmooth structure. The group focuses on the theoretical analysis and modeling of corresponding real-world problems as well as the development of efficient solution algorithms and their computational realization. Particular fields of interest involve generalized Nash equilibrium problems, quasi-variational inequalities, physics and model-based image processing, optimal control of learning-informed PDEs, stochastic optimization, as well as optimization problems of fluid flows. RG 8 actively contributes to the main application areas *Conversion, Storage, and Distribution of Energy*, *Quantitative Biomedicine*, *Optimization and Control in Technology and Economy*, *Flow and Transport*, as well as aspects of *Materials Modeling*.

Four new members joined the group during 2022. Denis Korolev is a new postdoc from Universität Koblenz with expertise in reduced basis methods. Mike Theiß is a Ph.D. student who transferred to RG 8 from Philipps-Universität Marburg. Sophie Gehricke has joined as a master's student, and Pia Pfau is the new secretary. Kostas Papafitsoros, who joined RG 8 in 2017, became lecturer at Queen Mary University of London. Jo Andrea Brüggemann successfully defended her dissertation entitled “A Class of Elliptic Obstacle-Type Quasi-Variational Inequalities with an Additional Volume Constraint: Theory and Solution Methods” in 2022, and Steven-Marian Stengl completed his dissertation with a defense set for 2023.

Selected research results

Analysis and boundary control of nonlinear transport in gas networks. Energy markets continue to be part of the group's research interest. In [4], a model for the gas market was studied by several members of the group and collaborators. Important economic features were considered along with a linearized and viscosity regularized version of the isothermal semilinear compressible Euler equation on a one-pipe network.

Research involved extending the analysis of the gas market carried out in [4] for the case of a m-pipe network ($m \geqslant 2$) within which, in each pipe, gas evolves according to the isothermal semilinear compressible Euler system

$$\frac{1}{c^2}\frac{\partial p}{\partial t} + \frac{\partial q}{\partial x} = 0 \tag{1a}$$

$$\frac{\partial q}{\partial t} + \frac{\partial p}{\partial x} = -\frac{\lambda}{2D}\frac{q|q|}{p} - \frac{g\sin(\alpha)p}{c^2} \tag{1b}$$

without linearization or regularization. In (1), the quantities p, q denote pressure and flux, respectively, while c, λ, D, g, and α are other physical constants coming from the modeling.

A framework was provided for constructing smooth local solutions to (1) on a tree-like passive network. The nonlinearity on the right-hand side of (1b) can degenerate in *vacuum* ($p = 0$) states and is the source of some of the challenges in the analysis. Building on the theory of [6], it was possible to obtain results with slightly more general assumptions on both the structure of the system and the smallness of the data. The extension of the theory from a 1-pipe to an m-pipe network is non-trivial due to the continuity conditions at the nodes, which lead to boundary coupling between the pipes.

In addition, a tracking-type minimization problem constrained by (1) along with pointwise state constraints was considered. This is a nonconvex optimal control problem since the state equation is not linearized or regularized. It is possible to show that an optimal control exists and provide first-order optimality conditions for this optimization problem.

Hybrid physics-informed neural networks for multiscale problems. The group continued its activities on optimal control of learning-informed PDEs. In the research project "Machine Learning for Simulation Intelligence in Composite Process Design," hybrid physics-informed neural networks for numerical homogenization of multiscale PDEs are being studied from an optimal control point of view. A fine-scale problem enters the objective by incorporating the PDE residual and boundary conditions. The ansatz for the solution $u \in U$ is a neural network $u_{\mathbb{N},n} \in \mathfrak{N}_{\theta,n}$ from some neural network class $\mathfrak{N}_{\theta,n}$, which plays the role of a control variable. A coarse-scale problem constrains the learning process, and its solution $y(u_{\mathbb{N},n}) \in Y$ plays the role of a state variable that is related to $u_{\mathbb{N},n}$ through homogenization. This gives rise to the PDE-constrained optimization problem

$$\inf_{(u_{\mathbb{N},n}, y)\in\mathfrak{N}_{\theta,n}\times Y} \mathcal{J}(u_{\mathbb{N},n}, y) := \|\mathcal{A}u_{\mathbb{N},n} - f\|_H + \|\mathcal{B}u_{\mathbb{N},n} - g\|_Z + \|\mathcal{R}_\delta u_{\mathbb{N},n} - y\|_Y, \tag{2}$$

$$\text{subject to: } \langle \mathcal{S}[u_{\mathbb{N},n}]y, v\rangle_{Y^*Y} = F(v) \quad \forall v \in Y.$$

A function space formulation of (2) was proposed and the individual components were studied. Special attention was paid to the interplay of regularity theory of PDEs, neural network approximation theorems, and the choice of activation functions. The existence of quasi-optimal controls was proven, and the Karush–Kuhn–Tucker (KKT) system for the discrete counterpart of (2) was derived. The examples from the composite material design were studied. In particular, the process of heat conduction in a medium whose properties are described by a multiscale coefficient, and fluid flow in a porous medium were considered. In these examples, suitable fine and coarse scale equations were identified and then coupled by homogenization methods.

Further research will focus on deepening the analysis, extensive numerical experiments, as well as on the development of efficient optimization algorithms in the aforementioned framework. In addition, new engineering insights will be considered to extend the modeling part.

Constrained mean field games. Several members of the group are studying a constrained mean field game coming from a noncooperative differential game with N rational players and interacting through a mean field term. At an individual level, the problem for player i has the following form:

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

where A^i_{ad} are box constraints for the control, X_{ad} are conic constraints for the state, and $\mathcal{AC}(0,T;\mathcal{P}(\mathbb{R}^d))$ is the space of all absolutely continous flows of probability measures. For the objective function we consider quadratic and ℓ^1 cost functionals. The nonsmoothness in the objective is crucial for good modeling and a better understanding of real-world phenomena.

Necessary and sufficient first-order optimality conditions were provided by treating couplings as fixed. Under regularity conditions, there exists a generalized Nash equilibrium for this constrained game. The main result is the derivation of a limiting model when the number of players goes to infinity. This was done by assuming that the players, their dynamics, and their objective functionals are symmetric. The resulting constrained mean field game consists of two coupled parts. The first one is a continuity equation, which describes the behavior of the whole crowd. The second one is a coupled forward-backward differential equation that describes the optimal trajectory of an representative agent of the crowd. More detail about this work can be found in the preprint [5].

A subsequent study will involve developing efficient algorithms to solve the constrained mean field game and studying mean field games involving stochastic dynamics without common noise.

Control of quasi-variational inequalities and risk-averse variational inequalities. The group continued its research in stochastic optimization in the function space setting with the study of the optimal control problem constrained by a random elliptic variational inequality of the form

$$\begin{aligned}&\min_{u\in U_{ad}} \ \mathcal{R}[\mathcal{J}(y)] + \varrho(u)\\ &\text{subject to} \quad y(\omega) \leq \psi(\omega): \quad \langle A(\omega)y(\omega) - f(\omega) - B(\omega)u, y(\omega) - v\rangle \leq 0 \quad \forall v: v \leq \psi(\omega),\end{aligned}$$

where U_{ad} is a set of controls, $\mathcal{R} \circ \mathcal{J}$ is a risk functional, and ϱ is the cost of the control u. This work resulted in the preprint [3]. Stationarity conditions were derived by studying the limit of the KKT-type optimality conditions for a smoothed problem with respect to the penalization parameter. This analytical approach served as the basis for a path-following stochastic approximation algorithm using variance reduction techniques, which was used to numerically solve a modified benchmark problem.

In addition, a number of papers progressing the state-of-the-art of sensitivity analysis and control of quasi-variational inequalities were published this year (in particular, [1, 2]) by some members of the group.

Further highlights in 2022

The Thematic Einstein Semester on “Mathematics of Imaging in Real-World Challenges” of the Berlin Mathematics Research Center MATH+ took place from October 2021 to March 2022 and was co-organized by RG 8. It consisted of a kick-off workshop, three plenary tandem talks, three tutorials, a hackathon event, and it concluded with the SIAM Conference on Imaging Science in March 2022, where several members gave talks.

In addition to the MATH+ project AA4-7 “Decision-making for energy network dynamics” (PIs: Falk Hante (Humboldt-Universität zu Berlin), Sebastian Pokutta (Zuse Institute Berlin), Michael Hintermüller) already in progress, three new projects started in 2022: EF1-15 “Robust multilevel training for artificial neural networks” (PIs: Carsten Gräser (Freie Universität Berlin) and Michael Hintermüller), EF1-17 “Data-driven robust model predictive control under distribution shift” (PIs: Jia-Jie Zhu from WG DOC and Michael Hintermüller), and EF3-12 “Integrated learning and variational methods for quantitative dynamic imaging” (PIs: Christoph Kolbitsch (Physikalisch-Technische Bundesanstalt), Tobias Schäffter (Technische Universität Berlin), and Michael Hintermüller). One new project was approved in the latest MATH+ call and will start in 2023: AA4-13 “Equilibria for distributed multi-modal energy systems under uncertainty.” This project is lead by Michael Hintermüller, Caroline Geiersbach, Pavel Dvurechensky (RG 6), and Aswin Kannan (Humboldt-Universität zu Berlin). In November 2022, Michael Hintermüller was elected speaker of MATH+. He additionally is serving as a scientist-in-charge of the MATH+ Emerging Field 3 (EF3) Model-Based Imaging.

Two projects were approved for the funding period (2022–2026) within the third phase of the Collaborative Research Center CRC/TRR 154 *Mathematical Modelling, Simulation, and Optimization Using the Example of Gas Networks*. Project B02 “Multicriteria optimization using the example of gas markets” was continued with the co-PIs Michael Hintermüller and Caroline Geiersbach, and a new project C08 “Stochastic gradient methods for almost sure state constraints for optimal control of gas flow under uncertainty” headed by Michael Hintermüller was approved.

The SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* continues to run successfully with much activity in terms of papers, and the annual meeting was held in the center of Berlin in October 2022, which was well attended and appreciated by the project members. Furthermore, a special issue book collecting the research achievements of the current (second) phase of the SPP is being compiled for publication under

Birkhäuser, giving each project in the SPP an opportunity to condense and provide an overview of their work. A Young Researchers' event and equal opportunities activities are also being organized by and for SPP members, and the SPP will support minisymposia at some upcoming conferences. RG 8 organized the annual meeting, and several members of the group presented their work.

The collaborative project ML4SIM "Machine Learning for Simulation Intelligence in Composite Process Design" between the Weierstrass Institute (PI: Michael Hintermüller) and the Leibniz-Institut für Verbundwerkstoffe (IVW), German Research Center for Artificial Intelligence (DFKI), Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Fraunhofer Institute for Industrial Mathematics (ITWM) started in January 2022 and is funded by the Leibniz Competition program. The project went through an initial phase in which the goals of each partner were defined and ways of possible cooperation were identified. Interim results were discussed at a consortium meeting held at IVW, November 2022.

Members of RG 8 actively contributed to international conferences, workshops, and seminars. Several members of the group presented at International Conference on Continuous Optimization (ICCOPT) at Lehigh University in July 2022 and the 93rd GAMM Annual Meeting in Aachen in August 2022. Other talks were given at the IFIP TC7 System Modeling and Optimization in Warsaw and the 15th International Conference on Mathematical and Numerical Aspects of Wave Propagation at ENSTA-Paris, both in July 2022.

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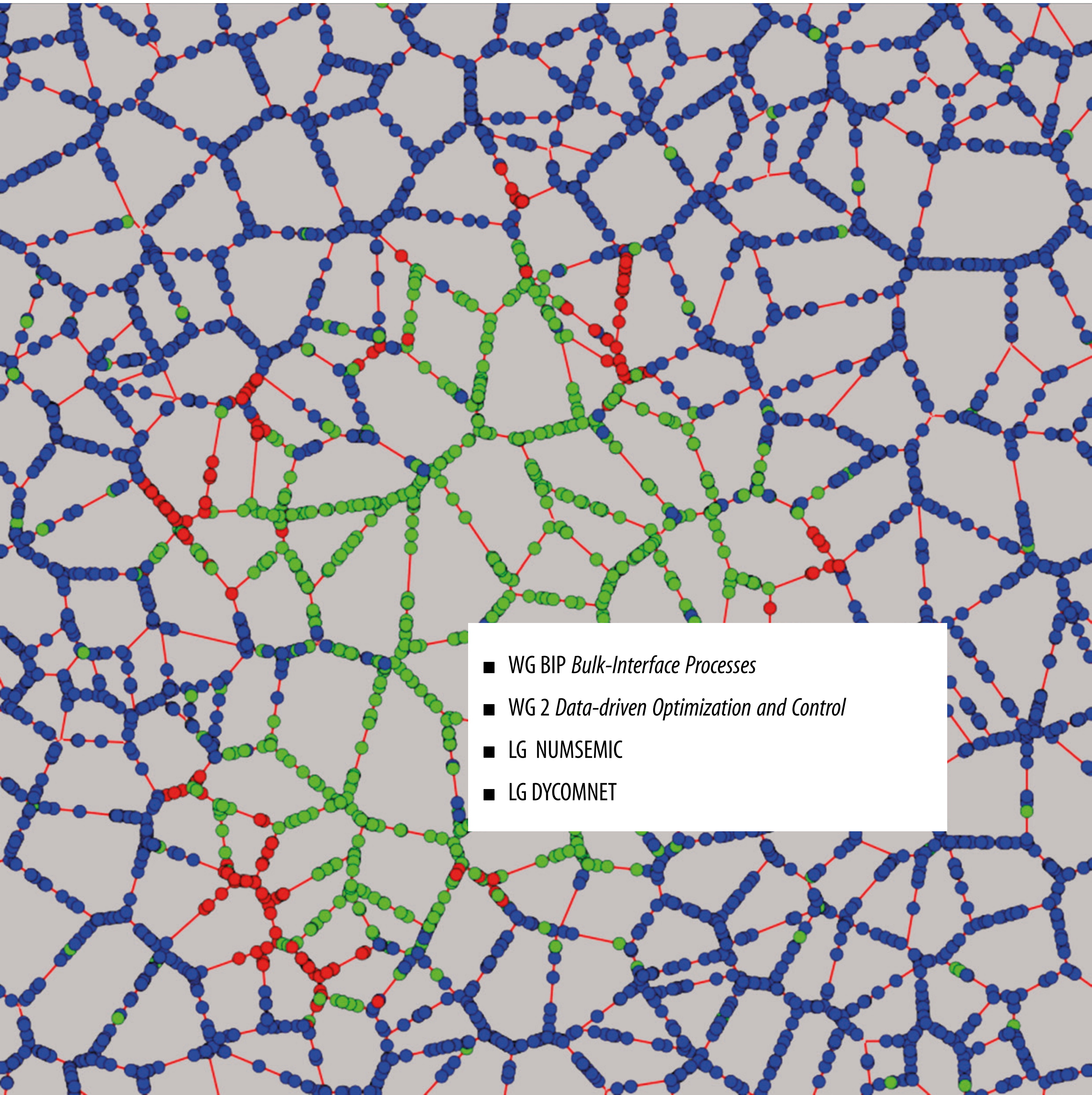
5 Flexible Research Platform



- WG BIP *Bulk-Interface Processes*
- WG 2 *Data-driven Optimization and Control*
- LG NUMSEMIC
- LG DYCOMNET

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

Head:	Prof. Dr. Marita Thomas
Team:	Prof. Priv.-Doz. Dr. Mohammad Hassan Farshbaf Shaker Dr. Dirk Peschka Sven Tornquist Andrea Zafferi
Secretary:	Andrea Eismann

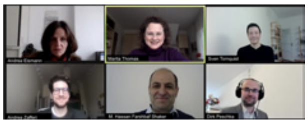


Fig. 1: *WG BIP, 2022, from left to right: A. Eismann, M. Thomas, S. Tornquist, A. Zafferi, M.H. Farshbaf-Shaker, D. Peschka*

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

In 2022, already in view of its planned termination in June 2023, the group saw big changes in its staff. First of all, two group members succeeded to obtain permanent professorships at a university, resp. at a university of applied sciences, in Berlin: In April 2022, M. Hassan Farshbaf Shaker started his new position as a W2-professor at the Hochschule für Technik und Wirtschaft Berlin (HTW Berlin) and thus left the WG BIP. Moreover, in summer 2022, Marita Thomas received a call for the W2-professorship for Applied Analysis at Freie Universität Berlin (FU Berlin), which she started in August 2022. She remains on a part-time position at the WIAS to successfully run WG BIP till its termination in June 2023. In the course of her call, it was possible to offer positions to Sven Tornquist and Andrea Zafferi at FU Berlin, where they plan to submit their Ph.D. theses in 2023 and may subsequently continue on postdoc positions. Sven Tornquist thus moved to FU Berlin in October 2022, and Andrea Zafferi will join the FU team in January 2023. Both of them will remain guests of WG BIP at WIAS till the termination of the group. Additionally, it is also planned to offer a guest professorship to Dirk Peschka at FU Berlin for the summer term 2023.

The research goal of WG BIP consists in developing mathematical methods for systems with bulk-interface processes. This concerns the thermodynamically consistent modeling of bulk-interface interaction with dissipative, Hamiltonian, and coupled dynamics, the theory for the existence and qualitative properties of solutions, and the derivation and justification of interfacial evolution laws.

The analytical results provide the basis for the development of numerical algorithms supporting simulations for applications with bulk-interface interaction. During the first funding period, WG BIP contributed with its research projects to the three WIA -main application areas *Nano- and Optoelectronics*, *Materials Modeling*, and *Flow and Transport*. Since the projects on mechanically strained optoelectronic devices are considered successfully closed for the time being, in the second funding period that started in July 2020, the group continues and intensifies its research on applications within the areas *Materials Modeling* and *Flow and Transport*, in particular, on:

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

with the long-term goal of directing the research within (1) and (2) towards applications in biology.

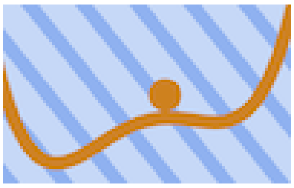
WG BIP also contributes to organizing the WIAS seminar on Materials Modeling and to the Langenbach Seminar on Nonlinear Partial Differential Equations.

The following summary reports on the research results and successes obtained in 2022 within the two topics (1) and (2):

In March 2022, the review for the third funding period of Collaborative Research Center CRC 1114 *Scaling Cascades in Complex systems* took place. As a member of the Scientific Board and prospective spokesperson, Marita Thomas took a leading role in helping prepare and shape the CRC for its third funding period. After a very successful defense, the CRC started its third funding period in July 2022 with Marita Thomas and Frank Noé (FU Berlin) as the team of speakers. In October 2022, Marita Thomas was once more confirmed in an election as the acting spokesperson for the DFG.

In the third funding period, Marita Thomas will be involved as PI in three projects with applications within topics (1) and (2): While project C09 "Dynamics of rock dehydration on multiple scales" has existed already since the second funding period and, as a joint collaboration with geoscientists from FU Berlin, will be based at FU Berlin for the third funding period, she is also involved in two new projects that were established with funding at WIAS: In collaboration with Martin Heida (RG 1 *Partial Differential Equations*), the project B09 "Materials with discontinuities on many scales" will develop novel models for multiscale fracture evolutions using stochastic and fractal homogenization methods in combination with tools from nonlinear partial differential equations theory and variational convergence methods. In project B09, Leon Schütz took up his work as a Ph.D. student in November 2022 as a member of RG 1. Moreover, in collaboration with Robert Patterson (RG 5 *Interacting Random Systems*) and Roland Netz (FU Berlin), the project C02 "Interface dynamics: Bridging stochastic and hydrodynamic descriptions" will investigate the dynamics of aerosole droplets starting from stochastic lattice models with exclusion processes, by considering their hydrodynamic limit and large deviations in order to obtain a related macroscopic reaction diffusion limit model. In October 2022, Julian Kern started his work as a Ph.D. student in this project as a member of RG 5. The reader is also referred to the research portrait on Marita Thomas authored by Dr. C. Pietschmann and published by Forschungsverbund Berlin e.V. in Verbundjournal no. 119, 2022.

March 2022 also saw the defense of the second funding period of the Priority Program 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates*. In this program, Dirk Peschka succeeded to acquire funding for three more years for his own DFG-funded position within the project "Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows." In the second funding period, Dirk Peschka's research within the project will focus on fluid structure interaction (multiphase flows with moving contact lines) and coupling to nonlinear diffusion via phase-field models.



Dissipative processes in elastic solids. The research of WG BIP is concerned with the development and mathematical analysis of models for damage and fracture in elastically deformable solids, both at small and at finite strains. The project "Nonlinear fracture dynamics: Modeling, analysis, approximation, and applications" of Marita Thomas in collaboration with Kerstin Weinberg (U Siegen) and Christian Wieners (KIT Karlsruhe) within the Priority Program SPP 2256 *Variational*

Methods for Predicting Complex Phenomena in Engineering Structures and Materials, aims to develop discretization methods for dynamic fracture and to extend them also to the nonlinear setting at finite strains. As a first step in this direction, an alternative discretization method for the dynamic phase-field fracture model from [1] was discussed in [2]. It uses a coupled first-order system for the momentum balance in combination with a discontinuous Galerkin approach. The performance of this scheme is also compared with alternative approaches like peridynamics.

Moreover, it was possible in [3] to cast well-known dynamic fracture and delamination models in the framework of GENERIC (General Equations of Non-Equilibrium Reversible Irreversible Coupling). For this, the GENERIC formalism was extended in [3] from thermodynamically closed systems to a general concept for systems with bulk-interface interaction. It makes use of the functional derivatives of energy and dissipation potentials with interfacial contributions and provides the governing equations of the GENERIC system rather in a weak formulation. In this way, the formulation naturally displays interfacial coupling conditions. As was demonstrated in [3] at the example of heat transfer, by regarding one of the bulk phases as a reservoir, the GENERIC formalism for bulk-interface systems can also be used to provide formulations suited for thermodynamically open systems.

In the MATH+ project AA2-9 “Variational methods for viscoelastic flows and gelation,” which saw its start in January 2021, mathematical models and corresponding structure-preserving models for viscoelastic solids coupled to phase-field evolution were developed in the context of geophysical flows and with applications in biology; see, e.g., [5].

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

In order to describe chemical reactions and reactive transport within rocks during subduction in project C09 a model for fluid-structure interaction was developed in [4]. It makes use of the framework of GENERIC for bulk-interface systems and also provides the governing equations with suitable coupling conditions in a weak form. Using suitable transformations between Lagrangian, Eulerian, and arbitrary configurations, it points out a concept for numerical implementation using ALE (Arbitrary Lagrangian Eulerian) methods.

As a part of the project “Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows” within the DFG-funded Priority Program SPP 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates*, advanced mathematical methods for coupling fluid flow with non-trivial substrate dynamics are investigated, e.g., fluid-structure interaction, reactive surfaces, and coupling flow over porous substrates. Highlights of the first funding period are the development of energy-based mathematical methods for coupled problems involving multiphase flows, finite strain viscoelasticity, and nonlinear diffusion, jointly with RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, cf. [5], and development of mathematical methods for moving contact lines. Additionally, higher-order schemes for thin-film problems were developed jointly with Luca Heltai (SISSA, WIAS Preprint no. 2887, 2021), and comparisons of hydrodynamic models and molecular dynamics models were performed jointly with Marcello Sega et al. (Universität Erlangen-Nürnberg, WIAS Preprint no. 2911, 2022). Based on these results, in the future it is the aim to develop robust mathematical methods for fluid-structure interaction and free boundary problems, coupling phase-field evolution, finite strain elasticity, and (sharp and diffuse) moving interfaces for biological applications.

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

Head: Dr. Jia-Jie Zhu
Team: Jamie Barnes
Dr. Andrei Pavlov
Secretary: Christine Schneider

WG DOC was established as a unit of the Flexible Research Platform at WIAS in June 2021, funded by WIAS budget resources. The group will go on interim review after the initial period of three years. In 2022, a Ph.D. student has left the group. Later, affected by the unexpected war in Europe, postdoctoral researcher Andrei Pavlov moved to Australia for family reasons. Fortunately, a new Ph.D. student, René Saitenmacher, will join the group in February 2023. In addition, a new postdoctoral scholar funded by the MATH+ has accepted our offer to join the group in March 2023.

WG DOC leader Jia-Jie Zhu gave a mini-course on Data-Driven Modeling and Optimization of Dynamical Systems under Uncertainty at Technische Universität Berlin in July 2022.

WG DOC's overarching goal is to study mathematical foundations and applications of machine learning and data-driven optimization, especially the enhancing of the robustness of learning decisions under data distribution shift — a pressing issue plaguing modern-day machine learning and intelligent control algorithms.

One of WG DOC's focal topics is the theory and application of distributionally robust optimization (DRO), an emerging topic born out of the study of data-driven optimization, robust optimization, and stochastic programming. It has deep connections with the minimax formulations in nonparametric statistics, as well as convex analysis, and optimal transport theory. Intuitively, DRO applies computational strategies developed for the classical robust optimization framework, but lifts the variables from the original input space to the space of probability measures.

Building upon our previous works in distributionally robust optimization and kernel methods using the kernel maximum mean discrepancy (MMD), e.g., [2, 1], we further expand our expertise in achieving robust learning and estimation under stronger forms of distributional perturbation — those caused by causal confounding and heterogeneity within the data sets. In [3], together with collaborators at the Max Planck Institute for Intelligent Systems, Tübingen, we invented a new estimation algorithm that beats state-of-the-art performance in conditional moment restriction for estimation. This paper was published in the Proceedings of the 39th International Conference on Machine Learning (ICML), a prestigious venue for machine learning research. In another follow-up work (submitted and under review), we further propose a novel framework using the kernel MMD geometry instead of the information divergences for enforcing conditional moment condition, which is the first framework in the generalized moment method literature that goes beyond re-weighting data points. Those works mark the beginning of a series of our investigation into learning invariant prediction under causal confounding, addressing one of the most pressing issues in machine learning today.

We also deepened our investigation of DRO in another direction of chance-constrained stochastic programming (CCSP), where we proposed the first novel distributionally robust CCSP algorithm that can handle nonlinear constraints with statistical guarantees [4]. CCSP is an important class of problems that are widely applied in practical optimization and engineering to probabilistically make robust decisions. We are currently cooperating with René Henrion (RG 4), an expert in CCSP at WIAS, on further works for nonlinear CCSP.

To fully attack the problem of robust optimization and learning, we are in the process of establishing cooperations with other experts at WIAS. For example, we are exploring novel applications of principled Wasserstein gradient flow theory, partial differential equations, and optimal transport, via interactions with experts such as Alexander Mielke (RG 1). We are also cooperating with Pavel Dvurechensky (RG 6) on continuous optimization for DRO and machine learning.

Last but not least, another focus of WG DOC is in data-driven modeling and control of dynamical systems. This research direction draws from the foundational works in kernel discrepancy measures and data-driven modeling schemes based in statistical learning theory. Currently, we aim to finish a work on characterizing the concentration and multistep estimation deviation of the Koopman models using the learning theory techniques coming from the kernel machine learning literature. In addition, our work in data-driven modeling using an approximate kernel method was published in 2022 [5].

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5.3 Leibniz Group NUMSEMIC “Numerical Methods for Innovative Semiconductor Devices”

Head:	Dr. Patricio Farrell
Team:	Dr. Yiannis Hadjimichael Dr. Daniel Fritsch Dilara Abdel Zeina Amer
Secretary:	Marion Lawrenz

The Leibniz Group NUMSEMIC was established on WIAS’ Flexible Research Plattform in January 2020 after successfully winning a grant within the Leibniz competition. For five years, it is funded by the Leibniz Association and covers three of WIAS’ main application areas: *Materials Modeling*, *Conversion, Storage and Distribution of Energy*, and *Nano- and Optoelectronics*. The aim of this group is to develop partial differential equation (PDE) models as well as physics-preserving numerical techniques for new semiconductor materials and technologies. Highlights this year include a top-ten submission together with Julien Moatti, INRIA Lille, for the 22nd International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD), as well as having been awarded an incubator project of the Berlin Mathematics Research Center MATH+ to study band energies in strained materials together with Christian Merdon (RG 3) and Costanza Manganelli (IHP).

The following four specific research topics drive our research:

- **Electro-mechanical models and simulations**, e.g., to understand transport in bent nanowires,
- **Opto-electronic imaging techniques** to detect fluctuations in crystals,
- Models and simulations of charge transport in **perovskite solar cells**,
- **Inclusion of atomistic effects** in drift-diffusion models.

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

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

Electro-mechanical models and simulations. Together with Christian Merdon (RG 3), Yiannis Hadjimichael and Patricio Farrell are developing numerical techniques to simulate charge transport in bent nanowires. The difficulty here is to combine the nonlinear van Roosbroeck system, which models charge transport in semiconductors, with an appropriate model from continuum mechanics to take into account the deformations. A model that describes the bending of nanowires due to a lattice number mismatch, as well as piezoelectric effects, was proposed and numerically solved using the finite element method. This work is a collaboration with the Paul-Drude-Institut für Festkörperelektronik (PDI).

Deriving and analyzing thermodynamically consistent models that describe charge-carrier transport in mechanically deformed semiconductors is the topic of the MATH+ project “Electro-mechanical coupling for semiconductor devices” which started in 2021. Apart from LG NUMSEMIC, this project involves Matthias Liero and Annegret Glitzky (both RG 1) as well as Barbara Zwicknagel from Humboldt-Universität zu Berlin. In general, it is important to understand how band-edge energies are impacted by general strain profiles. Daniel Fritsch investigates how to find the eigenvalues from a Bir–Pikus Hamiltonian and identify them with heavy hole, light hole, and split-off band edge energies. This work is in collaboration with the Leibniz Institute for High Performance Microelectronics (IHP).

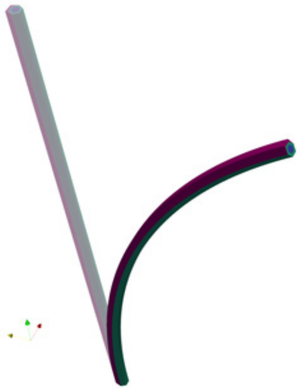

Fig. 2: *A bent nanowire*

Opto-electronic imaging techniques The non-destructive estimation of doping concentrations in semiconductor devices is of paramount importance for many applications ranging from crystal growth, the recent redefinition of the 1kg to defect and inhomogeneity detection. A number of technologies (such as light beam-induced current (LBIC), electron beam induced current (EBIC), and lateral photovoltage scanning (LPS)) have been developed, allowing the detection of doping variations via photovoltaic effects. The idea is to illuminate the sample at several positions, and detect the resulting voltage drop or current at the contacts. We model a general class of such photovoltaic technologies by ill-posed global and local inverse problems based on a drift-diffusion system that describes charge transport in a self-consistent electrical field. The doping profile is included as a parametric field. To numerically solve a physically relevant local inverse problem, we present three different data-driven approaches, based on least squares, multilayer perceptrons, and residual neural networks. Our data-driven methods reconstruct the doping profile for a given spatially varying voltage signal induced by a laser scan along the sample’s surface. The methods are trained on synthetic data sets (pairs of discrete doping profiles and corresponding photovoltage signals at different illumination positions) that are generated by efficient physics-preserving finite volume solutions of the forward problem. While the linear least square method yields an average absolute error around 10%, the nonlinear networks roughly halve this error to 5%, respectively [4]. Patricio Farrell works on this topic together with researchers from SISSA, Trieste, and the University of Florence.

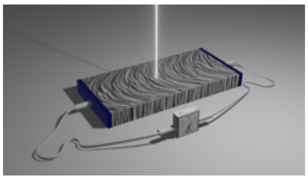

Fig. 3: *A laser scan along a crystal produces voltage signals that can help to detect inhomogeneities*

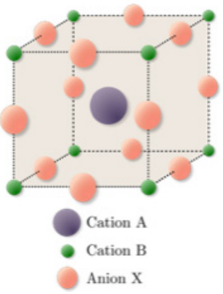

Fig. 4: *The perovskite unit cell*

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

Dilara Abdel and Patricio Farrell are working together with Petr Vágner on deriving thermodynamically consistent models for PSCs taking surface effects into account. With Nicola Courtier from University of Oxford alternative current density descriptions for the inclusion of volume exclusion effects are numerically compared [2]. The simulations are performed with `ChargeTransport.jl`, a software package developed in cooperation with Jürgen Fuhrmann (RG 3) for the simulation of charge transport in semiconductors. Apart from numerical simulations, also the numerical analysis, including entropy dissipation relationships, of the model was analyzed with colleagues from the University of Lille/INRIA Lille [3].

Coupling with atomistic effects. LG NUMSEMIC investigates together with researchers from Tyndall National Institute (Ireland), INRIA Lille and Thomas Koprucki (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` [5, 6].

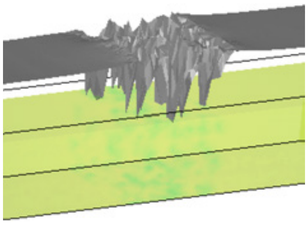

Fig. 5: *Random fluctuations in the band edge energy on atomic scale*

Comparison between HDG and FVM methods. Together with researchers from SISSA and the University of Florence, we are comparing the hybridizable discontinuous Galerkin (HDG) method with the finite volume method [1].

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

Head:	Prof. Dr. Benedikt Jahnel
Team:	Dr. Sanjoy Kumar Jhawar Alexander Hinsen Dr. Lukas Lüchtrath Anh Duc Vu Jonas Köppl
Secretary:	Christina van de Sand

The Leibniz junior research group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks* is cofunded by the Weierstrass Institute and the Leibniz Association through the *Leibniz Competition 2020*. 2022 is the second year within the anticipated five-year total runtime of the group. Broadly speaking, DYCOMNET’s goal is to perform state-of-the-art research in the domain of complex spatially distributed communication networks using methods from stochastic geometry and statistical mechanics. A prototypical example is the modeling and analysis of dynamic peer-to-peer networks via the theory of random point processes, interacting particle systems, and large deviations theory. DYCOMNET thrives to exhibit rigorous results, for example, for connectivity properties of such networks, manifesting themselves, e.g., via percolation phase transitions.

The DYCOMNET team further developed in 2022 with Alexander Hinsen leaving the institute (starting a career in industry and submitting his Ph.D. thesis in the near future) and two additional members joining the group. First, Jonas Köppl joined in September 2022 after a successful master’s thesis defense at Technische Universität Berlin and Lukas Lüchtrath in November after completion of his Ph.D. at Universität zu Köln. In April 2022, Benedikt Jahnel started his professorship at Technische Universität Braunschweig, leading DYCOMNET on a part-time contract.

Also in 2022, the group continued working on the probabilistic modeling and rigorous analysis of mobile device-to-device networks. Notable highlights here were the publication of the preprints [1], [2] in which a realistic multi-layer system of mobile devices in an urban topology can exchange messages only if they spend sufficiently long time in close proximity. The resulting connectivity graph is then first investigated in view of its percolation behavior. Here, most interestingly, an in-and-out of percolation with respect to the individual device velocities can be observed. The second part of the study is dedicated to the analysis of parameter regimes that feature extinction and survival of a malware introduced into the system at a typical point, with and without the presence of decentralized counter-measures; see Figure 6. These publications feature the latest results based on the collaboration with the French communication provider ORANGE.

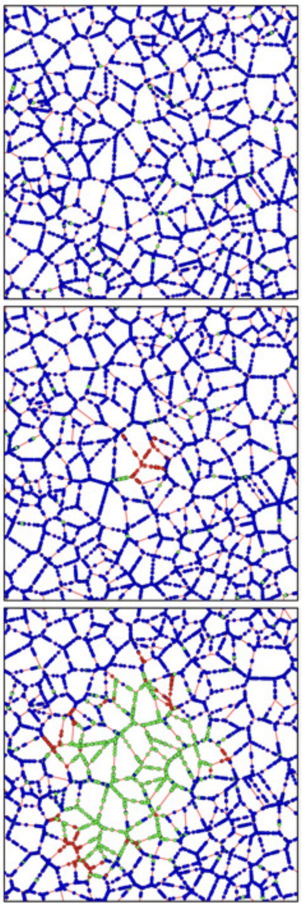

Fig. 6: *Propagation of malware (red) in a mobile device-to-device network in a street system. At initial time (up), there is one infected device present near the center, and the remaining devices are either susceptible (blue) or patch-holding devices (green). At some positive time (middle), further devices in the vicinity of the initially infected device became infected and started to make contact to the patch. At some later time (down), infected devices are only present along the boundary of the set.*

Still within the realm of percolation analysis, but on a more fundamental level, the publications [4], [5] present results for continuum percolation based on Poisson point processes in random environments. More precisely, in [5] the environment is given by a rectangular Manhattan-type grid that features infinite-range dependencies and is therefore very challenging to analyze rigorously;

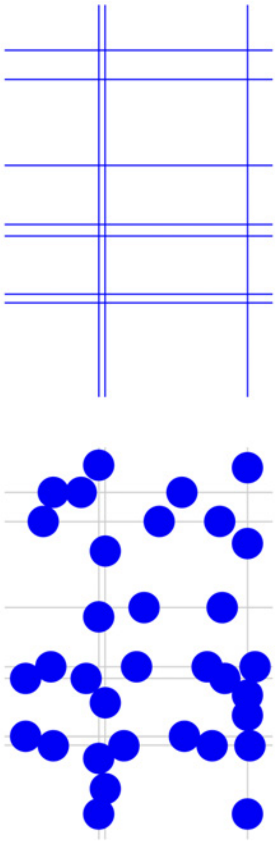

Fig. 1: *Construction of the Manhattan grid model: First, generate a random Manhattan grid (left). Second, place balls with random centers on the grid.*

see Figure 1 for an illustration. However, using a technical multi-scale approach and discretization arguments, non-trivial regimes for presence and absence of percolation can still be established. One particular consequence of the long-range dependencies is the absence of a sharp phase transition in the sense that in the subcritical regime the cluster-size distribution has exponentially light tails. This property, and more details about the percolation probability around the critical point, however, can be established in similar models where the environment features bounded-range dependencies. This is the main contribution of the work [4].

Also in 2022, members of DYCOMNET made contributions to the fundamental understanding of idealized physical systems inside and outside of their equilibrium states [3], [6]. More precisely, in [3] a variational description of the equilibrium states of a discrete version of an infinite-volume Bose-gas-type system is derived. This potentially provides a line of attack towards a deeper mathematical understanding of the famous Bose–Einstein condensation phenomenon. In [6], on the other hand, translation-invariant interacting particle systems are considered that possess at least one time-stationary Gibbs measure, which is not necessarily reversible. In a rather general framework, using the relative entropy as a Lyapunov function, attractor properties of the system are proven in the sense that any weak limit point of trajectories started in any translation-invariant measure is also a Gibbs measure for the same specification.

Finally, the success of DYCOMNET in 2022 is underlined by two awards given to Jonas Köppl. He won a Dies Mathematicus Award for the Best Master's Talk from the Mathematical Institute of Technische Universität Berlin, and he also won a Best DMV Student Talk Award in this year's Student Conference of the Deutsche Mathematiker-Vereinigung (DMV) and subsequently gave a presentation at the DMV Annual Meeting 2022 in Berlin. Benedikt Jahnel was involved as a co-organizer in the workshop on *"Recent Trends in Spatial Stochastic Processes"* at EURANDOM, Eindhoven University, within the Ambassador program, and the workshop on *"Random Point Processes in Statistical Physics"* within the DFG SPP 2265 *Random Geometric Systems*. Apart from many scientific presentations at conferences, DYCOMNET also contributed to the outreach of WIAS, for example, within the *Long Night of the Sciences Berlin*.

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A Facts and Figures

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

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

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

A.1.1 Offers of Professorships

1. M.H. Farshbaf Shaker, W2 Professorship, January 12, Hochschule für Technik und Wirtschaft Berlin (HTW Berlin), Fachbereich 2: Ingenieurswissenschaften – Technik und Leben.
2. T. Orenshtein, Assistant Professorship, March 1, The University of Milan-Bicocca, Department of Mathematics and Applications, Italy.
3. K. Papafitsoros, Lecturer, March 14, Queen Mary University of London, School of Mathematical Sciences, UK.
4. M. Thomas, W2 Professorship, March 24, Freie Universität Berlin, Institut für Mathematik.
5. J.-J. Zhu, Assistant Professorship, August 19, Free University of Amsterdam, School of Business and Economics, Department of Operation Analytics, the Netherlands.

A.1.2 Awards and Distinctions

1. P. Friz, *MATH+ Distinguished Fellowship*, December 12.
2. R. Henrion, *Member of Comité Scientifique International, Groupement de Recherche Mathématiques de l'Optimisation et Applications (GdR MOA), France*.
3. M. Hintermüller, *Chair of the Executive Board of the Berlin Mathematics Research Center MATH+*.
4. ———, *Chairperson of the Scientific Advisory Board of the INM – Leibniz-Institut für Neue Materialien, Saarbrücken*.
5. ———, *Member of the Integrative Research Institute for the Sciences IRIS Adlershof of the Humboldt-Universität zu Berlin*.
6. ———, *Spokesperson of MaRDI (Mathematical Research Data Initiative) – The NFDI Consortium of Mathematics*.
7. ———, *Spokesperson of Section 4, Technical Sciences and Engineering, of the initiative Berlin Research 50*.
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. ———, *Vice Chair of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization*.
12. S. Katz, *Best Student Paper Award at the ESCO 2022 Conference, June 13–17*.
13. J. Köppl, *Best DMV Student Talk Award of Deutsche Mathematiker-Vereinigung (DMV) student conference StuKon22*, August 10.
14. ———, *Dies Mathematicus Best Master's Talk Award, Technische Universität Berlin, Institut für Mathematik*, November 25.
15. A. Maltsi, *European Women in Mathematics Travel Grant*, May 15.

16. A. Mielke, *Chair of the Council of the Berlin Mathematics Research Center MATH+*.
17. ———, *MATH+ Distinguished Fellowship*, December 12.
18. L. Plato, *Dies Mathematicus Best Master's Degree Award, Technische Universität Berlin, Institut für Mathematik*, November 25.
19. ———, *Prize for one of the best master's degrees in the framework of the Dies Mathematicus, Technische Universität Berlin*, November 25.
20. M. Radziunas, *Honorary Associate Professor of Macquarie University 2021–2023, Sydney, Australia*.
21. H. Shafigh, *Dies Mathematicus Best Master's Degree Award, Technische Universität Berlin, Institut für Mathematik*, November 25.
22. ———, *Prize for one of the best master's degrees in the framework of the Dies Mathematicus, Technische Universität Berlin*, November 25.
23. A. Stephan, *WIAS Young Scientist's Grant*, November 14.
24. M. Thomas, *Nomination as a member of the Academia Net network*, 2022.

A.1.3 Habilitations

1. M. Eigel, *Adaptive Numerical Methods for High Dimensional Parametric PDEs*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, January 12.
2. M. Heida, *Geometric and Measure Theoretic Aspects of Stochastic Homogenization*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, May 4.
3. M. Liero, *Mathematical Analysis of Charge and Heat Flow in Organic Semiconductor Devices*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, July 31.

A.1.4 Defenses of Ph.D. Theses

1. J.A. Brüggemann, *A class of elliptic obstacle-type QVIs with volume constraints: Theory and methods*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, December 5.
2. M. Ebeling-Rump, *Phase-field approach to two-scale topology optimization*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, September 12.
3. R. Gruhlke, *Uncertainty quantification of material imperfections: Surrogates, upscaling and inference*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. D. Hömberg, Dr. M. Eigel, October 14.
4. Ch. Kwofie, *Large deviations of the throughput in multi-channel medium-access protocols*, University of Ghana, Department of Statistics and Actuarial Science, supervisor: Prof. Dr. W. König, April 6.
5. A. Maltsi, *A mathematical study of the Darwin–Howard–Whelan equations for Transmission Electron Microscopy*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, November 11.

A.1.5 Supervision of Undergraduate Theses

1. T. Both, *Parameteridentifikation für einen thermoinduzierten Koagulationsprozess* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, November 3.
2. F. Cevik, *Langzeitverhalten der angeregten Irrfahrt* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, February 26.
3. V. Dallmer, *Inverse Ungleichungen für die Stromlinien-Diffusions-Finite-Elemente-Methode* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, January 24.
4. J. Fehn, *Large deviations for a spatial particle model with coagulations* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, December 28.
5. A. Flöge, *Randomized box version of the interacting Bose gas* (master's thesis), Universität Potsdam, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Prof. Dr. S. Roelly, Prof. Dr. W. König, June 29.
6. M. Graham, *Eulerian and Lagrangian variational approaches for the modelling of viscoelastic materials* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. D. Peschka, February 27.
7. F. Haniel, *Eigenvalue asymptotics of the higher-order Anderson Hamiltonian with white noise potential* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. W. van Zuijlen, November 7.
8. H. Huang, *Characterisations of the phases in continuum percolation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof.Dr. W. König, Prof. Dr. B. Jahnel, November 11.
9. X. Jiang, *Erfolgsrate in ALOHA-Protokollen für Mediumszugang* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof.Dr. W. König, Prof. Dr. B. Jahnel, September 28.
10. S.M. Kaiser, *Effiziente numerische Verfahren für die Portfoliooptimierung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, August 21.
11. L. Kieslich, *Gelation in particle systems with coagulation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, April 5.
12. T. Konopka, *Optimale Steuerung eines raum-zeitlichen Modells für die Hochseefischerei* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, May 17.
13. J. Köppl, *Dynamical Gibbs variational principles for irreversible interacting particle systems* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. B. Jahnel, Prof. Dr. W. König, April 22.
14. Th.C. Le, *Phasenübergang in einem modifizierten freien Bosegas* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof.Dr. W. König, Prof. Dr. B. Jahnel, September 27.
15. Z. Li, *A method for modularity optimization based on total variance and signless total variance* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. V. John, Dr. Y. van Gennip, July 26.

16. C. Ly, *Large deviations of the empirical process of random walkers with reflecting boundaries in the Skorokhod topology* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. M. Renger, Prof. Dr. W. König, April 4.
17. C. Melnic, *H(div)-conforming finite elements for the Stokes equations* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, January 10.
18. L. Metz, *Burgers' equation* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, December 5.
19. J. Nguyen, *Eine mathematische Modellierung von Eierstockkrebs durch einen Multityp-Verzweigungsprozess* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Dr. N. Kurt, Prof. Dr. W. König, July 28.
20. M.-T. Nguyen, *Genetische Algorithmen für die multikriterielle Bilevel-Optimierung von Verkehrsmanagementproblemen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, May 18.
21. S.C. Paltra, *Investigations of the use of the monotropic programming framework to model, analyze and design gas networks* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, February 16.
22. T.Y.M. Paulin, *Das parabolische Anderson-Modell auf dem vollständigen Graphen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R.I.A. Patterson, August 5.
23. P.M. Reif, *Space-Mapping zur optimalen Steuerung stochastisch interagierender Partikelsysteme* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, August 18.
24. E. Schirren, *Gemischte Perkolation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, May 17.
25. E. Schmitz, *Analyticity of the capacity functional of the infinite cluster in the Boolean model* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, May 4.
26. H. Shafigh, *Strategien für Zugänge zu einem Kommunikationsmedium* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, August 3.
27. T. Siebert, *Multikriterielle Topologieoptimierung mit genetischen Algorithmen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, August 22.
28. D. Siemann, *Filterverfahren in der nichtlinearen Optimierung* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, January 7.
29. L.C. Stanzel, *Ein Mean-Field-Modell für das interagierende Bosegas* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. B. Jahnel, July 27.
30. R. Szatkowska, *Fixation of a two-particle Abelian network* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 14.
31. L. Teigeler, *Variable-Metrik-Verfahren in der Topologieoptimierung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, October 4.
32. T.C. Wieczorek, *Topologieoptimierung – Vergleich und Bewertung von Nebenbedingungen* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, August 14.

33. H. ZHOU, *Rekonstruktion hochdimensionaler Signale aus niederdimensionalen vertauschten Beobachtungen* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. M. Scheutzow, Prof. Dr. W. König, December 7.
34. F. SEVERING, *Instabilities in the context of the generalized nonlinear Schrödinger equation* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: PD Dr. U. Bandelow, Prof. K. Busch, November 24.

A.2 Grants[1]

European Union, Brussels

- **Seventh Framework Programme**

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

  The project ERC-2015-CoG no. 683164 takes part in RG 6 and was initially funded for the duration from September 2016 to August 2021. It has been extended to August 2022. Its purpose is to study a number of important problems in stochastic analysis, including the transfer of rough paths ideas to Hairer’s regularity structures, the study of rough volatility in quantitative finance, a pathwise view on stochastic Loewner evolution, and an understanding of the role of geometry in the pathwise analysis of fully nonlinear evolution equations. This project is run jointly with the Technische Universität Berlin.

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

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

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

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

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

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

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 was the joint operation of the Berlin Mathematics Research Center MATH+.

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

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

stories of the renowned Research Center MATHEON and the Excellence-Graduate School Berlin Mathematical School (BMS).

In 2022, WIAS dedicated considerable financial and personal resources to the Center: Its director, Prof. M. Hintermüller (RG 8) was elected speaker of MATH+ in November 2022. He, Prof. A. Mielke (RG 1, Chair of the MATH+ Council), Prof. W. König (RG 5), Prof. P. Friz (RG 6), Prof. V. Spokoiny (RG 6), Prof. M. Thomas (WG BIP), Dr. Chr. Bayer (RG 6), and Dr. R. Henrion (RG 4) were members of the MATH+ Council; Dr. U. Bandelow (RG 2), Scientist in Charge of the Application Area AA2 “Materials, Lights, Devices,” Prof. P. Friz (RG 6) and Dr. R. Henrion (RG 4), Scientists in Charge of the Application Area AA4 “Energy and Markets,” Prof. M. Hintermüller (RG 8) and Prof. V. Spokoiny (RG 6), Scientists in Charge of the Emerging Field EF3 “Model-based Imaging,” and Prof. W. König, Scientist in Charge of the Emerging Field EF4 “Particles and Agents;” 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)

AA2-6 “Modeling and simulation of multi-material electrocatalysis” (in RG 3 and RG 7)

AA2-9 “Variational methods for viscoelastic flows and gelation” (in WG BIP and RG 7)

AA2-10 “Electromechanical coupling for semiconductor devices” (in RG 1 and LG NUMSEMIC)

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)

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)

EF1-13 “Stochastic and rough aspects in deep neural networks” (in RG 6)

EF1-15 “Robust multilevel training of artificial neural networks” (in RG 8)

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

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

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

EF3-8 “Analysis of brain signals by Bayesian Optimal Transport” (in RG 6)

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

EF3-12 “Integrated learning and variational methods for quantitative dynamic imaging” (in RG 8)

EF4-1 “Influence of mobility on connectivity” (in RG 5 and LG DYCOMNET)

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

IN-7 “Electronic properties of gate-confined quantum dots in Si-Ge heterostructures for Qubit generation” (in RG 1)

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

Approved subprojects, starting in 2023:

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

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

EF1-22 “Bayesian optimization and inference for deep networks” (in RG 6)

EF1-25 “Wasserstein gradient flows for generalized transport in Bayesian inversion” (in RG 6)

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

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

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

  In December 2022, the SFB completed its third and last funding period. This interdisciplinary SFB combined groups from theoretical physics, applied mathematics, and computational neuroscience from four universities and research institutes in Berlin. WIAS participated with two subprojects. Subproject A3 “Self-organization and control in coupled networks and time-delayed systems” in RG 2 was focused on high-dimensional dynamics and localization phenomena in complex network systems and delay-differential equations. Subproject A5 “Pattern formation in coupled parabolic systems” in RG 1 studied pattern formation in reaction-diffusion systems and in models of fluid dynamics.

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

  The center began its work on October 1, 2014, and changed from the second into the third funding period in the middle of 2022, which will last until June 30, 2026. WIAS members participated until June 30, 2022, in the subprojects B01 “Fault networks and scaling properties of deformation accumulation” (in RG 1, with FU Berlin and GFZ Potsdam), C02 “Interface dynamics: Bridging stochastic and hydrodynamic descriptions” (in RG 1, with FU Berlin), C05 “Effective models for materials and interfaces with multiple scales” (in RG 1), and C08 “Stochastic spatial coagulation particle processes” (in RG 5). The subproject C09 “Dynamics of rock dehydration on multiple scales” (in WG BIP with FU Berlin) was worked on until Dec. 31, 2022. From July 1, 2022, WIAS staff participated in the subprojects B09 “Materials with discontinuities on many scales” (in RG 1 and WG BIP with FU Berlin) and C02 “Interface dynamics: Bridging stochastic and hydrodynamic descriptions” (in RG 5 and WG BIP, with FU Berlin).

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

  This center started in July 2017 and was initially funded for the duration of four years. In 2021, the second funding was granted for another four years until June 2025. It is coordinated by Universität Potsdam together with HU Berlin, TU Berlin, WIAS, Geoforschungszentrum Potsdam, and Universität Magdeburg. The research is focused on the seamless integration of large data sets into sophisticated computational models. When the computational model is based on evolutionary equations and the data set is time ordered, the process of combining models and data is called *data assimilation*.

The subproject A06 “Approximative Bayesian inference and model selection for stochastic differential equations (SDEs)” is carried out jointly between the TU Berlin, with the focus on variational Bayesian methods on combined state and drift estimation for SDEs, WIAS (in RG 6), on prior selection for semi- and non-parametric statistics applied to SDEs, and the Universität Potsdam, on sequential Monte Carlo methods for high-dimensional inference problems arising from SDEs.

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

RG 4 participates in this priority program with the subproject “Multi-scale failure analysis with polymorphic uncertainties for optimal design of rotor blades,” which is a collaboration with Prof. Yuriy Petryna at the TU Berlin. Main goals of the subproject are a possibilistic-probabilistic modeling of an adhesion layer described by a non-periodic random microstructure, and the numerical upscaling to a macroscopic random representation.

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

The Director of WIAS, Prof. Michael Hintermüller, is the coordinator of this priority program that was started in October 2016 with the aim to help solve some of the most challenging problems in the applied sciences that involve nondifferentiable structures as well as partial differential operators, thus leading to nonsmooth distributed parameter systems. The second funding period started in 2020 and was extended cost-neutrally until December 2024.

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

- **Priority Program SPP 2171: “Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates,”** Universität Münster

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

WIAS participates in this first funding period with the two subprojects “Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows” (in WG BIP; duration Sep. 2019 – Aug. 2022) 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 – Dec. 2022).

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

The aim of this priority program, whose first funding period started in July 2020, is the development of analytical and numerical tools for the solution of problems in the continuum mechanics of solids. The research in the priority program is grouped in three major research directions: multiscale and multiphysics problems, coupling of dimensions, and evolution of microstructure. Within this general scope, mathematical tools from the field of variational analysis are of great interest. They include the theories of homogenization, relaxation, Γ-convergence, and variational time evolution. WIAS contributes to the priority program with three subprojects: “Fractal and stochastic homogenization using variational methods” and “Analysis for thermo-mechanical models with internal variables" (both in RG 1) as well as "Nonlinear fracture dynamics: Modelling, analysis, approximation and applications" (WG BIP with Universität Siegen and Karlsruhe Institute of Technology).

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

  The head of RG 5, Prof. Wolfgang König, is the head 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.

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

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

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

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

  The first phase of this research unit has been funded since 2016, the second phase since 2019. One of the two spokespersons is Prof. Peter Friz (RG 6). The unit works on innovative methods for applying rough path theory to the analysis of stochastic partial differential equations (SPDEs), like rough flow transformations, paracontrolled distributions, and regularity structures, to push forward the understanding of the solution theory of various types of SPDEs and the analysis of the most important physical properties of the solution processes.

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

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

- **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 which in principle can be represented in neural and tensor networks. Main goals are the analysis of backward stochastic differential equation (BSDE) solutions and transport maps in terms of such compositions, the development of new tensor formats that are tailored to represent functions compositions, and the development of active and passive learning algorithms via optimal sampling techniques in a new COFNET format.

- **RFBR-DFG Cooperation: Joint German-Russian Research Projects**

  "Collective dynamics of heterogeneous networks of active elements" (in RG 2): The project was established jointly with the Institute of Applied Physics of the Russian Academy of Sciences (Nishny Novgorod) and is devoted to the investigation of the dynamics of large networks of active elements. Due to the pandemic situation, all traveling activities had to be cancelled, but a successful collaboration has been established on the basis of video conferencing and online communication.

- **Normalverfahren (Individual Grants)**

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

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

  "Computational multiscale methods for inverse estimation of effective properties of poroelastic tissues" (in RG 3)

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

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

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

  "Mathematische Modellierung und Simulation der Wechselwirkung von Substraten mit Strömungen durch verallgemeinerte Gradientenflüsse" (Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows; see SPP 2171, Dr. D. Peschka)

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

Leibniz-Gemeinschaft (Leibniz Association), Berlin

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

  "Leibniz-MMS: Mathematische Modellierung und Simulation" (Leibniz MMS: Mathematical Modeling and Simulation; January 2021 – December 2022, 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 ITWM, DFKI Kaiserslautern, and Leibniz IPF Dresden (January 2022 – December 2024)

Approved project:

"Excellence in Photonic Crystal Surface Emitting Lasers", contribution of RGs 2, 3 and LG NUMSEMIC to a Leibniz Association's Cooperative Excellence project led by the Ferdinand Braun Institute (FBH). Further partner: Center of Excellence for Photonic-Crystal Surface-Emitting Lasers at Kyoto University (April 1, 2023 – April 1, 2026)

Einstein Stiftung Berlin (Einstein Foundation Berlin)

- Thematic Einstein Semester "Mathematics of Imaging in Real-World Challenges" (October 2021 – March 2022, co-organized by RG 8)

Investitionsbank Berlin

- **Programm zur Förderung von Forschung, Innovationen und Technologien (*Pro*FIT)** (Support program for research, innovation and technology)

  "ReLkat – Reinforcement Learning für komplexe automatisierungstechnische Anwendungen" (Reinforcement Learning for complex automation engineering), Fraunhofer IPK, Berlin

  The project in collaboration with Signal Cruncher GmbH and Fraunhofer IPK in the realm of Industry 4.0 develops machine-learning algorithms for the efficiency optimization of industrial high-energy production processes. The algorithms have to work on-site with continuous updating of the current state and in real-time environments. Reinforcement Learning methods for high-dimensional nonlinear systems are realized with efficient low-rank tensor formats (in RG 4).

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

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

International projects

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

Mission-oriented research (example)

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

A.3 Membership in Editorial Boards[2]

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

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

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

A.4 Conferences, Colloquia, and Workshops

RANDOM GEOMETRIC SYSTEMS – FIRST ANNUAL CONFERENCE OF THE SPP 2265

Berlin, April 11–14
Organized by: WIAS (RG 5)
Supported by: DFG SPP 2265

The workshop was one of the main activities of the newly founded Priority Program SPP 2265 *Random Geometric Systems*. It was the first opportunity after the pandemic that the members of the SPP 2265 could meet on a larger scale, and many scientists took advantage of this. The conference offered a broad survey on all the topics of the Priority Program SPP 2265, like spatial point processes, percolation, random polytopes, phase transitions and much more. The program comprised two extended guest talks, presentation of 13 of the 25 projects of the SPP 2265, a series of crash courses for younger researchers on fundamental topics, and two brain storming discussion panels on hot open prolems. 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 69 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-Haus in Berlin-Dahlem.

The organizers were five members of the RG 5.

LEIBNIZ-MMS DAYS 2022

Potsdam, April 25–27
Organized by: WIAS, PIK
Supported by: MMS

After the Leibniz MMS Days as the central annual meeting of the Leibniz Network “Mathematical Modeling and Simulation” had to be postponed at short notice due to the pandemic in March 2020, this could be caught up from April 25 to 27, 2022, at the Potsdam Institute for Climate Impact Research (PIK). The meeting marked a successful relaunch of scientific face-to-face workshops, which are fundamentally important for this network structure, and was attended by 55 scientists from 20 institutions.

Three key-note talks were given by: Florian Dörfler (ETH Zurich) on data-enabled predictive control; Harald Pfeiffer (Max Planck Institute for Gravitational Physics – Albert Einstein Institute, Potsdam) on binary black hole coalescence: From numerical relativity to gravitational waves, and Luciano Rezzolla (Goethe-Universität, Frankfurt) on the first image of a black hole. There were general plenary contributions and discussions on MMS-related topics at large, and in particular on research software, the programming language Julia, research data, reproducibility, Open Science, data science, and other topics.

15TH ANNUAL ERC BERLIN-OXFORD YOUNG RESEARCHERS MEETING ON APPLIED STOCHASTIC ANALYSIS

Berlin, May 12–14
Organized by: WIAS (RG 6), TU Berlin, University of Oxford
Supported by: WIAS, University of Oxford, TU Berlin, DFG FOR 2402, DFG IRTG 2544, European Research Council, DataSig

Sixty-two participants attended the 15th Berlin-Oxford Workshop in May. As in previous years, the workshop continued the tradition of previous meetings, with focus on Applied Stochastic Analysis, including but not restricted to the resolution of ill-posed stochastic partial differential equations (SPDEs) to new ways of handling high-dimensional data. More specifically, talks were divided into sections on “Rough Paths and Regularity,” “Signatures and Data Science,” “Numerical Analysis/Mathematical Finance,” SPDEs, and “Further Topics in Stochastic Analysis.” (The 16th meeting took place in Oxford in December 2022, a 17th meeting is scheduled to take place in Berlin in April 2023.

RANDOM POINT PROCESSES IN STATISTICAL PHYSICS

Berlin, June 29 – July 1
Organized by: WIAS (RG 5 and LG DYCOMNET)
Supported by: DFG SPP 2265

This workshop discussed old and new results and old and new open problems from Statistical Physics around random point processes in discrete and continuous space. It brought together mathematicians and physicists and gave both communities opportunities to jump over the language barrier and to have cross-community discussions. Some of the main topics of the workshop were phase transitions, interacting many-body systems with extra features, Gibbs measures in continuum with marks and/or time-dependence, density functional theory and smectic phases. Twenty-one participants enjoyed respectively gave eight research talks and two minicourses on Gibbs measures in continuum and on the interacting Bose gas, respectively. All talks were given in presence in the wonderful location of the Harnack-Haus in Berlin-Dahlem.

The workshop was organized within the activities of the newly founded Priority Program SPP 2265 *Random Geometric Systems*.

The organizers were Benedikt Jahnel (LG DYCOMNET) and Wolfgang König (RG 5)

WORKSHOP ON NUMERICAL METHODS AND ANALYSIS IN CFD

Berlin, July 5–8
Organized by: WIAS (RG 3)
Supported by: Joint Seed Funding Call 2021 of the Humboldt-Universität zu Berlin and University of Zurich

This workshop was devoted to modern numerical methods for solving equations from fluid dynamics, such as Stokes and Navier–Stokes equations, convection-diffusion-reaction or reaction-diffusion equations, and coupled systems. Talks on numerical analysis topics covered, e.g., temporal and spatial discretizations, adaptive methods, and reduced-order methods. Talks devoted to applications presented, e.g., methods for flows in vascular tissues, for the simulation of rarefied gas flows, and for fluid-body interaction problems.

The workshop was attended by 47 participants from 11 countries.

STOCHASTIC & ROUGH ANALYSIS (SRA)

Berlin, August 22–26
Organized by: HU Berlin, FU Berlin, TU Berlin, WIAS (RG 6), and Universität Potsdam
Supported by: European Research Council, DFG FOR 2402, and DFG IRTG 2544

Eighty-six participants attended the SRA conference in August 2022 at Harnack House. This conference marked the end of ERC Project GPSART “Geometric Aspects in Pathwise Analysis and Related Topics” (PI: Peter Friz), hosted jointly at WIAS and Technische Universität Berlin since 2016. The conference also served as a platform to share progress among members of the DFG Research Unit FOR 2402 *Rough Paths, Stochastic Partial Differential Equations and Related Topics*, the second funding period of which is also nearing its end. Many international speakers, including Fields medallist Martin Hairer, made this conference a memorable event. The event was also targeted at early career researchers, in the audience there were many members of the Berlin-Oxford graduate school IRTG 2544. (WIAS Berlin is a host institution for all named projects.)

NONLINEAR WAVES AND TURBULENCE IN PHOTONICS 2022

Berlin, July 13–15
Organized by: WIAS (RG 2)

The Workshop “Nonlinear Waves and Turbulence in Photonics” was financially supported by WIAS. It brought together internationally renowned researchers working on theoretical, experimental, and applied aspects of the nonlinear wave-dynamics in optical systems as well as on mathematical methods for modeling and analysis of the nonlinear light propagation. The workshop featured a good balance between theory, experiment, and simulations and provided the participants with a platform to present their latest developments in the field, as well as to exchange ideas and knowledge. The subjects of the Workshop included: time-delayed systems in optics, dispersive and dissipative solitons, optical cavities, semiconductor- and fiber-lasers, non-Hermitian systems, exceptional points, extreme nonlinear optics, and optical wave turbulence. Due to the corona restrictions, the total number of participants was limited to 25, including the organizers. The program comprised 18 invited and 3 contributed talks, all on-site.

Symposium on the Occasion of Uwe Bandelow's 60th Anniversary
Berlin, August 30
Organized by: WIAS (RG 2)

On August 30, the WIAS organized a colloquium in honor of the 60th birthday of Priv.-Doz. Dr. Uwe Bandelow, who started his career at the WIAS in 1996 and, since 2005, has been the head of Research Group 2 *Laser Dynamics*. The scientific program comprised four invited talks on the topics of laser physics and nonlinear optics, highlighting the impact of Uwe Bandelow in these fields and pointing out future perspectives and new developments in this vibrant field of research.

Minisymposium for Young Researchers 2022 (Online Event)
Berlin, July 21
Organized by: WIAS (RG 2)

The online symposium for young researchers was financially supported by WIAS. It brought together several doctoral and master's students working in the field of nonlinear optics and photonics. The symposium was associated to the main Workshop "Nonlinear Waves and Turbulence in Photonics" (July 13–15). As the number of the main workshop contributors was limited due to the corona restrictions, the follow-up symposium gave several young scientists the opportunity to present their results and to become visible to the internationally renowned researchers participating in the main event. The program included six online talks devoted to solitons and nonlinear wave instabilities in optics, dispersion design, Kerr resonators and nonlinear light propagation in liquid crystals.

MathBio22 – Mathematical Models for Biological Multiscale Systems (Hybrid Format)
Berlin, September 12–14
Organized by: WIAS (RG 1 (Matthias Liero), RG 3 (Alfonso Caiazzo), RG 7 (Barbara Wagner), WG BIP (Dirk Peschka))
Supported by: Einstein Foundation Berlin, MATH+

At the Workshop, mathematical methods and topics were identified and discussed that bridge the gap in scale and complexity between microscopic descriptions of biological and biophysical systems with corresponding partial differential equation descriptions. The focus of the workshop was on the multiscale nature innate to biological processes connecting interacting biomolecules with complex systems such as cells, tissue, and organs to elucidate macroscopic phenomena. The event attracted an international audience and featured nine invited and 15 contributed talks.

Junior Female Researchers in Probability
Berlin, October 5–7
Organized by: IRTG 2544 Berlin-Oxford
Supported by: MATH+, HU Berlin, TU Berlin, WIAS

The goal of the workshop was to offer international 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. To cover various topics in probability and its applications, two keynote talks by outstanding female probabilists and four invited talks built the core of the program. Moreover, a number of contributed talks were chosen by the organizing committee among the submitted abstracts. Substantial financial support was given to many young females for travel and accommodation, and about 20–30 took this opportunity to present their Ph.D. work to a larger audience.

The workshop took place in hybrid format, and about 88 participants (by far not only females) were present in person at the wonderful location at the Tieranatomisches Theater (TA T) of the Humboldt-Universität zu Berlin in Berlin-Mitte. Most of the talks were given in presence, and all the participants that were present enjoyed having a direct communication after a long break, due to the pandemic.

This workshop was organized by a team of eight people, comprising with Alexandra Quitmann one member of the WIAS Research Group RG 5

ANNUAL MEETING OF THE DFG PRIORITY PROGRAMME 1962

Berlin, October 24–26
Organized by: WIAS (RG 8), HU Berlin
Supported by: DFG SPP 1962

The Annual Meeting of the Second Phase of the DFG Priority Programme (SPP) 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization*, organized by Amal Alphonse, Pia Pfau, and Michael Hintermüller with support from Sarah Essadi and Mike Theiss, took place from October 24 to 26 in Novotel in central Berlin.

A total of 49 participants attended the annual meeting of whom 45 were from outside WIAS. All but one of the 21 scientific projects in the SPP were represented by a talk of 25 minutes where a presentation of work done and results achieved in the project was given. In addition, a meeting for principal investigators also took place where important matter related to the upkeep of SPP issues as well as the future prospects for the SPP community were discussed since it was anticipated that this meeting would be the final one. At the same time, a Young Researchers' Meeting took also place, which helped to identify an organizational team (outside WIAS) who will be responsible for running a Young Researchers' event for the younger SPP members in 2023. In summary, the meeting was well attended, and participants greatly enjoyed the central location and quality of the venue.

MARDI ANNUAL WORKSHOP 2022 (HYBRID EVENT)

Berlin, November 9–11
Organized by: WIAS, Universität Stuttgart, Universität Leipzig, FIZ Karlsruhe
Supported by: MaRDI

WIAS hosted the 3-day second annual MaRDI Workshop in November 2022. The hybrid event saw 40 people meeting on site with up to 10–12 people online and was geared towards lessons learned in the past year, identifying potential gaps and themes for future development. The keynote delivered by Professor Martin Grötschel shared his experiences working in large collaborative projects similar to MaRDI and his vision of a mathematical research data infrastructure, helped in shaping discussions on linking of services to the MaRDI portal, development of research data management plans for mathematical data, and integrating the research community. Where the first workshop in 2021 provided a good start for the consortium, the second was focused on networking with the community and consortial cross collaboration.

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

1. O. Butkovsky, co-organizer, *Mini-Workshop "Regularization by Noise: Theoretical Foundations, Numerical Methods and Applications driven by Levy Noise"*, Mathematisches Forschungsinstitut Oberwolfach, February 13–20.
2. A. Caiazzo, co-organizer of the Minisymposium MS 129: "Biomechanical Model-Based MR Imaging, Inverse Problems, and Applications", *2022 SIAM Conference on Imaging Science (IS22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 21–25.
3. P. Dvurechensky, co-organizer of the Minisymposium MS 84: "Multi-Marginal Optimal Transport", *2022 SIAM Conference on Imaging Science (IS22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 21–25.
4. M. Eigel, member of the Organizing Committee, *Research School "High Dimensional Approximation and Deep Learning"*, Centre de Mathématiques Henri Lebesgue, Nantes, France, May 16–20.
5. Th. Eiter, co-organizer of the Minisymposium "Recent Developments in the Mathematical Analysis of Viscous Fluids", *SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 14–18.
6. ———, co-organizer, *Young Researchers' Forum on Mathematical Fluid Mechanics (Online Event)*, Waseda University, Tokyo, Japan, June 20–21.
7. P. Friz, co-organizer, *16th Oxford-Berlin Young Researcher's Meeting on Applied Stochastic Analysis*, University of Oxford, UK, December 8–10.
8. M. Heida, organizer of the Minisymposium "Homogenization of Random Singular Structures", *SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 14–18.
9. M. Hintermüller, member of the Organizing Committee, *2022 SIAM Conference on Imaging Science (IS22) (Online Event)*, Society for Industrial and Applied Mathematic, Philadelphia, USA, March 21–25.
10. ———, organizer of the Cluster "PDE-Constrained Optimization", *International Conference on Continuous Optimization – ICCOPT/MOPTA 2022*, Lehigh University, Bethlehem, Pennsylvania, USA, July 23–28.
11. D. Hömberg, member of the Organizing Committee, *ESGI 156 – The Norwegian Study Group with Industry*, Norwegian University of Science and Technology, Ålesund, Norway, June 13–17.
12. B. Jahnel, co-organizer, *Workshop "Recent Trends in Spatial Stochastic Processes"*, EURANDOM, Eindhoven, Netherlands, October 3–7.
13. Th. Koprucki, K. Tabelow, co-organizers of the Minisymposium 09 "The Future of Digital Infrastructures for Mathematical Research", *DMV Annual Meeting 2022*, Freie Universität Berlin, September 12–16.
14. R. Lasarzik, co-organizer of the Minisymposium MS47: "Generalized Solvability Concepts for Evolutionary PDEs and their Properties", *SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 14–18.
15. M. Liero, D. Peschka, M. Thomas, co-organizers of the Minisymposium "Energy-Based Mathematical Methods and Thermodynamics", *SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 14–18.

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

16. CH. MERDON, co-organizer of the Minisymposium MS142: "Structure-preserving Finite Element Methods in Computational Fluid Dynamics", *8th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 22)*, Nordic Association of Computational Mechanics, Oslo, Norway, June 5–9.
17. A. MIELKE, co-organizer of the Minisymposium "Nonlinear Parabolic Equations and Systems", *SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 14–18.
18. K. PAPAFITSOROS, co-organizer, *MATH+ Hackathon "Maths Meets Image"*, MATH+, Fabrik 23, The Classroom, Berlin, March 17–19.
19. ———, organizer of the Minisymposium "Recent Developments in Image Super-Resolution", *SIAM Conference on Imaging Science (IS22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 21–25.
20. V. SPOKOINY, organizer, *Rencontres de Statistique Mathématique*, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 12–16.
21. A. STEPHAN, co-organizer of the Minisymposium "Variational Evolution: Analysis and Multi-Scale Aspects", *SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event)*, Society for Industrial and Applied Mathematics, Philadelphia, USA, March 14–18.
22. M. WOLFRUM, Member of the Program Committee, *CRC 910: International Conference on Control of Self Organizing Nonlinear Systems*, Technische Universität Berlin, November 23–26.

A.6 Publications

A.6.1 Editorship of Proceedings and Collected Editions

[1] M. Hintermüller, R. Herzog, Ch. Kanzow, M. Ulbrich, St. Ulbrich, eds., *Non-Smooth and Complementarity-Based Distributed Parameter Systems: Simulation and Hierarchical Optimization*, vol. 172 of International Series of Numerical Mathematics, Birkhäuser, Springer Nature Switzerland AG, Cham, 2022, viii + 519 pages. DOI: 10.1007/978-3-030-79393-7.

Proceedings and Collected Editions (to appear)

[1] A.H. Erhardt, K. Tsaneva-Atanasova, G.T. Lines, E.A. Martens, eds., *Dynamical Systems, PDEs and Networks for Biomedical Applications: Mathematical Modeling, Analysis and Simulations*, Special Edition of Front. Phys., Sec. Statistical and Computational Physics, Frontiers, Lausanne, Switzerland.

[2] B. Wagner, M. Timme, eds., *Special Issue "The Mathematics in Renewable Energy"*, European Journal of Applied Mathematics, Springer Nature, Heidelberg et al.

A.6.2 Outstanding Contributions to Monographs

[1] M. Danilova, P. Dvurechensky, A. Gasnikov, E. Gorbunov, S. Guminov, D. Kamzolov, I. Shibaev, *Chapter: Recent Theoretical Advances in Non-convex Optimization*, A. Nikeghbali, P.M. Pardalos, A.M. Raigorodskii, M.T. Rassias, eds., vol. 191 of Springer Optimization and Its Applications, Springer, Cham, 2022, pp. 79–163. DOI: 10.1007/978-3-031-00832-0_3.

A.6.3 Articles in Refereed Journals[4]

[1] M. Brokate, M. Ulbrich, *Newton differentiability of convex functions in normed spaces and of a class of operators*, SIAM J. Optim., 32 (2022), pp. 1265–1287. DOI: 10.1137/21M1449531.

[2] P. Colli, G. Gilardi, E. Rocca, J. Sprekels, *Well-posedness and optimal control for a Cahn–Hilliard–Oono system with control in the mass term*, Discrete Contin. Dyn. Syst. Ser. S, 15 (2022), pp. 2135–2172. DOI: 10.3934/dcdss.2022001.

[3] P. Colli, G. Gilardi, J. Sprekels, *Optimal control of a phase field system of Caginalp type with fractional operators*, Pure Appl. Funct. Anal., 7 (2022), pp. 1597–1635.

[4] ———, *Well-posedness for a class of phase-field systems modeling prostate cancer growth with fractional operators and general nonlinearities*, Atti Accad. Naz. Lincei Rend. Lincei Mat. Appl., 33 (2022), pp. 193–228. DOI: 10.4171/rlm/969.

[5] P. Colli, A. Signori, J. Sprekels, *Analysis and optimal control theory for a phase field model of Caginalp type with thermal memory*, Commun. Optim. Theory, 2022 (2022), pp. 4/1–4/31. DOI: 10.23952/cot.2022.4.

[6] ———, *Optimal control problems with sparsity for tumor growth models involving variational inequalities*, J. Optim. Theory Appl., 194 (2022), pp. 25–58. DOI: 10.1007/s10957-022-02000-7.

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A.6.4 Contributions to Collected Editions

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A.7 Preprints, Reports

A.7.1 WIAS Preprints Series[5]

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[2] P. Colli, G. Gilardi, A. Signori, J. Sprekels, *Cahn–Hilliard–Brinkman model for tumor growth with possibly singular potentials*, Preprint no. 2939, WIAS, Berlin, 2022.

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[4] ———, *Optimal control of a nonconserved phase field model of Caginalp type with thermal memory and double obstacle potential*, Preprint no. 2949, WIAS, Berlin, 2022.

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[10] Ch. Bayer, Ch. Ben Hammouda, A. Papapantoleon, M. Samet, R. Tempone, *Optimal damping with hierarchical adaptive quadrature for efficient Fourier pricing of multi-asset options in Lévy models*, Preprint no. 2968, WIAS, Berlin, 2022.

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[17] M. Eigel, M. Haase, J. Neumann, *Topology optimisation under uncertainties with neural networks*, Preprint no. 2982, WIAS, Berlin, 2022.

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[19] M. Kirstein, M. Eigel, D. Sommer, *Tensor-train kernel learning for Gaussian processes*, Preprint no. 2981, WIAS, Berlin, 2022.

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[20] Th. Eiter, *On the regularity of weak solutions to time-periodic Navier–Stokes equations in exterior domains*, Preprint no. 2979, WIAS, Berlin, 2022.

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[37] M. Hintermüller, T. Keil, *Strong stationarity conditions for the optimal control of a Cahn–Hilliard–Navier–Stokes system*, Preprint no. 2924, WIAS, Berlin, 2022.

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[39] D. Hömberg, R. Lasarzik, L. Plato, *On the existence of generalized solutions to a spatio-temporal predator-prey system*, Preprint no. 2925, WIAS, Berlin, 2022.

[40] N. Engler, B. Jahnel, Ch. Külske, *Gibbsianness of locally thinned random fields*, Preprint no. 2910, WIAS, Berlin, 2022.

[41] A. Hinsen, B. Jahnel, E. Cali, J.-P. Wary, *Chase-escape in dynamic device-to-device networks*, Preprint no. 2969, WIAS, Berlin, 2022.

[42] Ch. Hirsch, B. Jahnel, St. Muirhead, *Sharp phase transition for Cox percolation*, Preprint no. 2922, WIAS, Berlin, 2022.

[43] B. Jahnel, J. Köppl, *Dynamical Gibbs variational principles for irreversible interacting particle systems with applications to attractor properties*, Preprint no. 2935, WIAS, Berlin, 2022.

[44] Ch. Ghribi, E. Cali, Ch. Hirsch, B. Jahnel, *Agent-based simulations for coverage extensions in 5G networks and beyond*, Preprint no. 2920, WIAS, Berlin, 2022.

[45] B. Jahnel, S.K. Jhawar, A.D. Vu, *Continuum percolation in a nonstabilizing environment*, Preprint no. 2943, WIAS, Berlin, 2022.

[46] O. Collin, B. Jahnel, W. König, *The free energy of a box-version of the interacting Bose gas*, Preprint no. 2914, WIAS, Berlin, 2022.

[47] V. John, P. Knobloch, O. Pártl, *A numerical assessment of finite element discretizations for convection-diffusion-reaction equations satisfying discrete maximum principles*, Preprint no. 2946, WIAS, Berlin, 2022.

[48] M. Kantner, L. Mertenskötter, *Improved laser linewidth estimation from self-heterodyne beat note measurements using parametric Wiener filters*, Preprint no. 2983, WIAS, Berlin, 2022.

[49] S. Katz, A. Caiazzo, V. John, *Impact of viscosity modeling on the simulation of aortic blood flow*, Preprint no. 2963, WIAS, Berlin, 2022.

[50] W. König, H. Shafigh, *Multi-channel ALOHA and CSMA medium-access protocols: Markovian description and large deviations*, Preprint no. 2985, WIAS, Berlin, 2022.

[51] Th. Koprucki, A. Maltsi, A. Mielke, *Symmetries in TEM imaging of crystals with strain*, Preprint no. 2938, WIAS, Berlin, 2022.

[52] R. Lasarzik, M.E.V. Reiter, *Analysis and numerical approximation of energy-variational solutions to the Ericksen–Leslie equations*, Preprint no. 2966, WIAS, Berlin, 2022.

[53] A. Afsardeir, A. Kapetanis, V. Laschos, K. Obermayer, *Risk-sensitive partially observable Markov decision processes as fully observable multivariate utility optimization problems*, Preprint no. 2977, WIAS, Berlin, 2022.

[54] J. Geuter, V. Laschos, *Generative adversarial learning of Sinkhorn algorithm initializations*, Preprint no. 2978, WIAS, Berlin, 2022.

[55] V. Laschos, A. Mielke, *Evolutionary variational inequalities on the Hellinger–Kantorovich and spherical Hellinger–Kantorovich spaces*, Preprint no. 2973, WIAS, Berlin, 2022.

[56] M. Liero, A. Mielke, G. Savaré, *Fine properties of geodesics and geodesic lambda-convexity for the Hellinger–Kantorovich distance*, Preprint no. 2956, WIAS, Berlin, 2022.

[57] Ch. Merdon, W. Wollner, *Pressure-robustness in the context of optimal control*, Preprint no. 2923, WIAS, Berlin, 2022.

[58] A. Mielke, *On two coupled degenerate parabolic equations motivated by thermodynamics*, Preprint no. 2937, WIAS, Berlin, 2022.

[59] R. Bazaes, A. Mielke, Ch. Mukherjee, *Stochastic homogenization of Hamilton–Jacobi–Bellman equations on continuum percolation clusters*, Preprint no. 2955, WIAS, Berlin, 2022.

[60] A. Mielke, T. Roubíček, *Qualitative study of a geodynamical rate-and-state model for elastoplastic shear flows in crustal faults*, Preprint no. 2954, WIAS, Berlin, 2022.

[61] R. Müller, M. Landstorfer, *Galilean bulk-surface electrothermodynamics and applications to electrochemistry*, Preprint no. 2984, WIAS, Berlin, 2022.

[62] O. Pártl, U. Wilbrandt, J. Mura, A. Caiazzo, *Reconstruction of flow domain boundaries from velocity data via multi-step optimization of distributed resistance*, Preprint no. 2929, WIAS, Berlin, 2022.

[63] A.K. Giri, P. Malgaretti, D. Peschka, M. Sega, *Hydrodynamics at the moving contact line*, Preprint no. 2911, WIAS, Berlin, 2022.

[64] A. Pimenov, A.G. Vladimirov, *Temporal solitons in an optically injected Kerr cavity with two spectral filters*, Preprint no. 2948, WIAS, Berlin, 2022.

[65] A. Roche, S. Slepneva, A. Kovalev, A. Pimenov, A.G. Vladimirov, M. Marconi, M. Giudici, G. Huyet, *Decoherence and turbulence sources in a long laser*, Preprint no. 2988, WIAS, Berlin, 2022.

[66] A. Quitmann, L. Taggi, *Macroscopic loops in the 3D double-dimer model*, Preprint no. 2944, WIAS, Berlin, 2022.

[67] ———, *Macroscopic loops in the Bose gas, Spin O(N) and related models*, Preprint no. 2915, WIAS, Berlin, 2022.

[68] M. Radziunas, *Calculation of steady states in dynamical semiconductor laser models*, Preprint no. 2961, WIAS, Berlin, 2022.

[69] A. Rathsfeld, *Simulating rough surfaces by periodic and biperiodic gratings*, Preprint no. 2989, WIAS, Berlin, 2022.

[70] R. Haller, H. Meinlschmidt, J. Rehberg, *Hölder regularity for domains of fractional powers of elliptic operators with mixed boundary conditions*, Preprint no. 2959, WIAS, Berlin, 2022.

[71] D.R.M. Renger, U. Sharma, *Untangling dissipative and Hamiltonian effects in bulk and boundary driven systems*, Preprint no. 2936, WIAS, Berlin, 2022.

[72] L. Schmeller, D. Peschka, *Gradient flows for coupling order parameters and mechanics*, Preprint no. 2909, WIAS, Berlin, 2022.

[73] M. Mirahmadi, B. Friedrich, B. Schmidt, J. Pérez-Ríos, *Mapping atomic trapping in an optical superlattice onto the libration of a planar rotor in electric fields*, Preprint no. 2972, WIAS, Berlin, 2022.

[74] D. Belomestny, J.G.M. Schoenmakers, *Primal-dual regression approach for Markov decision processes with general state and action space*, Preprint no. 2957, WIAS, Berlin, 2022.

[75] F. Severing, U. Bandelow, S. Amiranashvili, *Spurious four-wave mixing processes in generalized nonlinear Schrödinger equations*, Preprint no. 2975, WIAS, Berlin, 2022.

[76] G. Thiele, Th. Johanni, D. Sommer, J. Krüger, *Decomposition of a cooling plant for energy efficiency optimization using OptTopo*, Preprint no. 2980, WIAS, Berlin, 2022.

[77] M. Stöhr, M. Wolfrum, *Temporal dissipative solitons in the Morris–Lecar model with time-delayed feedback*, Preprint no. 2970, WIAS, Berlin, 2022.

[78] K. Ebrahimi-Fard, F. Patras, N. Tapia, L. Zambotti, *Shifted substitution in non-commutative multivariate power series with a view towards free probability*, Preprint no. 2945, WIAS, Berlin, 2022.

[79] M.G. Varzaneh, S. Riedel, A. Schmeding, N. Tapia, *The geometry of controlled rough paths*, Preprint no. 2926, WIAS, Berlin, 2022.

[80] P. Vágner, M. Pavelka, J. Fuhrmann, V. Klika, *A multiscale thermodynamic generalization of Maxwell–Stefan diffusion equations and of the dusty gas model*, Preprint no. 2947, WIAS, Berlin, 2022.

[81] T. Matsuda, W. van Zuijlen, *Anderson Hamiltonians with singular potentials*, Preprint no. 2976, WIAS, Berlin, 2022.

A.7.2 Preprints/Reports in other Institutions

[1] M. Brokate, C. Christof, *Strong stationarity conditions for optimal control problems governed by a rate-independent evolution variational inequality*, arXiv:2205.01196, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2205.01196.

[2] N. Ahmed, V. John, X. Li, Ch. Merdon, *Inf-sup stabilized Scott–Vogelius pairs on general simplicial grids for Navier–Stokes equations*, arXiv:2212.10909, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2212.10909.

[3] Ch. Bayer, M. Fukasawa, N. Shonosuke, *On the weak convergence rate in the discretization of rough volatility models*, arXiv:2203.02943, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2203.02943.

[4] Ch. Bayer, P.K. Friz, N. Tapia, *Stability of deep neural networks via discrete rough paths*, arXiv:2201.07566, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2201.07566.

[5] O. Butkovsky, K. Dareiotis, M. Gerencsér, *Strong rate of convergence of the Euler scheme for SDEs with irregular drift driven by Levy noise*, arXiv:2204.12926, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2204.12926.

[6] M. Alkousa, A. Gasnikov, P. Dvurechensky, A. Sadiev, L. Razouk, *An approach for non-convex uniformly concave structured saddle point problem*, arXiv:2202.06376, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2202.06376.

[7] P. Dvurechensky, S. Shtern, M. Staudigl, *A conditional gradient homotopy method with applications to semidefinite programming*, arXiv:2207.03101, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2207.03101.

[8] A. Gasnikov, A. Novitskii, V. Novitskii, F. Abdukhakimov, D. Kamzolov, A. Beznosikov, M. Takáč, P. Dvurechensky, B. Gu, *The power of first-order smooth optimization for black-box non-smooth problems*, arXiv:2201.12289, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2201.12289.

[9] V. Artem, A. Gasnikov, P. Dvurechensky, V. Spokoiny, *Accelerated gradient methods with absolute and relative noise in the gradient*, arXiv:2102.02921, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2102.02921.

[10] A. Erhardt, E. Wahlén, J. Weber, *Bifurcation analysis for axisymmetric water waves*, arXiv:2202.01754, arXiv, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2202.01754.

[11] St. Piani, P. Farrell, W. Lei, N. Rotundo, L. Heltai, *Data-driven solutions of ill-posed inverse problems arising from doping reconstruction in semiconductors*, arXiv:2208.00742, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2208.00742.

[12] ———, *A weighted hybridizable discontinuous Galerkin method for drift-diffusion problems*, arXiv:2211.02508, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2211.02508.

[13] M. O'Donovan, P. Farrell, J. Moatti, T. Streckenbach, Th. Koprucki, St. Schulz, *Impact of random alloy fluctuations on the carrier distribution in multi-color (In,Ga)N/GaN quantum well systems*, arXiv.2209.11657, Cornell University, Ithaca, 2022. DOI: 10.48550/arXiv.2209.11657.

[14] C. Bellingeri, P.K. Friz, S. Paycha, R. Preiss, *Smooth rough paths, their geometry and algebraic renormalization*, arXiv:2111.15539, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2111.15539.

[15] P.K. Friz, A. Hocquet, K. Lê, *Rough stochastic differential equations*, arXiv:2106.10340, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2106.10340.

[16] G.R. Barrenechea, V. John, P. Knobloch, *Finite element methods respecting the discrete maximum principle for convection-diffusion equations*, arXiv:2204.07480, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2204.07480.

[17] B. García-Archilla, V. John, J. Novo, *POD-ROMs for incompressible flows including snapshots of the temporal derivative of the full order solution*, arXiv:2206.09123, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2206.09123.

[18] A. Jha, V. John, P. Knobloch, *Adaptive grids in the context of algebraic stabilizations for convection-diffusion-reaction equations*, arXiv:2007.08405, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2007.08405.

[19] V. John, X. Li, Ch. Merdon, H. Rui, *Inf-sup stabilized Scott–Vogelius pairs on general simplicial grids by Raviart–Thomas enrichment*, arXiv:2206.01242, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2206.01242.

[20] P. Ral, A.K. Giri, V. John, *Instantaneous gelation and nonexistence for the Oort–Hulst–Safronov coagulation model*, arXiv:2206.02035, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2206.02035.

[21] S. Katz, A. Caiazzo, B. Moreau, U. Wilbrandt, J. Brüning, L. Goubergrits, V. John, *Impact of turbulence modeling on the simulation of blood flow in aortic coarctation*, arXiv:2208.14217, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2208.14217.

[22] J. Kern, *The Skorokhod topologies: What they are and why we should care*, arXiv:2210.16026, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2210.16026.

[23] N. Djurdjevac Conrad, J. Köppl, A. Djurdjevac, *Feedback loops in opinion dynamics of agent-based models with multiplicative noise*, arXiv:2209.07151, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2209.07151.

[24] T. Boege, R. Fritze, Ch. Görgen, J. Hanselman, D. Iglezakis, L. Kastner, Th. Koprucki, T. Krause, Ch. Lehrenfeld, S. Polla, M. Reidelbach, Ch. Riedel, J. Saak, B. Schembera, K. Tabelow, M. Weber, *Research-data management planning in the German mathematical community*, arXiv:2211.12071, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2211.12071.

[25] A. Kroshnin, E. Stepanov, D. Trevisan, *Infinite multidimensional scaling for metric measure spaces*, arXiv:2201.05885, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2201.05885.

[26] P. Gracar, L. Lüchtrath, Ch. Mönch, *Finiteness of the percolation threshold for inhomogeneous long-range models in one dimension*, arXiv:2203.11966, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2203.11966.

[27] M. Oliva, T. Flissikowsky, M. Góra, J. Lähnemann, J. Herranz, R. Lewis, O. Marquardt, M. Ramsteiner, L. Geelhaar, O. Brandt, *Carrier recombination in highly uniform and phase-pure GaAs/(Al,Ga)As core/shell nanowire arrays on Si(111): Mott transition and internal quantum efficiency*, arXiv:2211.17167, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2211.17167.

[28] F. Delarue, W. Salkeld, *Probabilistic rough paths II Lion–Taylor expansions and random controlled rough paths*, arXiv:2203.01185, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2203.01185.

[29] V. Spokoiny, *Dimension free non-asymptotic bounds on the accuracy of high dimensional Laplace approximation*, arXiv:2204.11038, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2204.11038.

[30] ———, *Finite samples inference and critical dimension for stochastically linear models*, arXiv:2201.06327, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2201.06327.

[31] Y.-W. Sun, K. Papagiannouli, V. Spokoiny, *High dimensional change-point detection: A complete graph approach*, arXiv:2203.08709, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2203.08709.

[32] J.M. Oeschger, K. Tabelow, S. Mohammadi, *Axisymmetric diffusion kurtosis imaging with Rician bias correction: A simulation study*, bioRxiv2022.03.15.484442, Cold Spring Harbor Laboratory, bioRxiv, Laurel Hollow, NY, USA, 2022. DOI: 10.1101/2022.03.15.484442.

[33] S. Mohammadi, T. Streubel, L. Klock, A. Lutti, K. Pine, S. Weber, L. Edwards, P. Scheibe, G. Ziegler, J. Gallinat, S. Kuhn, M. Callaghan, N. Weiskopf, K. Tabelow, *Error quantification in multi-parameter mapping facilitates robust estimation and enhanced group level sensitivity*, bioRxiv: 2022.01.11.475846, Cold Spring Harbor Laboratory, NY, USA, 2022. DOI: 10.1101/2022.01.11.475846.

[34] K. Ebrahimi-Fard, F. Patras, N. Tapia, L. Zambotti, *Shifted substitution in non-commutative multivariate power series with a view toward free probability*, arXiv:2204.01445, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2204.01445.

[35] M. Ghani Varzaneh, S. Riedel, A. Schmeding, N. Tapia, *The geometry of controlled rough paths*, arXiv:2203.05946, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2203.05946.

[36] Y. Nemmour, H. Kremer, B. Schölkopf, J.-J. Zhu, *Maximum mean discrepancy distributionally robust nonlinear chance-constrained optimization with finite-sample guarantee*, arXiv:2204.11564, Cornell University, Ithaca, USA, 2022. DOI: 10.48550/arXiv.2204.11564.

A.8 Talks and Posters

A.8.1 Scientific Talks (Invited)

1. M. Brokate, *Newton derivatives of convex functionals*, Conference on Multiple Scale Systems, Silesian University, Opava, Czech Republic, January 16.
2. ———, *Rate independent evolutions*, Charles University, Department of Numerical Mathematics, Prague, Czech Republic, March 10.
3. ———, *Rate independent evolutions: Derivatives and control*, Universität Kiel, Department of Mathematics, April 29.
4. ———, *Derivatives of hysteresis operators*, MURPHYS 2022 – Interdisciplinary Conference on Multiple Scale Systems, Systems with Hysteresis, May 29 – June 3, Ostravice, Czech Republic, May 30.
5. ———, *Strong stationarity for an optimal control problem for a rate independent evolution*, Conference on Differential Equations and Their Applications (EQUADIFF 15), Minisymposium NAA-03: “Evolution Differential Equations with Application to Physics and Biology”, July 11–15, Masaryk University, Brno, Czech Republic, July 12.
6. M. Kniely, *Global renormalized solutions and equilibration of reaction-diffusion systems with nonlinear diffusion (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium “Bridging Gradient Flows, Hypocoercivity and Reaction-Diffusion Systems”, March 14–18, March 14.
7. ———, *Global solutions to a class of energy-reaction-diffusion systems*, Conference on Differential Equations and Their Applications (EQUADIFF 15), Minisymposium NAA-03 “Evolution Differential Equations with Application to Physics and Biology”, July 11–15, Masaryk University, Brno, Czech Republic, July 12.
8. J. Sprekels, *Deep quench approach and sparsity in the optimal control of a phase field model for tumor growth*, PHAse field MEthods in applied sciences (PHAME 2022), May 23–27, Istituto Nazionale di Alta Matematica, Rome, Italy, May 27.
9. A. Alphonse, *Directional differentiability and optimal control for quasi-variational inequalities (online talk)*, “Partial Differential Equations and their Applications” Seminar, University of Warwick, Mathematics Institute, UK, January 25.
10. ———, *Risk-averse optimal control of elliptic random variational inequalities*, SPP 1962 Annual Meeting 2022, October 24–26, Novotel Berlin Mitte, October 25.
11. Ch. Bayer, *Optimal stopping, machine learning, and signatures*, Seminar Stochastic Numerics Research Group, King Abdullah University of Science and Technology, Thuval, Saudi Arabia, January 31.
12. ———, *RKHS regularization of singular local stochastic volatility McKean–Vlasov models (online talk)*, Mini-Workshop “Regularization by Noise: Theoretical Foundations, Numerical Methods and Applications driven by Levy Noise”, February 13–20, Mathematisches Forschungsinstitut Oberwolfach, February 14.
13. ———, *Efficient Markovian approximation to rough volatility models*, Rough Volatility Meeting, Imperial College London, UK, March 16.
14. ———, *Simulating rough volatility models (online talk)*, MathFinance 2022 Conference (Online Event), March 21–22, March 22.
15. ———, *Machine learning techniques in computational finance*, 2 talks, Stochastic Numerics and Statistical Learning: Theory and Applications Workshop, May 15–28, King Abdullah University, Computer, Electrical and Mathematical Sciences and Engineering Division, Thuwal, Saudi Arabia, May 22.

16. ———, *Efficient Markovian approximation of rough stochastic volatility models (online talk)*, Aarhus/SMU Volatility Workshop (Online Event), Aarhus University, Department of Economics and Business, Denmark, May 31.

17. ———, *Optimal stopping with signatures*, ISOR Colloquium, June 13–14, Universität Wien, Department of Statistics and Operations Research, Austria, June 13.

18. ———, *Optimal stopping with signatures*, Oberseminar, Martin-Luther-Universität Halle Wittenberg, Institut für Mathematik, June 14.

19. ———, *Optimal stopping with signatures*, Advances in Mathematical Finance and Optimal Transport, June 27–30, Scuola Normale Superiore di Pisa, Centro di Ricerca Matematica Ennio De Giorgi, Italy, June 28.

20. ———, *Optimal stopping with signatures*, Rough Analysis and Data Science Workshop 2022, July 26–27, Imperial College London, Department of Mathematics, UK, July 27.

21. ———, *Stability of deep neural networks via discrete rough paths*, New Interfaces of Stochastic Analysis and Rough Paths, September 4–9, Banff International Research Station, Canada, September 8.

22. ———, *Optimal stopping with signatures*, Séminaire Bachelier, Institut Henri Poincaré, Paris, France, December 16.

23. M. BONGARTI, *Boundary feedback stabilization of a critical nonlinear JMGT equation with Neumann-undissipated part of the boundary*, IFIP TC7 System Modeling and Optimization, July 4–8, University of Technology, Warsaw, Poland, July 4.

24. ———, *Nonlinear gas transport on a network of pipelines*, IFIP TC7 System Modeling and Optimization, July 4–8, University of Technology, Warsaw, Poland, July 4.

25. ———, *Boundary feedback stabilization of a critical nonlinear JMGT equation with Neumann-undissipated part of the boundary*, Waves Conference 2022, July 24–29, ENSTA Institut Polytechnique de Paris, France, July 25.

26. ———, *Boundary stabilization of nonlinear dynamics of acoustics waves under the JMGT equation (online talk)*, Early Career Math Colloquium, University of Arizona, Tucson, USA, October 12.

27. ———, *Boundary stabilization of nonlinear dynamics of acoustic waves under the JMGT equation*, Oberseminar Partielle Differentialgleichungen, Universität Konstanz, November 17.

28. S. BRENEIS, *Markovian approximations for rough volatility models*, Seminar Stochastic Numerics Research Group, King Abdullah University of Science and Technology, Thuval, Saudi Arabia, January 26.

29. ———, *An error representation formula for the log-ode method*, 15th Berlin-Oxford Young Researcher's Meeting on Applied Stochastic Analysis, May 12–14, WIAS & TU Berlin, May 14.

30. ———, *Markovian approximations of rough volatility models*, Mathematics of Random Systems Summer School 2022, September 25–30, University of Oxford, St Hugh's College, UK, September 29.

31. ———, *An error representation formula for the log-ode method*, 16th Oxford-Berlin Young Researcher's Meeting on Applied Stochastic Analysis, December 8–10, University of Oxford, UK, December 9.

32. O. BUTKOVSKY, *Regularisation by noise for SDEs: State of the art & open problems*, Mini-Workshop "Regularization by Noise: Theoretical Foundations, Numerical Methods and Applications driven by Levy Noise", February 13–20, Mathematisches Forschungsinstitut Oberwolfach, February 16.

33. ———, *Strong rate of convergence of the Euler scheme for SDEs with irregular drift driven by Levy noise*, 15th Berlin-Oxford Young Researcher's Meeting on Applied Stochastic Analysis, May 12–14, WIAS & TU Berlin, May 12.

34. ———, *Weak and mild solutions of SPDEs with distributional drift (online talk)*, 42nd Conference on Stochastic Processes and their Applications (Online Event), June 27 – July 1, Wuhan University, School of Mathematics and Statistics, Chinese Society of Probability and Statistics, China, June 28.
35. ———, *Regularization by noise for L_p drifts: The case for Burkholder–Rosenthal stochastic sewing*, Stochastic & Rough Analysis, August 22–26, Harnack House, August 23.
36. ———, *Regularization by noise for SDEs and SPDEs beyond the Brownian case*, Open Japanese-German Conference on Stochastic Analysis and Applications, September 19–23, Westfälische Wilhelms-Universität Münster, September 19.
37. ———, *Strong rate of convergence of the Euler scheme for SDEs with irregular drift driven by Levy noise*, Numerical Analysis and Applications of SDEA, September 25 – October 1, Banach Center, Bedlewo, Poland, September 28.
38. ———, *Regularization by noise for SDEs and SPDEs beyond the Brownian case*, Oberseminar Analysis - Probability, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Fakultät für Mathematik und Informatik, Lepzig, November 1.
39. ———, *Regularization by noise for SDEs and SPDEs beyond the Brownian case (online talk)*, Webinar on Stochastic Analysis 2022 (Online Event), Beijing Institute of Technology, School of Mathematics and Statistics, China, November 8.
40. J.C. De los Reyes, *Bilevel learning for inverse problems*, Seminar SFB 1060, Universität Bonn, Fachbereich Mathematik, April 14.
41. P.-É. Druet, *Global existence and weak-strong uniqueness for isothermal ideal multicomponent flows*, Against the Flow, October 18–22, Polish Academy of Sciences, Będlewo, Poland, October 19.
42. P. Dvurechensky, *Multimarginal optimal transport by accelerated alternating minimization (online talk)*, SIAM Conference on Imaging Science (IS22) (Online Event), Minisymposium MS94: “Multi-Marginal Optimal Transport”, March 21–25, March 24.
43. ———, *Accelerated alternating minimization methods*, 20th French German Portuguese Conference in Optimization, May 3–6, University of Porto, School of Economics and Management, Portugal, May 5.
44. ———, *Generalized self-concordant analysis of Frank–Wolfe algorithms*, 19th Workshop on Advances in Continuous Optimization (EUROPT 2022), July 29–30, NOVA University Lisbon, School of Science and Technology, Portugal, July 30.
45. M. Eigel, *An empirical adaptive Galerkin method for parametric PDEs*, Workshop “Adaptivity, High Dimensionality and Randomness” (Hybrid Event), April 4–8, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, April 6.
46. ———, *Empirical adaptive Galerkin FEM for parametric PDEs*, 10th International Conference on Curves and Surfaces, Minisymposium 13 “High dimensional Approximation and PDEs”, June 20–24, Arcachon, France, June 23.
47. ———, *Adaptive Galerkin FEM for non-affine linear parametric PDEs*, Computational Methods in Applied Mathematics (CMAM 2022), MS06: “Computational Stochastic PDEs”, August 29 – September 2, Technische Universität Wien, Austria, August 29.
48. Th. Eiter, *Energy-variational solutions for a viscoelastoplastic fluid model (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium “Generalized Solvability Concepts for Evolutionary PDEs and their Properties”, March 14–18, March 16.
49. ———, *Junior Richard von Mises Lecture: On time-periodic viscous flow around a moving body*, Richard von Mises Lecture 2022, Humboldt-Universität zu Berlin, June 17.

50. ———, *Resolvent estimates for the flow past a rotating body and existence of time-periodic solutions*, CEMAT Seminar, University of Lisbon, Center for Computational and Stochastic Mathematics, Portugal, July 27.

51. ———, *On uniformity of the resolvent estimates associated with time-periodic flow past a rotating body*, Germany-Japan Workshop on Free and Singular Boundaries in Fluid Dynamics and Related Topics (Hybrid Event), August 10–12, Heinrich-Heine-Universität Düsseldorf, August 10.

52. ———, *Time-periodic maximal Lp regularity by R-boundedness in the context of incompressible viscous flows*, Research Seminar Function Spaces, Friedrich-Schiller-Universität Jena, November 4.

53. ———, *Existence of time-periodic flows in domains with oscillating boundaries*, International Workshop on Multiphase Flows: Analysis, Modelling and Numerics, December 5–9, Waseda University, Tokyo, Japan, December 6.

54. S. ESSADI, *Constrained deterministic non-smooth mean field games*, 92th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2022), DFG Priority Program 1962 “Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization”, August 15–19, Rheinisch-Westfälische Technische Hochschule Aachen, August 16.

55. ———, *Constrained mean field games: Analysis and algorithms*, SPP 1962 Annual Meeting 2022, October 24–26, Novotel Berlin Mitte, October 25.

56. P. FARRELL, *Numerical methods for innovative semiconductors devices*, Leibniz-Institut für Innovative Mikroelektronik (IHP), July 26.

57. P. FRIZ, *Local vol under rough vol*, Rough Volatility Workshop, March 15–16, Imperial College London, UK, March 16.

58. ———, *A theory of rough differential equations (online talk)*, Webinar on Stochastic Analysis (Online Event), Beijing Institute of Technology, School of Mathematics and Statistics, China, March 31.

59. ———, *Rough stochastic analysis*, Stochastic Analysis and Stochastic Partial Differential Equations: A Celebration of Marta Sanz-Solé’s Mathematical Legacy, May 30 – June 3, Centre de Recerca Matemàtica (CRM), Barcelona, Spain, June 2.

60. ———, *Rough stochastic analysis*, Conference in Honor of S. R. S. Varadhan’s 80th Birthday, June 13–17, Jeju Shinhwa World Marriott Resort, Seoul, Korea (Republic of), June 13.

61. ———, *Rough SDEs, rough semimartingales*, Advances in Mathematical Finance and Optimal Transport, June 27 – July 1, Scuola Normale Superiore di Pisa, Centro di Ricerca Matematica Ennio De Giorgi, Italy, June 28.

62. ———, *Weak rates for rough vol (online talk)*, New Interfaces of Stochastic Analysis and Rough Paths, September 4–9, Banff International Research Station, Canada, September 6.

63. ———, *Itô and Lyons in tandem*, Open Japanese-German Conference on Stochastic Analysis and Applications, September 19–23, Westfälische Wilhelms-Universität Münster, Institut für Mathematische Stochastik, September 20.

64. C. GEIERSBACH, *Optimality conditions and regularization for stochastic optimization with almost sure state constraints (online talk)*, 2022 SIAM Conference on Imaging Science (IS22) (Online Event), Minisymposium “Stochastic Iterative Methods for Inverse Problems”, March 21–25, March 25.

65. ———, *Optimality conditions and regularization for OUU with almost sure state constraints (online talk)*, SIAM Conference on Uncertainty Quantification (Hybrid Event), Minisymposium 24 “PDE-Constrained Optimization Under Uncertainty”, April 12–15, Atlanta, Georgia, USA, April 12.

66. ———, *Shape optimization under uncertainty: Challenges and algorithms*, Helmut Schmidt Universität Hamburg, Mathematik im Bauingenieurwesen, April 26.

67. ———, *Optimality conditions and regularization for stochastic optimization with almost sure state constraints*, International Conference on Continuous Optimization – ICCOPT/MOPTA 2022, Cluster "PDE-Constrained Optimization", July 23–28, Lehigh University, Bethlehem, Pennsylvania, USA, July 26.

68. ———, *Optimization with almost sure state constraints*, 92th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2022), Session 19 "Optimization of Differential Equations", August 15–19, Rheinisch-Westfälische Technische Hochschule Aachen, August 16.

69. ———, *State constraints in stochastic optimization*, PGMO DAYS 2022, Session 15F: "New Developments in Optimal Control Theory, Part II", November 28–30, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF Lab Paris-Saclay, Palaiseau, France, November 30.

70. ———, *Game-theoretical modeling for green hydrogen markets*, Future WiNS: New Energies for a Sustainable World, December 7–9, Humboldt-Universität zu Berlin, December 9.

71. M. HEIDA, *Homogenization on locally Lipschitz random domains (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium "Disordered Media and Homogenization", March 14–18, March 15.

72. ———, *Measure theoretic aspects of stochastic homogenization*, Seminar Interacting Random Systems (Hybrid Event), WIAS Berlin, April 20.

73. ———, *Homogenization on randomly perforated domains*, Block Course "Multiscale Problems and Homogenization" at Freie Universität Berlin from Nov. 10 to Dec. 15, 2022, Berlin Mathematical School & Berlin Mathematics Research Center MATH+, November 17.

74. H. HEITSCH, *An algorithmic approach for solving optimization problems with probabilistic/robust (probust) constraints (online talk)*, TRR154 Summer School on Modelling, Simulation and Optimization for Energy Networks (Online Event), June 8–9, June 8.

75. R. HENRION, *Probabilistic constraints via spherical-radial decomposition. Part I (online talk)*, Seminar on Variational Analysis and Optimization, Western Michigan University, Kalamazoo, USA, February 4.

76. ———, *Probabilistic constraints via spherical-radial decomposition. Part II (online talk)*, Western Michigan University, Kalamazoo, USA, February 11.

77. ———, *Controlled polyhedral sweeping processes: Existence, stability, and optimality conditions (online talk)*, Seminar on Variational Analysis and Optimization, University of Michigan, Department of Mathematics, Ann Arbor, USA, February 17.

78. ———, *A turnpike property for a discrete-time linear optimal control problem with probabilistic constraints*, Workshop on Optimal Control Theory, June 22–24, Institut National des Sciences Appliquées Rouen Normandie, France, June 24.

79. ———, *A turnpike property for an optimal control problem with chance constraints*, PGMO DAYS 2022, Session 15F: "New Developments in Optimal Control Theory, Part II", November 28–30, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF Lab Paris-Saclay, Palaiseau, France, November 30.

80. M. HINTERMÜLLER, *Optimization with learning-informed differential equations*, Robustness and Resilience in Stochastic Optimization and Statistical Learning: Mathematical Foundations, May 20–24, Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy, May 24.

81. ———, *Optimization subject to learning informed PDEs*, International Conference on Continuous Optimization – ICCOPT/MOPTA 2022, Cluster "PDE-Constrained Optimization", July 23–28, Lehigh University, Bethlehem, Pennsylvania, USA, July 27.

82. ———, *Optimization with learning-informed differential equation constraints (online talk)*, Workshop on Control Problems (Online Event), October 17–20, Technische Universität Dortmund, October 17.

83. ———, *PDE-constrained optimization with learning-informed structures (online talk)*, Optimization in Oslo (OiO) Seminar, Simula Research Laboratory, Norway, December 7.

84. ———, *A descent algorithm for the optimal control of ReLU neural network informed PDEs based on approximate directional derivatives (online talk)*, Workshop 2: Structured Optimization Models in High-Dimensional Data Analysis, December 12–16, National University of Singapore, Institute for Mathematical Sciences, December 15.

85. D. Hömberg, *On two-scale topology optimization (online talk)*, Workshop "Practical Inverse Problems and Their Prospects" (Online Event), March 2–4, Kyushu University, Japan, March 4.

86. ———, *A phasefield approach to two-scale topology optimization*, DNA Seminar (Hybrid Event), Norwegian University of Science and Technology, Department of Mathematical Sciences, Norway, March 14.

87. K. Hopf, *Relative entropies and stability in strongly coupled parabolic systems (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium "Variational Evolution: Analysis and Multi-Scale Aspects", March 14–18, March 16.

88. ———, *The Cauchy problem for a cross-diffusion system with incomplete diffusion*, Annual Workshop of the GAMM Activity Group "Analysis of PDEs" 2022, October 5–7, Institute of Science and Technology Austria (ISTA), Klosterneuburg, October 5.

89. T. Iyer, *Preferential attachment trees with neighbourhood influence*, Probability Seminar, Universität zu Köln, Department Mathematik/Informatik, April 29.

90. ———, *The influence of competition on genealogical trees associated with explosive age-dependent branching processes*, Oberseminar Stochastik, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, November 16.

91. B. Jahnel, *Phase transitions and large deviations for the Boolean model of continuum percolation for Cox point processes (online talk)*, Probability Seminar University Padua, Università di Padova, Dipartimento di Matematica, Italy, March 25.

92. ———, *First-passage percolation and chase-escape dynamics on random geometric graphs*, Spring School on Random Geometric Graphs, March 28 – April 1, Technische Universität Darmstadt, Fachbereich Mathematik, March 30.

93. ———, *Stochastic geometry for telecommunications*, Leibniz MMS Days 2022, April 25–27, Potsdam-Institut für Klimafolgenforschung (PIK), April 26.

94. ———, *Malware propagation in mobile device-to-device networks (online talk)*, Joint H2020 AI@EDGE and INSPIRE-5G Project Workshop – Platforms and Mathematical Optimization for Secure and Resilient Future Networks (Online Event), Paris, France, November 8–9, November 8.

95. W. König, *The free energy of a box-version of the interacting Bose gas*, SPP 2265 Workshop on Random Spatial Networks, March 14–17, Universität zu Köln, Mathematisches Institut, March 17.

96. ———, *A large-deviations principle for all the components in a sparse inhomogeneous Erdős–Rényi graph*, Workshop: Interacting Particle Systems and Hydrodynamic Limits, March 21–25, Université Montreal, Centre de Recherches de Mathématiques, Canada, March 22.

97. ———, *The free energy of a box version of the interacting Bose gas*, Quantum Many Body System and Interacting Particles: In Honor of Herbert Spohn, June 20–24, Westfälische Wilhelms-Universität Münster, June 24.

98. ———, *Many-body Systems and the Interacting Bose Gas (minicourse)*, 2 talks, Random Point Processes in Statistical Physics, June 29 – July 1, Harnack House, Berlin, June 30 – July 1.

99. ———, *Self-repellent Brownian bridges in the interacting Bose gas*, Oberseminar, Universität zu Köln, Mathematisches Institut, December 7.

100. J. Köppl, *Dynamical Gibbs variational principles for irreversible interacting particle systems and applications to attractor properties*, DMV Annual Meeting 2022, Section 12: “Probability, Computational Stochastics, and Financial Mathematics”, September 12–16, Freie Universität Berlin, September 15.

101. ———, *Dynamical Gibbs variational principles for irreversible interacting particle systems and applications to attractor properties*, BMS–BGSMath Junior Meeting 2022, September 5–7, Universitat de Barcelona, Spain, October 6.

102. Th. Koprucki, *MaRDI – The Mathematical Research Data Initiative within the German National Research Data Infrastructure (NFDI)*, 1st MaRDI Workshop on Scientific Computing, October 26–28, Westfälische Wilhelms-Universität Münster, October 26.

103. A. Kroshnin, *Robust k-means clustering in Hilbert and metric spaces*, Rencontres de Statistique Mathématique, December 12–16, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 13.

104. J. Leake, *Lorentzian polynomials on cones and the Heron–Rota–Welsh conjecture*, Workshop “The Laguerre-Pólya Class and Combinatorics”, March 13–19, Mathematisches Forschungsinstitut Oberwolfach, March 18.

105. M. Liero, *From diffusion to reaction-diffusion in thin structures via EDP-convergence (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium “Bridging Gradient Flows, Hypocoercivity and Reaction-Diffusion Systems”, March 14–18, March 14.

106. ———, *The impact of modeling, analysis, and simulation on organic semiconductor development (online talk)*, ERCOM Meeting 2022 (Hybrid Event), March 25–26, European Research Centers on Mathematics, Bilbao, Spain, March 26.

107. ———, *Analysis of an electrothermal drift-diffusion model for organic semiconductor devices*, PHAse field MEthods in applied sciences (PHAME 2022), May 23–27, Istituto Nazionale di Alta Matematica, Rome, Italy, May 24.

108. ———, *EDP-convergence for evolutionary systems with gradient flow structure*, 92th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2022), Minisymposium 4 “Evolution Equations with Gradient Flow Structure”, August 15–19, Rheinisch-Westfälische Technische Hochschule Aachen, August 16.

109. E. Magnanini, *Limit theorems for the edge density in exponential random graphs*, Third Italian Meeting on Probability and Mathematical Statistics, June 13–16, University of Bologna, Italy, June 15.

110. Ch. Merdon, *Recent advances for pressure-robust discretisations of the incompressible Navier–Stokes equations (online talk)*, SIAM Annual Meeting 2022, MS87: “Recent Developments in Mathematical Analysis and Numerics for Incompressible Flow and Related Problems (Hybrid Event)”, July 11–15, David L. Lawrence Convention Center, Pennsylvania, USA, July 14.

111. ———, *Recent advances in pressure-robust finite element methods (online talk)*, 15th World Congress on Computational Mechanics & 8th Asian Pacific Congress on Computational Mechanics (Online Event), July 31 – August 5, Japan Convention Services, Congress Secretariat, Yokohama, Japan, August 2.

112. A. Mielke, *On the longtime behavior of solutions to a coupled degenerate parabolic system motivated by thermodynamics (online talk)*, Nonlinear Waves and Coherent Structures Webinar Series (Online Event), University of Massachusetts, Amherst, USA, January 25.

113. ———, *On the existence and longtime behavior of solutions to a degenerate parabolic system (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium MS43: “Nonlinear Parabolic Equations and Systems”, March 14–18, March 16.

114. ———, *Gamma convergence for evolutionary problems: Using EDP convergence for deriving nontrivial kinetic relations*, Calculus of Variations. Back to Carthage, May 16–20, Carthage, Tunisia, May 18.

115. ———, *Existence and longtime behavior of solutions to a degenerate parabolic system*, Journées Équations aux Dérivées Partielles 2022, May 30 – June 3, Centre National de la Recherche Scientifique, Obernai, France, May 31.

116. ———, *Gradient flows in the Hellinger–Kantorovich space*, 92th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2022), Minisymposium 4 "Evolution Equations with Gradient Flow Structure", August 15–19, Rheinisch-Westfälische Technische Hochschule Aachen, August 16.

117. ———, *Convergence of a split-step scheme for gradient flows with a sum of two dual dissipation potentials*, Nonlinear Evolutionary Equations and Applications 2022, September 6–9, Technische Universität Chemnitz, September 8.

118. ———, *Convergence to thermodynamic equilibrium in a degenerate parabolic system*, DMV Annual Meeting 2022, Section 09 "Applied Analysis and Partial Differential Equations", September 12–16, Freie Universität Berlin, September 13.

119. ———, *Gradient flows: Existence and Gamma-convergence via the energy-dissipation principle*, 3 talks, Horizons in Non-linear PDEs, September 26–30, Universität Ulm, September 26–27.

120. ———, *On time-splitting methods for gradient flows with two dissipation mechanisms*, Annual Workshop of the GAMM Activity Group "Analysis of PDEs" 2022, October 5–7, Institute of Science and Technology Austria (ISTA), Klosterneuburg, October 7.

121. K. PAPAFITSOROS, *Automatic distributed parameter selection of regularization functionals via bilevel optimization (online talk)*, SIAM Conference on Imaging Science (IS22) (Online Event), Minisymposium "Statistics and Structure for Parameter and Image Restoration", March 21–25, March 22.

122. ———, *Total variation methods in image reconstruction*, Institute Colloquium, Foundation for Research and Technology Hellas (IACM-FORTH), Institute of Applied and Computational Mathematics, Heraklion, Greece, May 3.

123. ———, *Optimization with learning-informed nonsmooth differential equation constraints*, Second Congress of Greek Mathematicians SCGM-2022, Session Numerical Analysis & Scientific Computing, July 4–8, National Technical University of Athens, July 6.

124. P. PELECH, *Balanced-viscosity solutions for a Penrose–Fife model with rate-independent friction (hybrid talk)*, Oberseminar "Mathematik in den Naturwissenschaften", Julius-Maximilians-Universität Würzburg, December 8.

125. D. PESCHKA, *Discretization of compressible Stokes flow using Hamiltonian and Onsager structures*, Workshop on Numerical Methods and Analysis in CFD, July 5–8, WIAS Berlin, July 5.

126. L. PLATO, *Biological pest control – Analysis and numerics for a spatio-temporal predator-prey system (online talk)*, Technische Universität Berlin, Institut für Mathematik, January 10.

127. ———, *Generalized solutions in the context of a nonlocal predator-prey model (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium "Generalized Solvability Concepts for Evolutionary PDEs and their Properties", March 14–18, March 16.

128. A. QUITMANN, *Macroscopic loops in the Spin O(N) and related models (online talk)*, Percolation Today (Online Event), Eidgenössische Technische Hochschule Zürich, Switzerland, February 15.

129. ———, *Macroscopic loops in a random walk loop soup*, Spring School on Random Geometric Graphs, March 28 – April 1, Technische Universität Darmstadt, Fachbereich Mathematik, March 31.

130. ———, *Macroscopic loops in an interacting random walk loop soup*, Focused Research: Graphical Representations of Spin Systems, September 5–7, University of Bristol, Heilbronn Institute for Mathematical Research, Bristol, UK, September 6.

131. A. Quitmann, *Macroscopic loops in interacting random walk loop soups*, Oberseminar AG Stochastik, Technische Universität Darmstadt, Fachbereich Mathematik, November 3.

132. ———, *Macroscopic loops in interacting random walk loop soups*, Oberseminar Wahrscheinlichkeitstheorie, Ludwig-Maximilians-Universität, Mathematisches Institut, Munich, November 14.

133. M. Radziunas, *Modeling and simulation of semiconductor lasers for high emission power applications*, 25th International Conference Mathematical Modelling and Analysis, May 30 – June 2, Vilnius Gediminas Technical University, Druskininkai, Lithuania, June 1.

134. ———, *Steady states in dynamical semiconductor laser models and their analysis (online talk)*, 22nd International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) (Online Event), September 12–16, Politecnico di Torino, Italy, September 12.

135. J. Rehberg, *Explicit Lp-estimates for second-order divergence operators*, Oberseminar Analysis und Angewandte Mathematik, Universität Kassel, June 9.

136. ———, *On non-autonomous and quasilinear parabolic equations*, Oberseminar AG Analysis, Technische Universität Darmstadt, December 8.

137. M. Renger, *Variational structures beyond gradient flows — Part II (online talk)*, Seminar on Variational Evolutionary Problems and Related Problems (Online Event), Technische Universität Dresden, Fakulät für Mathematik, January 19.

138. W. Salkeld, *Random controlled rough paths (online talk)*, Thursdays Seminar (Online Event), Technische Universität Berlin, Institut für Mathematik, March 10.

139. ———, *Random controlled rough paths*, 15th Berlin-Oxford Young Researcher's Meeting on Applied Stochastic Analysis, May 12–14, WIAS & TU Berlin, May 12.

140. ———, *Lions calculus and rough mean-field equation*, 2 talks, Journées TRAG 2022, May 30 – June 1, Université Paris Nanterre, GdR TRAG (TRAjectoires ruGueuses), May 30–31.

141. L. Schmeller, *Gradient flows for coupling order parameters and mechanics*, Universitá di Brescia, Mathematical Analysis, Italy, June 14.

142. C. Sirotenko, *Dictionary learning for an inverse problem in quantitative MRI (online talk)*, SIAM Conference on Imaging Science (IS22) (Online Event), Minisymposium "Recent Advances of Inverse Problems in Imaging", March 21–25, March 25.

143. ———, *Dictionary learning for an in inverse problem in quantitative MRI*, 92th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2022), Session 21 "Mathematical Signal and Image Processing", August 15–19, Rheinisch-Westfälische Technische Hochschule Aachen, August 16.

144. V. Spokoiny, *Laplace approximation in high dimension*, Workshop "Re-thinking High-dimensional Mathematical Statistics", May 16–20, Mathematisches Forschungsinstitut Oberwolfach, May 17.

145. ———, *Bayesian optimization by Laplace iterations*, Workshop on Statistical Inference and Convex Optimization, June 13–15, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, France, June 13.

146. ———, *Bayesian inference for nonlinear inverse problems*, SFB 1294 Annual Meeting 2022, September 13–14, Universität Potsdam, Institut für Mathematik, September 13.

147. A. Stephan, *EDP-convergence for a linear reaction-diffusion systems with fast reversible reaction (online talk)*, SIAM Conference on Analysis of Partial Differential Equations (PD22) (Online Event), Minisymposium MS11: "Bridging Gradient Flows, Hypocoercivity and Reaction-Diffusion Systems", March 14–18, March 14.

148. A. Stephan, *EDP-convergence for gradient systems and applications to fast-slow chemical reaction systems*, Block Course "Multiscale Problems and Homogenization" at Freie Universität Berlin from Nov. 10 to Dec. 15, 2022, Berlin Mathematical School & Berlin Mathematics Research Center MATH+, November 24.

149. K. Tabelow, *Neural MRI*, Tandem tutorial “Mathematics of Imaging’ ’, Berlin Mathematics Research Center MATH+, February 18.

150. N. Tapia, *The moving frame method for iterated-integrals signatures: Orthogonal invariants (online talk)*, Arbeitsgruppenseminar Analysis (Online Event), Universität Potsdam, Institut für Mathematik, January 28.

151. ———, *Transport and continuity equations with (very) rough noise*, Mini-Workshop “Regularization by Noise: Theoretical Foundations, Numerical Methods and Applications driven by Levy Noise”, February 13–19, Mathematisches Forschungsinstitut Oberwolfach, February 18.

152. ———, *Stability of deep neural networks via discrete rough paths*, 15th Berlin-Oxford Young Researcher’s Meeting on Applied Stochastic Analysis, May 12–14, WIAS & TU Berlin, May 13.

153. ———, *Signature methods in numerical analysis*, International Conference on Scientific Computation and Differential Equation (SciCADE 2022), July 25–29, University of Iceland, Faculty of Physical Sciences, Reykjavík, Iceland, July 25.

154. ———, *Stability of deep neural networks via discrete rough paths (online talk)*, Rough Analysis and Data Science Workshop 2022, July 26–27, Imperial College London, Department of Mathematics, UK, July 27.

155. ———, *Generalized iterated-sums signatures*, New Interfaces of Stochastic Analysis and Rough Paths, September 4–9, Banff International Research Station, Canada, September 9.

156. M. Theiss, *Constrained MFG: Analysis and algorithms*, SPP 1962 Annual Meeting 2022, October 24–26, Novotel Berlin Mitte, October 25.

157. M. Thomas, *First-order formulation for dynamic phase-field fracture in visco-elastic materials*, Beyond Elasticity: Advances and Research Challenges, May 16–20, Centre International de Rencontres Mathématiques, Marseille, France, May 16.

158. ———, *First-order formulation for dynamic phase-field fracture in visco-elastic materials*, PHAse field MEthods in applied sciences (PHAME 2022), May 23–27, Istituto Nazionale di Alta Matematica, Rome, Italy, May 25.

159. W. van Zuijlen, *Anderson Hamiltonians with singular potentials*, 15th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis, May 12–14, WIAS Berlin, May 13.

160. W. van Zuijlen, *Weakly self-avoiding walk in a random potential*, Forschungsseminar Wahrscheinlichkeitstheorie, Universität Potsdam, Institut für Mathematik, October 24.

161. ———, *Weakly self avoiding walk in a random potential*, Seminar, UFR de Mathématiques, Université Paris Cité, France, December 14.

162. Y. Vargas, *Cumulant-to-moment relations from Hopf algebras*, 15th Berlin-Oxford Young Researcher’s Meeting on Applied Stochastic Analysis, May 12–14, WIAS & TU Berlin, May 12.

163. ———, *Combinational moment-to-cumulant formulas in free probability*, Technische Universität Graz, Institut für Diskrete Mathematik, Austria, June 2.

164. ———, *Primitive basis for the Hopf algebra of permutations*, Séminaire de Combinatoire, Université Gustave Eiffel, Laboratoire d’Informatique Gaspard Monge, Marne-la-Vallée, France, July 1.

165. M. Wolfrum, *Stability properties of temporal dissipative solitons in DDEs (online talk)*, Delay Days Utrecht 2022 (Hybrid Event), Hasselt University, Utrecht, Netherlands, May 12.

166. ———, *Dynamics of excitable units with noise and coupling*, Nonlinear Science: Achievements and Perspectives, September 26–28, Universität Potsdam, September 28.

167. A. Zass, *Gibbs point process on path space: Existence, cluster, cluster expansion and uniqueness*, Oberseminar zur Stochastik, Otto-von-Guericke-Universität Magdeburg, Fakultät für Mathematik, January 20.

168. ———, *Marked Gibbs point processes: A path space example*, Workshop “New Trends in Point Process Theory”, February 28 – March 2, Karlsruher Institut für Technologie (KIT), Fakultät für Mathematik, February 28.

169. ———, *Existence of infinite-volume marked Gibbs point processes: A path space example*, Third Italian Meeting on Probability and Mathematical Statistics, June 13–16, University of Bologna, Italy, June 15.

170. ———, *Interacting diffusions as marked Gibbs point processes*, Seminar of Stochastic Geometry, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, October 11.

171. J.-J. Zhu, *Kernel methods for distributionally robust machine learning and optimization*, Vrije Universiteit Amsterdam, Department of Operations Analytics, Netherlands, July 28.

172. ———, *Distributionally robust learning and optimization in MMD geometry*, KU Leuven, STADIUS Center for Dynamical Systems, Signal Processing, and Data, Belgium, September 9.

173. H. Kremer, J.-J. Zhu, K. Muandet, B. Schölkopf, *Functional generalized empirical likelihood estimation for conditional moment restrictions (spotlight, online talk)*, ICML 2022: 39th International Conference on Machine Learning (Online Event), July 18–23, Baltimore, USA, July 19.

174. J.-J. Zhu, F. Nüske, *Data-Driven Modeling and Optimization of Dynamical Systems under Uncertainty (Ph.D. 16-hour minicourse)*, 8 talks, IRTG 2544 Stochastic Analysis in Interaction, Technische Universität Berlin, July 11–14.

A.8.2 Talks for a More General Public

1. B. Jahnel, *Die Poesie der Logik*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2022, WIAS at Leibniz Association Headquarters, July 2.
2. ———, *Zufällige Geometrie und das Internet der Ding*, Studium Generale, Technische Universität Braunschweig, Institut für Mathematische Stochastik, October 25.
3. J. Kern, *Betrunkene in der Mathematik*, Kongresssimulation MATh.en.JEANS, French Embassy Berlin, October 7.
4. ———, *Darwin und die Mathematik*, Schülerworkshop, WIAS Berlin, November 30.
5. W. König, *Das Bosegas im Lichte der Wahrscheinlichkeitstheorie*, Online Event via Webex, Berliner Mathematische Gesellschaft, February 10.
6. D.R.M. Renger, *Funktionen von Funktionen*, 25. Berliner Tag der Mathematik (25th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
7. H. Stephan, *Talk for students: Was sind Zahlen? Paradoxa mit reellen Zahlen*, 25. Berliner Tag der Mathematik (25th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
8. ———, *Talk for teachers: Was sind Zahlen? Intuition vs. Axiomatik in der Mathematik*, 25. Berliner Tag der Mathematik (25th Berlin Day of Mathematics), Freie Universität Berlin, Institut für Mathematik, April 30.
9. ———, *Mathematik in der Theorie und im Leben*, 2 talks, Schülerworkshop, WIAS Berlin, November 30.

A.8.3 Posters

1. A. Caiazzo, *Displacement & pressure reconstruction from MRE images in an in silico brain model*, ISMRM Workshop on Magnetic Resonance Elastography, Charité, Berlin, August 25–26.
2. P. Farrell, *Data-driven solutions of ill-posed inverse problems arising from doping reconstruction in semiconductors*, AI4Science 2022 : AI for Science, NASSMA Workshop, Rabat, Morocco, December 12–16.

3. D. Fritsch, *Identifying and efficiently computing band-edge energies for charge transport simulations in strained materials*, MATH+ Day 2022, Technische Universität Berlin, November 18.
4. A. Gerdes, *Synchronization patterns in globally coupled Stuart–Landau oscillators*, French-German WE-Heraeus-Seminar : Outstanding Challenges in Nonlinear Dynamics, Les Houches, France, March 20–25.
5. ———, *Synchronization patterns in globally coupled Stuart–Landau oscillators*, Leibniz MMS Days 2022, Potsdam, April 25–27.
6. ———, *Synchronization patterns in globally coupled Stuart–Landau oscillators*, Dynamics Days Europe 2022, Aberdeen, UK, August 22–26.
7. Y. Hadjimichael, O. Marquardt, Ch. Merdon, P. Farrell, *Band structures in highly strained 3D nanowires*, 22th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) (Online Event), Italy, September 12–16.
8. Ch. Keller, J. Fuhrmann, M. Landstorfer, B. Wagner, *Development of an ion-channel model-framework for in-vitro assisted interpretation of current voltage relations*, MATH+-Day 2022, Technische Universität Berlin, November 18.
9. M. Landstorfer, A. Selahi, M. Heida, M. Eigel, *Recovery of battery ageing dynamics with multiple timescales*, MATH+-Day 2022, Technische Universität Berlin, November 18.
10. A. Maltsi, *Symmetries in TEM images of strained crystals*, “European Women in Mathematics” General Meeting 2022, Espoo, Finland, August 22–26.
11. L. Mertensкötter, M. Kantner, U. Bandelow, H. Wenzel, *Non-Markovian noise in semiconductor lasers*, MATH+ Day 2022, Technische Universität Berlin, November 18.
12. W. Salkeld, *Lions calculus and regularity structures*, Probability and Mathematical Physics 2022, Helsinki, Finland, June 28 – July 4.
13. St. Schindler, *Convergence to self-similar profiles for a coupled reaction-diffusion system on the real line*, CRC 910: Workshop on Control of Self-Organizing Nonlinear Systems, Wittenberg, September 26–28.
14. L. Schmeller, *Multi-phase dynamic systems at finite strain elasticity*, Summer School: Mathematical Models for Bio-Medical Sciences, Lake Como, Italy, June 20–24.
15. F. Severing, *Nonlinear Schrödinger Equation – Flawless description of modulation instability?*, Student Chapter Poster Session (SCPS) 2022 (Online Event), Sussex, UK, February 20.
16. ———, *How numerics add to the instabilities of the generalised nonlinear Schrödinger equation*, Nonlinear Waves and Turbulence in Photonics 2022, Berlin, July 14–15.
17. M. Stöhr, *Bifurcations and instabilities of temporal dissipative solitons in DDE-systems with large delay*, CRC 910: Workshop on Control of Self-Organizing Nonlinear Systems, Wittenberg, September 26–28.
18. ———, *Bifurcations and instabilities of temporal dissipative solitons in DDE-systems with large delay*, International Conference on Control of Self Organizing Nonlinear Systems, Potsdam, November 23–26.
19. W. van Oosterhout, *Analysis of a poro-visco-elastic material model*, Summer School: Mathematical Models for Bio-Medical Sciences, Lake Como, Italy, June 20–24.
20. Y. Vargas, *Algebraic combinatorics of moment-to-cumulant relations*, Summer School in Algebraic Combinatorics, Kraków, Poland, July 11–15.
21. U. Wilbrandt, *ParMooN – Recent developments and application*, Leibniz MMS Days (Hybrid Event), Potsdam, April 25–27.
22. H. Kremer, J.-J. Zhu, K. Muandet, B. Schölkopf, *Functional generalized empirical likelihood estimation for conditional moment restrictions*, ICML 2022: 39th International Conference on Machine Learning (Online Event), Baltimore, USA, July 18–23.

A.9 Visits to other Institutions[6]

1. Ch. Bayer, King Abdullah University of Science and Technology, Stochastic Numerics Research Group, Thuval, Saudi Arabia, January 24 – February 4.
2. ———, Universitiy of Calgary, Department of Mathematics & Statistics, Canada, August 30 – September 3.
3. C. Belponer, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Mathematical Analysis, Modeling, and Applications, Trieste, Italy, October 17–28.
4. ———, Universität Augsburg, Numerische Mathematik, November 7–10.
5. S. Breneis, King Abdullah University of Science and Technology, Stochastic Numerics Research Group, Thuval, Saudi Arabia, January 24 – February 4.
6. ———, May 14–28.
7. O. Butkovsky, University of Edinburgh, CMS Bayes Centre, UK, May 9–29.
8. A. Caiazzo, Universität Augsburg, Numerische Mathematik, November 7–10.
9. J.C. De los Reyes, Technische Universität Dortmund, Fakultät Mathematik, March 7–11.
10. ———, Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI and Universität Bonn, Fachbereich Mathematik, Bonn, April 11–14.
11. P. Dvurechensky, Université Catholique de Louvain (UCL), Center for Operations Research and Econometrics, Belgium, August 1–5.
12. Th. Eiter, University of Lisbon, Center for Computational and Stochastic Mathematics, Portugal, July 24–30.
13. P. Farrell, Universidad de Buenos Aires, Department of Mathematics, Argentina, November 24–27.
14. C. Geiersbach, Université de Pau, Laboratoire de Mathématiques et de leurs Applications, Pau, France, June 5–11.
15. D. Hömberg, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, March 7–25.
16. ———, November 1–11.
17. T. Iyer, Westfälische Wilhelms-Universität Münster, Fachbereich Mathematik und Informatik, November 15 – December 17.
18. V. John, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, March 14–18.
19. W. König, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica “Ulisse Dini”, Firenze, Italy, October 10–21.
20. ———, Universität zu Köln, Mathematisches Institut, December 5–9.
21. J. Köppl, University of New South Wales, School of Mathematics and Statistics, Sydney, Australia, October 10 – November 11.
22. J. Leake, Technische Universität Braunschweig, Carl-Friedrich-Gauß-Fakultät, June 13–17.
23. O. Marquardt, Yerevan State University, Faculty of Radiophysics, Armenia, September 24 – October 22.
24. M. O’Donovan, Tyndall National Institute, Cork, Ireland, December 19–23.
25. A. Quitmann, Universitá di Roma “La Sapienza”, Mathematics Department, Italy, January 3 – March 9.
26. ———, University of Oxford, Department of Statistics, Oxford, UK, May 14 – July 4.

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[6] Only stays of more than three days are listed.

27. A. QUITMANN, Ludwig-Maximilians-Universität, Mathematisches Institut, Munich, November 10–15.
28. J. REHBERG, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fachbereich Mathematik, August 8–11.
29. ———, Technische Universität Darmstadt, Fachbereich Mathematik, December 6–9.
30. L. SCHMELLER, Universitá di Brescia, Mathematical Analysis, Italy, May 28 – June 19.
31. A. STEPHAN, Westfälische Wilhelms-Universität Münster, Institut für Analysis und Numerik, November 14–18.
32. N. TAPIA, University of Trento, Dipartimento di Matematica, Italy, November 30 – December 3.
33. W. VAN ZUIJLEN, Radboud University Nijmegen, Department of Mathematics, Nijmegen, Netherlands, March 16–21.
34. ———, August 3–8.
35. ———, September 13–16.
36. ———, Université Paris Cité, UFR de Mathématiques, France, December 12–16.
37. ———, Radboud University Nijmegen, Department of Mathematics, Nijmegen, Netherlands, December 21, 2022 – January 3, 2023.
38. Y. VARGAS, Technische Universität Graz, Institut für Diskrete Mathematik, Austria, May 30 – June 8.
39. ———, Université Clermont-Auvergne, Laboratoire de Mathématiques Blaise Pascal, Aubière, France, June 19–26.
40. ———, Université Gustave Eiffel, Laboratoire d’Informatique Gaspard Monge, Marne-la-Vallée, France, June 29 – July 3.
41. ———, Universität Greifswald, Institut für Mathematik und Informatik, July 5–8.

A.10 Academic Teaching[7]

Winter Semester 2021/2022

1. U. Bandelow, *Online: Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. Ch. Bayer, *Online: Fortgeschrittene Themen der Finanzmathematik - Machine Learning with Financial Applications* (lecture), Technische Universität Berlin, 2 SWS.
3. A. Caiazzo, *Hybrid: Lineare Algebra für Physiker* (lecture), Freie Universität Berlin, 4 SWS.
4. ———, *Hybrid: Lineare Algebra für Physiker* (practice), Freie Universität Berlin, 4 SWS.
5. M. Eigel, *Hochdimensionale Approximation und statistisches Lernen* (lecture), Technische Universität Berlin, 4 SWS.
6. P. Friz, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
7. J. Fuhrmann, *Online: Wissenschaftliches Rechnen (Scientific Computing)* (lecture), Technische Universität Berlin, 4 SWS.
8. A. Glitzky, A. Mielke, B. Zwicknagl, *Online and Hybrid: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
9. R. Henrion, *Optimization Problems with Probabilistic Constraints* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. ———, *Optimization Problems with Probabilistic Constraints* (practice), Humboldt-Universität zu Berlin, 1 SWS.
11. D. Hömberg, *Online: Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
12. V. John, *Aufbaumodul: Numerik IV* (lecture), Freie Universität Berlin, 2 SWS.
13. ———, *Aufbaumodul: Numerik IV* (practice), Freie Universität Berlin, 2 SWS.
14. V. Spokoiny, *Nonparametric Statistics (M29)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
15. ———, *Nonparametric Statistics (M29)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
16. 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.
17. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
18. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
19. W. van Zuijlen, *Theory of Function Spaces and Applications (Hybrid)* (lecture), Freie Universität Berlin, 2 SWS.
20. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Online: Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

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[7] SWS = semester periods per week

Summer Semester 2022

1. J. Sprekels, *Block Lecture as Professor by contract in Evolution Equations at the Dipartimento di Matematica "Felice Casorati," Università Degli Studi di Pavia, for the 2021/2022 Academic Year: Optimal Control of Parabolic Equations (24 hours between April 20 and May 13)* (lecture), Università degli Studi di Pavia, – SWS.
2. U. Bandelow, *Online: Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
3. U. Bandelow, S. Amiranashvili, *Nichtlineare Dynamik in der Photonik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
4. M. Eigel, *Neural Networks and Tensor Formats for High-Dimensional Approximations* (lecture), Technische Universität Berlin, 2 SWS.
5. P. Friz, *Wahrscheinlichkeitstheorie III* (lecture), Technische Universität Berlin, 4 SWS.
6. ———, *Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
7. A. Glitzky, A. Mielke, B. Zwicknagl, *Online and Hybrid: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
8. M. Hintermüller, *Online: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
9. B. Jahnel, *Probabilistic Methods in Telecommunications* (lecture), Technische Universität Braunschweig, 4 SWS.
10. ———, *Wahrscheinlichkeitstheorie und diskrete Finanzmathematik* (lecture), Technische Universität Braunschweig, 4 SWS.
11. V. John, *Masterseminar Numerical Mathematics* (lecture), Freie Universität Berlin, 2 SWS.
12. ———, *Numerik I* (lecture), Freie Universität Berlin, 4 SWS.
13. W. König, *Probabilistic Methods in Telecommunications* (lecture), Technische Universität Berlin, 2 SWS.
14. ———, *Probabilistic Methods in Telecommunications* (seminar), Technische Universität Berlin, 2 SWS.
15. 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.
16. V. Spokoiny, P. Dvurechensky, J.-J. Zhu, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
17. K. Tabelow, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
18. M. Thomas, *Analysis 1 (Mathematik für Physiker I)* (lecture), Freie Universität Berlin, 4 SWS.
19. ———, *Analysis 1 (Mathematik für Physiker I)* (practice), Freie Universität Berlin, 2 SWS.
20. W. van Zuijlen, *SPDEs: Classical and New* (lecture), Freie Universität Berlin, 2 SWS.
21. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Online: Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/Technische Universität Berlin, 2 SWS.

Winter Semester 2022/2023

1. U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.

2. TH. EITER, M. LIERO, *Mehrdimensionale Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
3. J. FUHRMANN, *Advanced Topics from Scientific Computing* (lecture), Technische Universität Berlin, 2 SWS.
4. A. GLITZKY, A. MIELKE, M. THOMAS, B. ZWICKNAGL, *Online and Hybrid: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
5. M. HINTERMÜLLER, *Online: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
6. K. HOPF, *Nichtlineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
7. ———, *Nichtlineare partielle Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
8. B. JAHNEL, *Introduction to Probability Theory* (lecture), Technische Universität Braunschweig, 4 SWS.
9. ———, *Probabilistic Methods in Telecommunications* (lecture), Technische Universität Braunschweig, 3 SWS.
10. V. JOHN, *Basismodul: Numerik II* (lecture), Freie Universität Berlin, 4 SWS.
11. O. MARQUARDT, *SPHInX-Tutorial 2022 (10 ninety-minute lectures from September 27 to October 20)* (lecture), Yerevan State University, - SWS.
12. CH. MERDON, *Numerik gewöhnlicher Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
13. ———, *Numerik gewöhnlicher Differentialgleichungen* (practice), Humboldt-Universität zu Berlin, 2 SWS.
14. A. MIELKE, *Ausgewählte Themen der angewandten Analysis: Gradientensysteme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
15. R.I.A. PATTERSON, *Mathematik für Geowissenschaftler* (lecture), Freie Universität Berlin, 2 SWS.
16. V. SPOKOINY, *Nonparametric Statistics (M29)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
17. ———, *Nonparametric Statistics (M29)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
18. V. SPOKOINY, M. REISS, S. GREVEN, W. HÄRDLE, A. CARPENTIER, *Online and Hybrid: Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
19. V. SPOKOINY, P. DVURECHENSKY, J.-J. ZHU, *Online and Hybrid: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
20. H. STEPHAN, *Funktionalanalytische Methoden in der klassischen Physik (lineare Theorie)* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
21. K. TABELOW, *Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
22. M. THOMAS, *Analysis I* (lecture), Freie Universität Berlin, 4 SWS.
23. ———, *Variational Methods and Gamma-Convergence* (seminar), Freie Universität Berlin, 2 SWS.
24. ———, *Analysis I* (practice), Freie Universität Berlin, 1 SWS.
25. M. WOLFRUM, B. FIEDLER, I. SCHNEIDER, E. SCHÖLL, *Online: 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, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica “Ulisse Dini”, Firenze, Italy, April 1–15.
2. ———, July 2–7.
3. S. Andres, University of Manchester, Department of Mathematics, UK, December 19–22.
4. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, May 8 – June 24.
5. D. Belomestny, Universität Duisburg-Essen, Fakultät für Mathematik, Essen, January 18–21.
6. L. Berlyand, Pennsylvania State University, Department of Mathematics, University Park, PA, USA, November 7–10.
7. M. Biskup, University of California, Los Angeles, Department of Mathematics, Los Angeles, USA, December 18–22.
8. M. Brokate, Technische Universität München, Zentrum Mathematik, Garching, January 1 – December 31.
9. Y. Chen, National University of Singapore, Department of Statistics & Applied Probability, Singapore, March 14–20.
10. G. Dong, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – September 20.
11. S. Fischer, Ludwig-Maximilians-Universität München, Institut für Statistik, München, October 1, 2022 – September 30, 2023.
12. N. Forien, Sapienza Università di Roma, Dipartimento di Matematica “Guido Castelnuovo”, Italy, October 16–22.
13. K. Gambaryan, Yerevan State University, Faculty of Radiophysics, Armenia, July 15–30.
14. A. Grauer, Universität zu Köln, Mathematisches Institut, Köln, October 11–14.
15. N. Hao, University College London, Department of Mathematics, London, UK, October 12–18.
16. O. Huber, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – June 30.
17. M. Kasprzak, University of Luxembourg, Department of Mathematics, Esch-sur-Alzette, Luxembourg, November 27 – December 2.
18. M. Kniely, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, March 1, 2022 – February 29, 2024.
19. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, June 6–10.
20. ———, September 1–9.
21. R. Kraaij, Delft University of Technology, Faculty of Electrical Engineering, Mathematics & Computer Science, Delft, Netherlands, May 16–20.
22. R. Kravchenko, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, January 1 – June 30.
23. H. Kremer, Max Planck Institute for Intelligent Systems, Empirical Inference Department, Tübingen, December 13–16.
24. Ch. Kwofie, University of Energy and Natural Resources, School of Sciences, Sunyani, Ghana, June 7–17.

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[8] Only stays of more than three days are listed.

25. Z. LAKDAWALA, Lahore University of Management Sciences, Syed Babar Ali School of Science and Engineering, Pakistan, May 18 – June 15.

26. ———, July 7–20.

27. J. LATZ, Heriot-Watt University, School of Mathematical and Computer Sciences, Department of Actuarial Mathematics and Statistics, Edinburgh, UK, November 7–14.

28. L. LÜCHTRATH, Universität zu Köln, Department Mathematik/Informatik, Köln, June 21–24.

29. Y. LUO, Max Planck Institute for Intelligent Systems, Empirical Inference Department, Tübingen, December 4–9.

30. K. MACKENZIE, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, June 6–12.

31. A. MARTINI, University of Oxford, Department of Statistics, Oxford, UK, June 13–16.

32. A. MASSING, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, September 11–15.

33. J. MOATTI, Université de Lille, Laboratoire Paul Painlevé, Villeneuve-d'Ascq, France, May 10 – July 31.

34. J. MURA, Universidad Técnica Federico Santa María, Department of Mechanical Engineering, Santiago, Chile, May 16–27.

35. Y. NEMMOUR, Max Planck Institute for Intelligent Systems, Empirical Inference, Tübingen, December 13–16.

36. H. NI, University College London, Department of Mathematics, UK, October 13–20.

37. L. ODUNLAMI, Humboldt-Universität zu Berlin, Institut für Mathematik, November 1, 2022 – May 31, 2023.

38. P. PÉREZ-AROS, Universidad de O'Higgins, Instituto de Ciencias de la Ingeniería, Rancagua, Chile, June 6–11.

39. ST. PIANI, International School for Advanced Studies, Trieste, Italy, March 23 – April 8.

40. ———, April 25 – May 6.

41. M. REDMANN, Martin Luther University of Halle Wittenberg, Institute of Mathematics, Halle, May 2–6.

42. T. ROUBÍČEK, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, November 19 – December 19.

43. Y. SAMET, Rheinisch-Westfälische Technische Hochschule Aachen, Fachgruppe Mathematik, Aachen, October 24–28.

44. M. SLOWIK, Universität Mannheim, Fakultät für Wirtschaftsinformatik und Wirtschaftsmathematik, December 19–22.

45. M. STAUDIGL, Maastricht University, School of Business and Economics, Netherlands, August 15–18.

46. L. TAGGI, Sapienza Università di Roma, Dipartimento di Matematica, Italy, December 6–12.

47. Q.T.S. VOGEL, New York University Shanghai, Institute of Mathematical Sciences, Shanghai, China, July 12–16.

48. D. WALTER, Humboldt-Universität zu Berlin, Institut für Mathematik, October 10, 2022 – October 9, 2023.

49. K. WIŚNIEWSKI, Warsaw University of Technology, Faculty of Physics, Warsaw, Poland, July 11–16.

50. Y. WU, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, October 12–18.

51. M. ZHOU, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, June 6–12.

A.11.2 Scholarship Holders

1. O. Burylko, National Academy of Sciences of Ukraine, Kiev, MATH+ Fellowship for Mathematicians from Ukraine, November 1, 2022 – April 30, 2023.
2. M. Kniely, Universität Graz, Austria, Erwin Schrödinger-Auslandsstipendium, March 1, 2022 – February 29, 2024.
3. X. Li, Shandong University, China, China Scholarship Council, January 22 – December 23.

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, February 4 – December 31.
2. M. Reiter, Technische Universität Berlin, Institut für Mathematik, supervisor: Dr. R. Lasarzik, doctoral candidate, April 1 – December 31.

A.12 Guest Talks

1. G. Acosta, University of Buenos Aires, Department of Mathematics, Argentina, *Nonlocal models related problems*, July 21.
2. N. Akhmediev, Australian National University, Research School of Physics, Canberra, Australia, *Rogue waves: Sasa–Satsuma and Uwe Bandelow*, August 30.
3. C. Amendola, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Research Group in Nonlinear Algebra, Leipzig, *Likelihood geometry of correlation models (hybrid talk)*, May 4.
4. S. Baldassarri, Universitá di Firence, Dipartimento di Matematica e Informatica "Ulisse Dini", Florence, Italy, *Critical Droplets and sharp asymptotics for Kawasaki dynamics with strongly anisotropic interactions*, April 6.
5. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Divergence-free finite element methods for an inviscid fluid model*, June 7.
6. D. Belomestny, Universität Duisburg-Essen, Fakultät für Mathematik, *Achieving optimal sample complexity in reinforcement learning via upper solutions (hybrid talk)*, January 19.
7. T. Böhnlein, Technische Universität Darmstadt, Fachbereich Mathematik, *On necessary and sufficient conditions for Gaussian estimates of elliptic operators subject to mixed boundary conditions (hybrid talk)*, November 17.
8. O.A. Burylko, National Academy of Sciences of Ukraine, Institute of Mathematics, and Potsdam Institute for Climate Impact Research, Berlin, *Symmetry breaking yields chimeras in two small populations of Kuramoto-type oscillators*, May 24.
9. A. Carpentier, Universität Potsdam, Institut für Mathematik, *Optimal ranking for crowd-sourcing (hybrid talk)*, June 15.
10. F. Cottini, Università degli Studi di Milano-Bicocca, Dipartimento di Matematica e Applicazioni, Italy, *Gaussian limits for subcritical chaos*, June 1.
11. N. Courtier, University of Oxford, Department of Engineering Science, UK, *Part I: Accurate and adaptable charge transport modelling of perovskite solar cells using IonMonger (hybrid talk)*, March 24.
12. ———, *Part II: Parameter/state estimation using the measure-moment approach to polynomial optimisation (hybrid talk)*, March 24.
13. O. Cronie, Chalmers University of Technology & University of Gothenburg, Department of Mathematical Sciences, Sweden, *Point process learning: A cross-validation-based approach to statistics for point processes (hybrid talk)*, October 19.
14. B. de Wolff, Vrije Universiteit, Faculty of Science, Mathematics, Amsterdam, Netherlands, *Delayed feedback stabilization & unconventional symmetries*, June 14.
15. M.F. Djete, Université Paris Dauphine, École Polytechnique, Paris, France, *Non-regular McKean–Vlasov equations and calibration problem in local stochastic volatility models (online talk)*, September 27.
16. A. Djurdjevac, Zuse Institute Berlin, Computational Humanities, *Approximation of the Dean–Kawasaki equation*, February 23.
17. P.L. Dragotti, Imperial College London, Department of Electrical and Electronic Engineering, UK, *Computational imaging and sensing: Theory and applications (online talk)*, May 30.
18. C. Duval, Université de Paris, Unité de Formation et de Recherches Mathématiques et Informatique, France, *Interacting Hawkes processes with multiplicative inhibition (online talk)*, February 16.
19. M. Egert, Technische Universität Darmstadt, Fachbereich Mathematik, *Four critical numbers for elliptic systems with block structure (hybrid talk)*, November 16.

20. R. Eisenberg, Rush University, Department of Physiology & Biophysics, Chicago, USA, *From Maxwell to mitochondria (online talk)*, September 29.
21. O. Esen, Gebze Technical University, Faculty of Science, Mathematics, Gebze, Turkey, *On geometry of Vlasov plasma (online talk)*, May 11.
22. St. Evje, University of Stavanger, Applied and Computational Mathematics, Norway, *A cell-fluid-matrix model to understand how aggressive cancer cell behavior possibly is linked to elevated fluid pressure (online talk)*, July 12.
23. A. Fermanian, Université Paris Sciences & Lettres, Mines ParisTech, Center for Computational Biology, France, *Framing RNN as a kernel method: A neural ODE approach (online talk)*, August 30.
24. N. Forien, Sapienza Università di Roma, Dipartimento di Matematica “Guido Castelnuovo”, Italy, *Sleepy frogs playing ping-pong on an overcrowded torus: The supercritical phase of Activated Random Walks*, October 19.
25. D. Frazier, Monash University, Department of Econometrics and Business Statistics, Melbourne, Australia, *Guaranteed robustness via semi-modular posterior inference (hybrid talk)*, October 19.
26. E. Gladin, Humboldt-Universität zu Berlin, Berlin Mathematical School, *Algorithm for constrained Markov decision process with linear convergence*, October 18.
27. A. Grauer, Universität zu Köln, Department Mathematik/Informatik, *Short paths in scale-free geometric random graphs*, October 12.
28. W.K. Härdle, Humboldt-Universität zu Berlin, BRC Blockchain Research Center, *DAI the digital art index (hybrid talk)*, April 20.
29. D. Heydecker, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *From LDPs of the Kac process to the H-Theorem*, December 7.
30. Z. Hlávka, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, *Testing dependencies in functional time series*, May 18.
31. R. Jack, University of Cambridge, Yusuf Hamied Department of Chemistry, UK, *Examples of hydrodynamic behaviour in two-species exclusion processes (online talk)*, September 19.
32. P. Jacob, ESSEC Business School, Information Systems, Decision Sciences and Statistics, Paris, France, *Some methods based on couplings of Markov chain Monte Carlo algorithms (online talk)*, January 26.
33. M. Kasprzak, University of Luxembourg, Department of Mathematics, Esch-sur-Alzette, Luxembourg, *How good is your Laplace approximation? Finite-sample error bounds for a variety of useful divergences (hybrid talk)*, November 30.
34. M. Kniely, Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, *From energy- to electro-energy-reaction-diffusion systems (hybrid talk)*, April 27.
35. M. Koser, Humboldt-Universität zu Berlin, Institut für Mathematik, *Pattern formation in certain frustrated spin systems (hybrid talk)*, June 1.
36. R. Kraaij, Delft University of Technology, Faculty of Electrical Engineering, Mathematics & Computer Science, Netherlands, *Large deviations for weakly coupled slow-fast systems via the comparison principle of an associated Hamilton–Jacobi equation*, May 18.
37. H. Kremer, Y. Nemmour, Max Planck Institute for Intelligent Systems, Empirical Inference Department, Tübingen, *Distributionally robust machine learning via conditional moment restrictions*, December 14.
38. Z. Lakdawala, Lahore University of Management Sciences, Syed Babar Ali School of Science and Engineering, Pakistan, *On water wave dynamics using physics informed neural networks*, July 12.

39. J. Latz, Heriot-Watt University, School of Mathematical and Computer Sciences, Department of Actuarial Mathematics and Statistics, Edinburgh, UK, *Analysis of stochastic gradient descent in continuous time*, November 10.
40. X. Li, Shandong University, The School of Mathematics, China, *Two divergence-free reconstructions for Navier–Stokes simulations regarding EMA and robust estimates of kinetic energy error (hybrid talk)*, March 10.
41. ———, *Inf-sup stabilized Scott–Vogelius elements for incompressible flows*, December 13.
42. G. Ligorio, Humboldt-Universität zu Berlin, Institut für Physik, *Neuromorphic device development: From modification of surfaces to modification of functions (hybrid talk)*, June 23.
43. Ch. Ling, Technische Universität Berlin, Institut für Mathematik, *Singular SDEs and PDEs*, May 4.
44. L. Lüchtrath, Universität zu Köln, Department Mathematik/Informatik, Köln, *The various phases of long-range inhomogeneous percolation*, June 22.
45. Y. Luo, Max Planck Institute for Intelligent Systems, Empirical Inference Department, Tübingen, *Spectral representation learning for conditional moment models*, December 5.
46. G. Malinovsky, King-Abdullah University of Science and Technology, Computer, Electrical and Mathematical Sciences and Engineering Division, Thuwal, Saudi Arabia, *Yes! Local gradient steps provably lead to communication acceleration! Finally! (online talk)*, June 21.
47. A. Martini, University of Oxford, Department of Statistics, Oxford, UK, *An additive-noise approximation to Keller–Segel–Dean–Kawasaki dynamics*, June 14.
48. A. Massing, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, *CutFEM: Discretizing geometry and partial differential equations*, September 13.
49. A. Menafoglio, Politecnico Milano, Department of Mathematics, Italy, *Object oriented data analysis in Bayes spaces: From distributional data to the analysis of complex shapes (online talk)*, February 2.
50. J. Moatti, Université de Lille, Laboratoire Paul Painlevé, France, *A structure preserving hybrid finite volume scheme for semi-conductor models on general meshes*, June 2.
51. M. Multerer, Università della Svizzera Italiana, Euler Institute, Lugano, Switzerland, *Samplets: Construction and scattered data compression*, October 13.
52. M. Myllymäki, Natural Resources Institute Finland (Luke), Bioeconomy and Environment, *Global envelopes with applications to spatial statistics and functional data analysis*, June 8.
53. M. Neuss-Radu, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Mathematik, Erlangen, *Effective models for nonlinear drift-diffusion of multiple species in porous media (online talk)*, May 18.
54. F. Nie, Technische Universität Berlin, Institut für Mathematik, *The stochastic F-KPP equation and on/off branching coalescing Brownian motion*, March 23.
55. A. Nota, Università degli Studi dell'Aquila, Dipartimento di Ingegneria e Scienze dell'Informazione e Matematica, Italy, *Stationary non-equilibrium solutions for coagulation equations (online talk)*, April 26.
56. F. Nüske, Universität Paderborn, Lehrstuhl für Angewandte Mathematik, *Tensor-based methods for learning the Koopman semigroup (online talk)*, January 11.
57. M.A. Olshanskii, University of Houston, Department of Mathematics, Texas, USA, *Numerical analysis of surface fluids (online talk)*, June 20.
58. T. Paul, Humboldt-Universität zu Berlin, Institut für Mathematik, *Modelling interactions of mutation, dormancy and transfer*, February 9.
59. P. Pérez-Aros, Universidad de O'Higgins, Instituto de Ciencias de la Ingeniería, Rancagua, Chile, *Inner Moreau envelope of nonsmooth conic chance constrained optimization problems*, June 7.

60. Y. Petrova, Instituto de Matemática Pura e Aplicada, Rio de Janeiro, Brazil, *On the impact of dissipation ratio on vanishing viscosity solutions of Riemann problems for chemical flooding models (online talk)*, May 10.
61. St. Piani, International School for Advanced Studies, Trieste, Italy, *HDG methods for the van Roosbroeck model*, March 31.
62. M. Redmann, Martin Luther University of Halle Wittenberg, Institute of Mathematics, Halle, *Solving high-dimensional optimal stopping problems using model order reduction (hybrid talk)*, May 3.
63. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, *Magnetism in the planet Earth and its mathematical modelling (hybrid talk)*, November 30.
64. A. Särkkä, Chalmers University of Technology and University of Gothenburg, Mathematical Sciences, Gothenburg, Sweden, *Anisotropy analysis and modelling of spatial point patterns (hybrid talk)*, November 16.
65. C. Schillings, Freie Universität Berlin, Institut für Mathematik, *The convergence of the Laplace approximation and noise-level-robust computational methods for Bayesian inverse problems (hybrid talk)*, November 9.
66. A. Schlömerkemper, Julius-Maximilians-Universität Würzburg, Insitut für Mathematik, *A discussion of two models extending the Cahn–Hilliard equation to a temperature-dependent setting (hybrid talk)*, October 11.
67. A. Schmidt, Universität Bremen, Zentrum für Technomathematik, Bremen, *Multi scale models for a tool grinding process*, September 13.
68. J. Schmidt-Hieber, University of Twente, Electrical Engineering, Mathematics and Computer Science (EEMCS), Enschede, Netherlands, *Overparametrization and the bias-variance dilemma (hybrid talk)*, November 2.
69. R. Schubert, Universität Bonn, Hausdorff Center for Mathematics, *A variational approach to data-driven problems in fluid mechanics (hybrid talk)*, November 23.
70. L. Schülen, Technische Universität Berlin, Institut für Theoretische Physik, *The solitary route to chimera states*, May 17.
71. S. Schwarzacher, Charles University Prague, Department of Mathematical Analysis, Czech Republic, *A variational approach to fluid-structure interactions (online talk)*, January 12.
72. E. Scornet, Ecole Polytechnique Paris, Centre de Mathématiques Appliquées, France, *Variable importance in random forests (online talk)*, February 9.
73. U. Sharma, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Variational structures beyond gradient flows (online talk)*, February 2.
74. A. Shilnikov, Georgia State University, Neuroscience Institute, Department of Mathematics and Statistics, Atlanta, USA, *Long saga of in-depth modeling of two swim CPGs in two sea slugs (online talk)*, May 20.
75. E. Sonnendrücker, Max-Planck-Institut für Plasmaphysik, Numerische Methoden in der Plasmaphysik, Garching, *Geometric numerical methods for models from plasma physics (online talk)*, May 31.
76. A. Srivastava, Florida State University, Department of Statistics, USA, *Statistical shape analysis of complex natural structures (hybrid talk)*, June 29.
77. M. Staudigl, Maastricht University, School of Business and Economics, Netherlands, *Stochastic relaxed inertial forward-backward-forward splitting for monotone inclusions in Hilbert spaces (hybrid talk)*, August 16.
78. K. Stinson, Universität Bonn, Hausdorff Center for Mathematics, *A gradient flow perspective for weak solutions of the Mullins–Sekerka flow and an application to lithium-ion batteries (hybrid talk)*, October 26.
79. Y. Sun, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *High dimensional change-point detection: A complete graph approach (online talk)*, January 18.
80. A. Thorpe, University of New Mexico, Hybrid Systems and Control Lab, Albuquerque, USA, *Stochastic optimal control & safety via kernel embeddings: A data-driven approach*, April 12.

81. S. Tikhomirov, Instituto de Matemática Pura e Aplicada, Rio de Janeiro, Brazil, *Mixing zone in miscible displacement: Application in polymer flooding and theoretical attempts of improving (online talk)*, May 10.
82. D. Tuarev, Imperial College London, Faculty of Natural Sciences, Department of Mathematics, London, UK, *Non-ergodicity and stable coherent motions in systems of mutually repelling particles with arbitrarily high kinetic energy*, September 27.
83. Q. Vogel, New York University Shanghai, Institute of Mathematical Sciences, China, *Infinite loops – The limit of the Feynman representation of the Bose gas (online talk)*, February 2.
84. ———, *The variational principle and the Bose gas*, July 13.
85. Th. Wagenhofer, Technische Universität Berlin, Berlin Mathematical School (BMS), *Reconstructing volatility: Pricing of index options under rough volatility (hybrid talk)*, November 29.
86. M. Wahl, Humboldt-Universität zu Berlin, Institut für Mathematik, *Functional estimation in log-concave location-scale families (hybrid talk)*, January 12.
87. J. Wang, Peking University, Department of Mechanics and Engineering Science, College of Engineering, China, *Performance optimization of model predictive control algorithm and its application (online talk)*, September 28.
88. S. Wohlfeil, Ferdinand-Braun-Institut, Berlin, *Experimental investigations of passively modelocked ridge-waveguide and tapered lasers emitting at 830 nm (online talk)*, February 10.
89. M. Yamakou, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Data Science, Erlangen, *Transitions between weak-noise-induced resonance phenomena in a multiple timescales neural system*, May 3.
90. N. Zakiyeva, Zuse-Institut Berlin, Applied Algorithmic Intelligence Methods, *Modeling and forecasting the dynamics of the natural gas transmission network in Germany with the demand and supply balance constraint*, April 27.

A.13 Software

ARKS – Adversarially Robust Kernel Smoothing (contact: J.-J. Zhu, phone: +49 30/20372-339, e-mail: jia-jie.zhu@wias-berlin.de)

ARKS is a large-scale implementation of kernel methods for distributionally robust optimization. It is based on the idea of using a diffusion process to robustify the learning algorithms.

More information: https://github.com/christinakouridi/arks

AWS – Adaptive Weights Smoothing (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

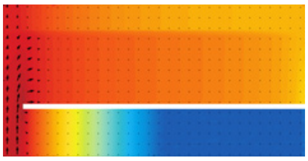
`AWS` is a contributed package within the R-Project for Statistical Computing containing a reference implementation of the **A**daptive **W**eights **S**moothing algorithms for local constant likelihood and local polynomial regression models. Binaries for several operating systems are available from 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.

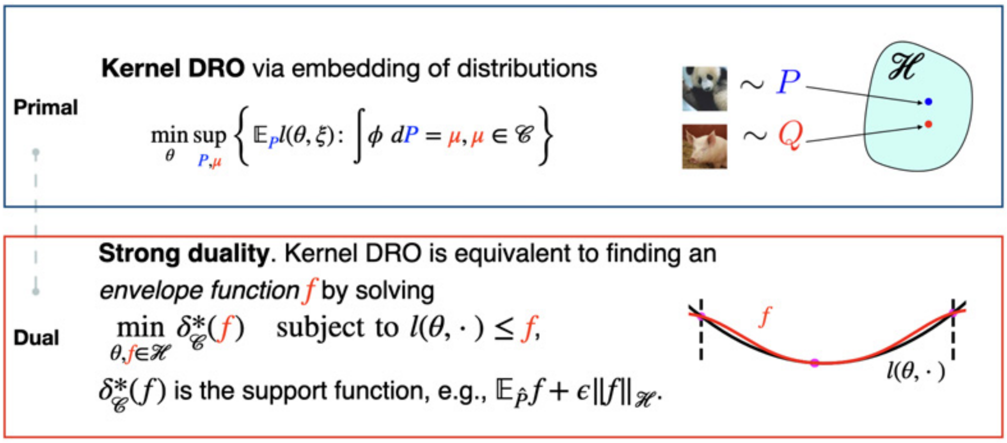
Please find further information under https://www.wias-berlin.de/software/ddfermi/.

DiPoG (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@wias-berlin.de)

The program package `DiPoG` (**D**irect and **i**nverse **P**roblems for **o**ptical **G**ratings) provides simulation and optimization tools for periodic diffractive structures with multilayer stacks.

The direct solver computes the field distributions and efficiencies of given gratings for TE and TM polarization as well as, under conical mounting, for arbitrary polygonal surface profiles. The inverse solver deals with the optimal design of gratings, realizing given optical functions, for example, far-field patterns, efficiency, or phase profiles. The algorithms are based on coupled generalized finite/boundary elements and gradient-type optimization methods.

For detailed information please see https://www.wias-berlin.de/software/DIPOG/.



K-DRO – Kernel Distributionally Robust Optimization (contact: J.-J. Zhu, phone: +49 30/20372-339, e-mail: jia-jie.zhu@wias-berlin.de)

K-DRO is the software implementation of Kernel Distributionally Robust Optimization (DRO), a robust machine learning and optimization algorithm that can handle nonlinear non-convex loss and model functions. It is based on a dual reformulation that turns a DRO problem into a kernel learning problem. The intuition is to find a smooth kernel function that majorizes the original loss, as demonstrated in the illustration above.

More information: https://github.com/jj-zhu/kdro

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.radziunas@wias-berlin.de)

`LDSL-tool` (**L**ongitudinal **D**ynamics in **S**emiconductor **L**asers) is a **tool** for the simulation and analysis of the nonlinear longitudinal dynamics in multisection semiconductor lasers and different coupled laser devices. This software is used to investigate and design laser devices that exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, mutual synchronization, and frequency entrainment by an external modulated optical or electrical signal.

`LDSL-tool` combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.

Detailed information: https://www.wias-berlin.de/software/ldsl

WIAS-MeFreSim (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@wias-berlin.de)

`WIAS-MeFreSim` allows for the three-dimensional simulation of induction heat treatment for workpieces made of steel using single- and multi-frequency currents. It is the aim of the heat treatment to produce workpieces with hard, wear-resistant surface and soft, ductile core. The boundary layer of the workpiece is heated up by induced eddy currents and rapidly cooled down by the subsequent quenching process. The resulting solid-solid phase transitions lead to a hardening of the surface of the workpiece.

`WIAS-MeFreSim` is based on the WIAS software `pdelib`. It solves coupled systems of PDEs consisting of Maxwell's equations, the heat equation, and the equations of linear elasticity.

Fore more information see https://www.wias-berlin.de/software/MeFreSim/.

MMD-DR-CCSP – Maximum Mean Discrepancy Distributionally Robust Nonlinear Chance-Constrained Programming (contact: J.-J. Zhu, phone: +49 30/20372-339, e-mail: jia-jie.zhu@wias-berlin.de)

MMD-DR-CCSP applies the Kernel Distributionally Robust Optimization methodology. Compared with other DR-CCSP algorithm, it can handle nonlinear chances constraints with computable finite-sample guarantees.

More information: https://github.com/yasnem/CC_Tutorial_TUB_Oxford

ParMoon (contact: A. Caiazzo, phone: +49 30/20372-332, e-mail: alfonso.caiazzo@wias-berlin.de)

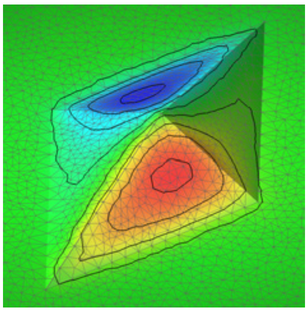
`ParMooN` is a flexible finite element package for the solution of steady-state and time-dependent convection-diffusion-reaction equations, incompressible Navier–Stokes equations, and coupled systems consisting of these types of equations, like systems coupling free flows and flows in porous media.

Please find more information under http://cmg.cds.iisc.ac.in/parmoon/.

Important features of `ParMooN` are

- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, non-conforming, discontinuous, higher-order, vector-valued, isoparametric, with bubbles),
- the use of implicit time-stepping schemes (θ-schemes, DIRK schemes, Rosenbrock–Wanner schemes),
- the application of a multiple-discretization multi-level (MDML) preconditioner in Krylov subspace methods,
- tools for using reduced-order models based on proper orthogonal decomposition (POD) are available,
- hybrid parallelization with MPI and OpenMP.

`ParMooN` is a joint development with the group of Prof. S. Ganesan (IISc Bangalore) and the group of Prof. G. Matthies (TU Dresden).



Displacement (y-component) from FEM simulation of elastic relaxation of a pyramidal InAs quantum dot with a rhomboidal base in GaAs matrix. Used as input for TEM image simulation.

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, T. Streckenbach, phone: +49 30/20372-476, e-mail: timo.streckenbach@wias-berlin.de)

`pdelib` is a collection of software components that are useful to create simulators and visualization tools for partial differential equations. The main idea of the package is modularity, based on a bottom-up design realized in the C++ programming language. Among others, it provides

- iterative solvers for linear and nonlinear systems of equations,
- sparse matrix structures with preconditioners and direct solver interfaces,
- dimension-independent simplex grid handling in one, two, and three space dimensions,
- finite-volume-based solution of coupled parabolic reaction-diffusion-convection systems and pressure-robust discretizations for Navier–Stokes,
- finite-element-based solution of variational equations (especially thermoelasticity) with goal-oriented error estimators,
- optimization tool box,
- parallelization on SMP architectures,
- graphical output during computation using OpenGL,
- scripting interface based on the languages Python and Lua,
- graphical user interface based on the FLTK toolkit,
- modular build system and package manager for the installation of third-party software used in the code.

Please see also https://www.wias-berlin.de/software/pdelib/.

PDELib.jl (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de,
T. Streckenbach, phone: +49 30/20372-476, e-mail: timo.streckenbach@wias-berlin.de,
Ch. Merdon, phone: +49 30/20372-452, e-mail: christian.merdon@wias-berlin.de)

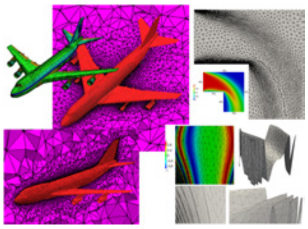
`PDELib.jl` is being developed as the successor of `pdelib` in the Julia programming language. It is a collection of open source Julia packages dedicated to the handling of sparse matrices, mesh generation, and visualization. It wraps the Julia package `VoronoiFVM.jl` that implements the Voronoi box-based finite volume method for nonlinear systems of partial differential equations and the Julia package `GradientRobustMultiPhysics.jl` implementing gradient robust finite element methods in Julia.

Please see also https://github.com/WIAS-BERLIN/PDELib.jl.

SPHInX (contact: O. Marquardt, phone: +49 30/20372-474, e-mail: oliver.marquardt@wias-berlin.de)

`SPHInX` is an open-source C++ library for materials simulation hosted by the Max-Planck-Institut für Eisenforschung GmbH in Düsseldorf. The multiband $\mathbf{k}\cdot\mathbf{p}$ and continuum elasticity modules of SPHInX for the calculation of elastic and optoelectronic properties of semiconductor heterostructures are maintained at WIAS Berlin.

Please see https://sxrepo.mpie.de/.



Adapted tetrahedral meshes and anisotropic meshes for numerical methods and scientific computation

TetGen (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de)

`TetGen` is a mesh generator for three-dimensional simplex meshes as they are used in finite volume and finite element computations. It generates the Delaunay tetrahedralization, Voronoi diagram, and convex hull for three-dimensional point sets. For three-dimensional domains with piecewise linear boundary, it constructs constrained Delaunay tetrahedralizations and quality tetrahedral meshes. Based on recent research on fundamental algorithms for the generation of tetrahedral meshes, the new version 1.6 provides improvements with respect to the quality of the created meshes and the speed for their creation.

More information is available at https://www.wias-berlin.de/software/tetgen/.

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 of the new code and the support of running projects.

For more information please see https://www.wias-berlin.de/software/tesca/.

WIAS Software Collection for Imaging (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

`adimpro` is a contributed package within the R-Project for Statistical Computing that contains tools for image processing, including structural adaptive smoothing of digital color images. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

The AWS for AMIRA (TM) plugin implements a structural adaptive smoothing procedure for two- and three-dimensional images in the visualization software AMIRA (TM). It is available in the Zuse Institute Berlin's version of the software for research purposes (http://amira.zib.de/).

WIAS Software Collection for Neuroscience (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

`dti` is a contributed package within the R-Project for Statistical Computing. The package contains tools for the analysis of diffusion-weighted magnetic resonance imaging data (dMRI). It can be used to read dMRI data, to estimate the diffusion tensor, for the adaptive smoothing of dMRI data, the estimation of the orientation density function or its square root, the estimation of tensor mixture models, the estimation of the diffusion kurtosis model, fiber tracking, and for the two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org). The multi-shell position-orientation adaptive smoothing (msPOAS) method for dMRI data is additionally available within the ACID toolbox for SPM (http://www.diffusiontools.com).

`fmri` is a contributed package within the R-Project for Statistical Computing that contains tools to analyze fMRI data with structure-adaptive smoothing procedures. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

`qmri` is the third R-package in this collection that contains functions for the analysis of magnetic resonance imaging data acquired in the multi-parameter mapping framework 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).