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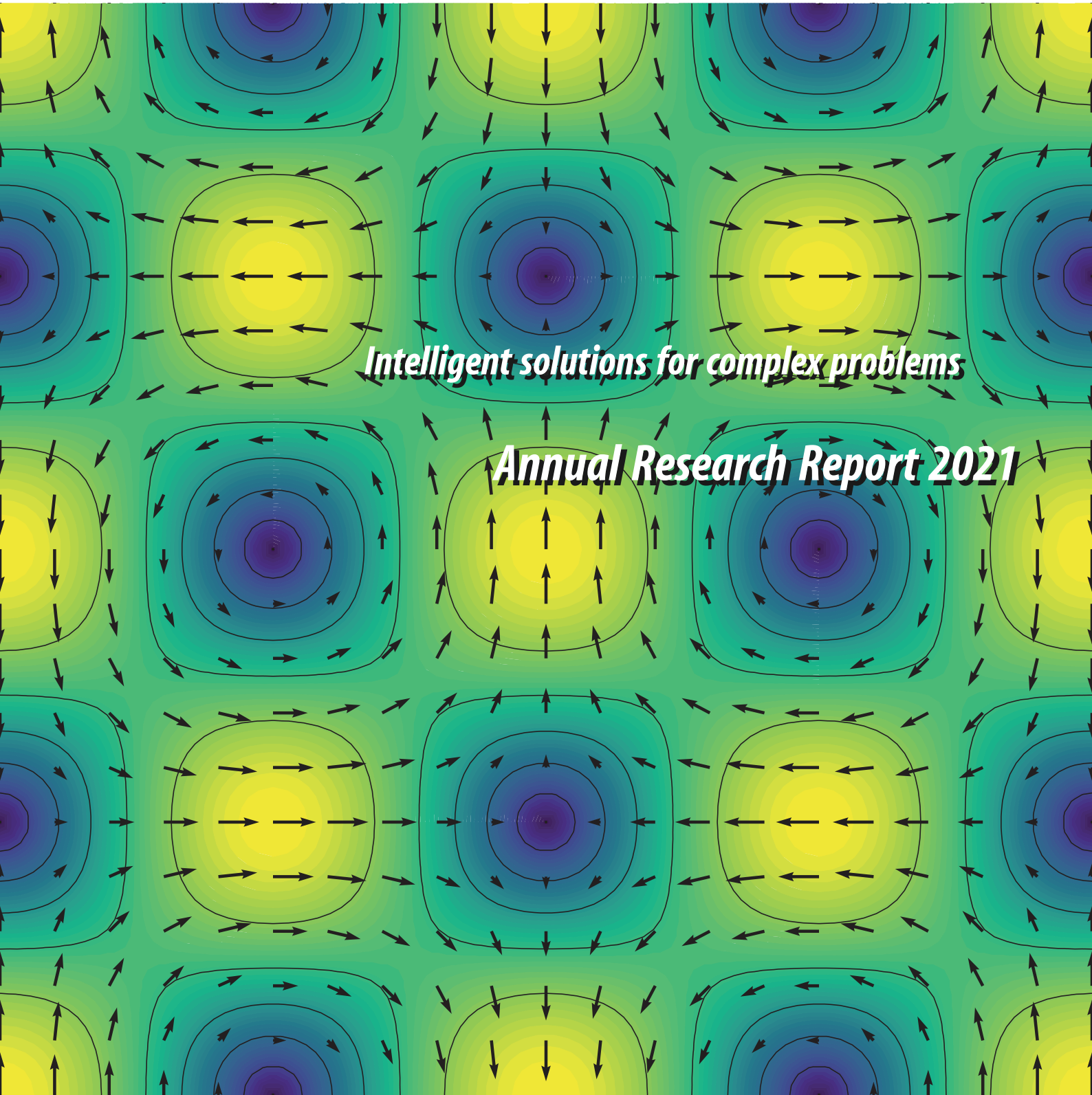
Weierstrass Institute for Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2021

Cover figure: Plot of the velocity field of a planar lattice flow, which is a popular benchmark example for the study of finite element discretisations for the Navier-Stokes equations. It has several interesting properties, namely that it keeps its shape in time (it just looses energy through diffusion), and its convective term actually is a gradient that should be balanced by the pressure. Gradient-robust discretisations that preserve the orthogonality between divergence-free test functions and gradients can resolve the flow much better than classical methods without this property.

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Prof. Dr. 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 Report 2021. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2021.

The persistent pandemic situation again demanded a lot from us in 2021, especially in the first and in the last quarter of the year. The many adjustments and changes to our work processes that we implemented since 2020 in order to achieve our goals helped us to a large extent. The overall situation, however, remained exhausting and stressfull. Every member of staff did what (s)he could to contribute to the smooth running of the institute and to ensure that all the aims of the institute for 2021 could be achieved.

Not least because of this solidarity, some outstanding successes were recorded and excellent projects were brought to the institute in 2021. On the scientific side, the many newly acquired MATH+ projects, the successes in the Leibniz competition and, of course, MaRDI show the enormous creativity and radiance of the institute. In the administrative area, milestones have been reached in the electronization of work processes, which support us in the increased mobile work caused by the pandemic.

The WIAS recruited a Leibniz Junior Group on “Probabilistic Methods for Dynamic Communication Networks”, which will be funded for five years from 2021. Headed by Benedikt Jahnel, it examines the connection intervals of devices in mobile D2D (device-to-device) networks with a static infrastructure with a view to increasing connectivity.

To promote young scientists, another Weierstraß group – with a term of three years and headed by Jia-Jie Zhu – was set up on the flexible research platform in June 2021 on the promising and highly innovative area of “Data-Driven Optimization and Control”.

WIAS is among the five cooperation partners of the Cluster of Excellence Berlin Mathematics Research Center MATH+, with its Director one of its three spokespersons. The reporting year brought WIAS 9 new MATH+ projects starting 2022, ranging from the development of an ion-channel model framework for in-vitro assisted interpretation of current voltage relations to volatile electricity markets and battery storage to gate-confined quantum dots for Qubit generation.

The Secretariat of the International Mathematical Union (IMU), permanently based at WIAS since 2011, lead by the head of WIAS Research Group 4 *Nonlinear Optimization and Inverse Problems* and IMU Treasurer Prof. Dietmar Hömberg, organized one year late each due to the pandemic the International Congress on Mathematical Education (ICME 14) in hybrid format in Shanghai, China, and the 100th anniversary of the IMU on September 27 and 28, 2021, in Strasbourg, France.

The WIAS purposefully expanded its area of research data management. A big success was the acquisition of the “Mathematical Research Data Initiative (MaRDI)”, the consortium of mathematics in the National Research Data Infrastructure (NFDI) coordinated by the WIAS. The library area was modernized and developed into a center for research data management at the WIAS with a new manager, who is now part of the directorate. Together with the MaRDI officer and another position yet to be filled for research software engineering with reference to MaRDI, and some experienced employees from science and the field of computing technology, WIAS now has a competent team for research data management.

Our *work and family* team made the compatibility of work and family the focus of a strategy workshop on July 9, 2021. It is preparing our Institute for its next re-audit in 2022 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.

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 2022

M. Hintermüller

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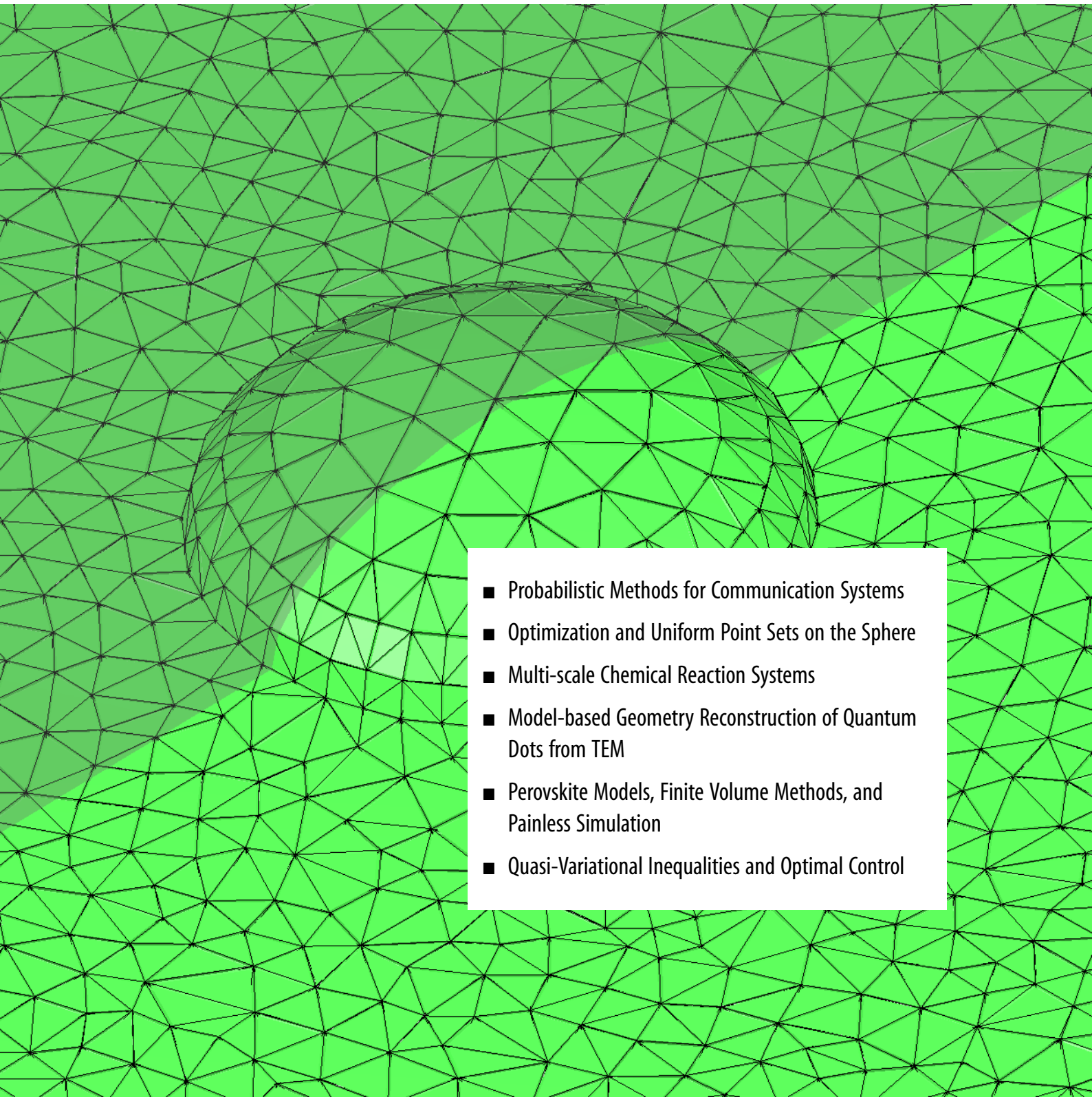
1 Scientific Highlights



- Probabilistic Methods for Communication Systems
- Optimization and Uniform Point Sets on the Sphere
- Multi-scale Chemical Reaction Systems
- Model-based Geometry Reconstruction of Quantum Dots from TEM
- Perovskite Models, Finite Volume Methods, and Painless Simulation
- Quasi-Variational Inequalities and Optimal Control

1.1 Probabilistic Methods for Communication Systems

Alexander Hinsen and Benedikt Jahnel

The steadily increasing demand for fast and reliable data exchange in communications systems presents network operators worldwide with major challenges, but also opportunities. A very important aspect of this state of affairs is the strongly increasing use of connected machines as part of the internet of things (IoT) as well as smart devices such as mobile phones, tablets, or even self-driving cars; see Figure 1 (left).

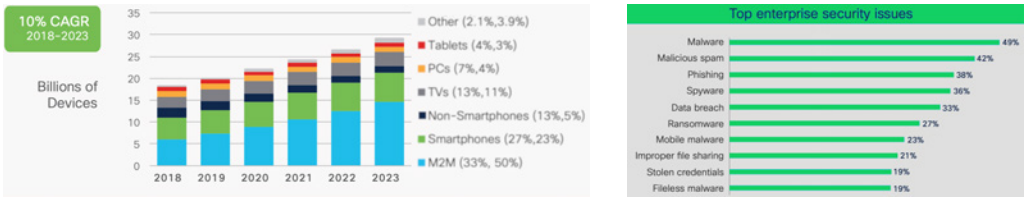


Fig. 1: *Left: Growth of communications driven by machine-to-machine and smartphone connections. Right: Network security breaches driven by malware attacks.* Cisco Annual Internet Report (2018–2023) White Paper

This situation is also reflected in the 5G (5th generation mobile network) specifications as well as in the negotiations for subsequent standards, which envisage faster connections, higher throughput, more capacity over enhanced mobile broadband, and highly reliable, low-latency communications to enable the system to support time-critical applications such as car-to-car communications as well as inter-machine connectivity.

In this context, *device-to-device (D2D) communications* is considered one of the key concepts that permeates a wide range of use cases. On the one hand, D2D systems have the potential to relieve today's cellular networks of at least some of the system pressure. On the other hand, D2D communications can provide, for example, faster and more robust connectivity. However, from an operator's perspective, D2D systems are much less controllable than traditional cellular networks, due to their dependence on individual user behavior. This lack of control is exacerbated when devices are *mobile* and the system is very dense due to the widespread use of connectable devices. Therefore, to correctly predict the performance and vulnerabilities of D2D systems, detailed and comprehensive modeling and analysis is essential. Here, a natural approach is to study the uncertainties of the system using *probabilistic methods*.

The starting point is the modeling of *random locations and movement* of the smart devices within their environment. Based on this information, the *transmission mechanism* between any pair of devices must be represented with an appropriate level of detail. Then, already the *connection times* in a sparse *cellular network* that is augmented by D2D communications, with a large but finite number of allowed D2D hops, is a significant performance indicator for a feasible D2D application; see below for more details in this direction.

A particularly relevant aspect of D2D networks is the *spread of malware* through the system. Due to the lack of central control, proximity-based sabotage software or viruses such as, for example, *Cabir, CommWarrior, or HummingBad* can potentially spread undetected in such networks. In this context, modeling and analyzing the unchecked infiltration of malware into D2D systems is already of immense relevance; see Figure 1 (right) and our results on limiting shapes of infected

regions below. The natural next step then is to design and evaluate possible decentralized countermeasures against malware attacks, for which we present a short summary of our research at the end.

Stochastic geometry in telecommunications

In order to describe the system with all its uncertainties, we use methods from probability theory, more precisely from *stochastic geometry* [6]. In the first step, we associate to each device located at X_i an interaction zone given by an open disk $B_r(X_i)$ of radius r centered at X_i, where $2r$ is the range in which the device X_i can communicate in a peer-to-peer fashion. In other words, any pair of devices whose associated disks have nonempty intersection are connected by an edge, forming a random graph, the so-called *Gilbert graph* $\mathcal{G}_r(X)$, where $X = \{X_i\}_{i\in I}$ is the set of all device locations; see Figure 2 for an illustration. In absence of any refined statistical information on the spatial distribution of the devices, the null model is given by the stationary *Poisson point process*. This is a family of random point measures that enjoys strong spatial independence. It has one parameter, the spatial average density of the points. The associated *Poisson–Gilbert graph* is the fundamental object of the theory of *continuum percolation*, which investigates statistical properties of the *connected components* of the graph. In particular, it has been observed already in the early 1960s that there exists a phase transition in the density parameter for the almost-sure absence, respectively unique existence, of an infinite connected component $\mathcal{C}$ in $\mathcal{G}_r(X)$. This is the celebrated *phase transition of percolation*, which also has strong links to statistical physics (e.g., the probabilistic description of liquid-vapor phase transitions) and can be interpreted as an indicator for the D2D system to feature only local, respectively global, connectivity.

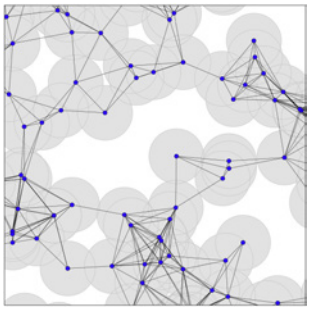


Fig. 2: *Realization of randomly placed devices (blue). Black edges are drawn whenever two devices have overlapping interaction zones (gray).*

The Poisson–Gilbert graph can serve as a model for a static pure D2D connectivity network, or as a snapshot for an otherwise *mobile system*. For example, considering the use case of car-to-car communications, the mobility of the nodes is of crucial importance for the system. Fortunately, *point-process theory* provides also a versatile framework for the modeling of mobile nodes, via the use of *markings*. More precisely, we can associate with each device location X_i an attribute, for example a trajectory Γ_i that represents the path of X_i. Then, the location of the device X_i at time $t \geq 0$ is given by $X_i(t) = X_i + \Gamma_i(t)$. Natural choices for these mobility models are, for example, independent and identically distributed (i.i.d.) *random walks* or *random-waypoint models* in continuous time and continuous space; see Figure 3 for an illustration. Mobile connectivity graphs now give rise to a new class of questions, for example, concerning the time at which a device makes contact with a large cluster, or the amount of time that it can communicate over large distances. Here is where the DYCOMNET group within WIAS makes contributions; see the following section for details.

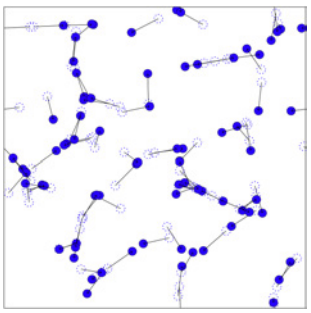


Fig. 3: *Realization of initial device positions (dotted blue) and their respective positions at a fixed positive time (blue), with arrows indicating the corresponding displacement.*

On the other hand, in connectivity graphs such as the Poisson–Gilbert graph, edges represent the possibility to transmit data from device to device, but the actual flow of messages is not represented. In order to incorporate this flow, a standard modeling approach is known under the name *first-passage percolation*, which plays also a big role in the probabilistic analysis of space-time epidemiological events. Here, a *passage time* τ_e is associated to every edge e in the graph. If, at time zero, a message is placed at a vertex X_i; then, the set of vertices $\mathcal{H}_t(X_i)$ that have received

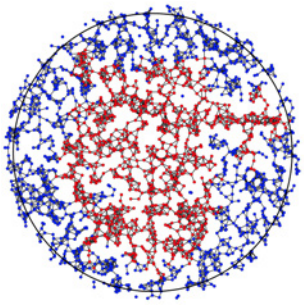


Fig. 4: *Realization of first-passage percolation on a Gilbert graph at some positive time. Vertices in $\mathcal{H}_t(o)$ are indicated in red.*

the message by some positive time $t > 0$, is given by

$$\mathcal{H}_t(X_i) = \Big\{ X_j \in X \colon \exists \text{ path } \gamma \text{ in } \mathcal{G}_r(X) \text{ starting in } X_i \text{ and ending in } X_j, \text{ such that } \sum_{e\in\gamma} \tau_e \le t \Big\};$$

see Figure 4 for an illustration. Note that the set $\mathcal{H}_t(X_i)$ cannot be larger than the connected component of X_i in $\mathcal{G}_r(X)$. In the case that the connected component of X_i is infinite, then questions about the asymptotic speed of data propagation, the limiting geometry of the reachable device set, and properties of the shortest paths (geodesics) become highly relevant, but nontrivial. One particular use case is given by the propagation of malware in pure D2D systems with and without the presence of counter-measures. Also here, the DYCOMNET group performs research within WIAS, and we present details in the last section.

Connection intervals in mobile D2D networks

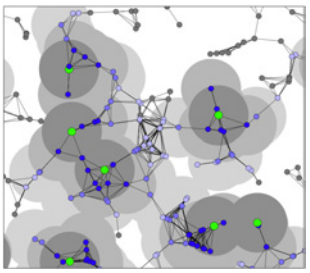


Fig. 5: *Realization of infrastructure nodes (green) and devices (blue and grey). The grey areas indicate the k-hop coverage zones of the infrastructure where $k = 1$ is dark grey, $k = 2$ is grey, and $k = 3$ is light grey. Correspondingly, dark blue devices are connected to the infrastructure directly, blue devices need one intermediate hop, light blue ones need two hops, and grey devices need at least three hops.*

Although pure D2D systems are already in use today, for example in sensor networks or disaster-rescue ad-hoc networks, in the foreseeable future, D2D systems will be mainly deployed as an extension to more traditional cellular networks. We thus consider a homogeneous Poisson point process $Y = \{Y_j\}_{j\in J}$ of *infrastructure nodes* with intensity $\lambda_S > 0$ in addition to the marked Poisson point process of *mobile nodes* $X(t)$ as presented above. We are interested in the times at which a typical device X_o is connected to the infrastructure in at most k hops

$$\Xi_k = \{t \in \mathbb{R} \colon X_o(t) \overset{k}{\rightsquigarrow}_t Y\},$$

where $\overset{k}{\rightsquigarrow}_t$ means that a connection is possible with at most k hops in $\mathcal{G}_r(X(t) \cup Y)$; see Figure 5 for an illustration. Our main interest lies in the distribution of *connection intervals* of the typical device. For this problem, we consider the length of maximal uninterrupted connection time intervals around a given time t

$$I(t, \Xi_k) = \sup_{a\le b \colon t\in[a,b]\subset\Xi_k} (b-a),$$

where $I(t, \Xi_k) = 0$ if $t \notin \Xi$. Using this formula, we define the *k-hop connection-interval measure*

$$\tau_T(\mathrm{d}\ell, \mathrm{d}t) = \frac{1}{T} \int_{[0,T]\cap\Xi_k} \delta_{(I(s,\Xi_k),s/T)}(\mathrm{d}\ell, \mathrm{d}t)\mathrm{d}s,$$

where δ is the Dirac measure. Here, T is the time horizon. Let us highlight that τ_T encodes a number of important network characteristics. For example, the integral $\tau_T(f)$ for $f(\ell, t) = 1$ is the *time-averaged connection time of the typical node*, and $T\tau_T(f)$ for $f(\ell, t) = 1\{\ell > 0\}/\ell$ is the *number of connection intervals* in $[0, T]$. We analyze τ_T in an asymptotic regime of large time horizons $T \uparrow \infty$, many hops $k \uparrow \infty$, and sparse infrastructure $\lambda_S \downarrow 0$, coupled as

$$\lambda_S(T)|B_{k/\mu}(o)| = c \qquad \text{and} \qquad \lambda_S(T) = T^{-\alpha}, \tag{1}$$

with parameters $\alpha, c > 0$, and where $\mu > 0$ is the so-called *stretch factor* of the Poisson–Gilbert graph in the supercritical percolation regime. This is the asymptotic quotient of the graph distance and the Euclidean distance between two distant sites in $\mathcal{C}$. Note that the constant c can be inter-

preted as the expected number of infrastructure nodes in the reachable region.

For the mobility scheme, we assume the trajectories Γ_i to be i.i.d. random walks, starting from zero, i.e., devices sequentially move with constant speed to random waypoints that are independently drawn from an isotropic probability measure $\kappa(\mathrm{d}x)$; see Figure 6 for an illustration. Now, our main results in [4, 5] establish distributional limits of τ_T, as $T \uparrow \infty$ under the scaling (1), for three different regimes that depend on α. First, for $\alpha < d/2$, we have

$$\tau_T(\mathrm{d}\ell, \mathrm{d}t) \xrightarrow{\mathrm{D}} \mathbb{E}[\delta_{I_o(N)}(\mathrm{d}\ell)]\mathrm{d}t,$$

where $I_o(N) = I(0, \Xi_\infty \cap (\cup_{j\le N} \Xi_\infty^{o,j}))$ with N an independent Poisson random variable with intensity c. Here, $(\Xi_\infty^{o,j})_{j\ge 1}$ is a family of i.i.d. copies of Ξ_∞^o where

$$\Xi_\infty^o = \{t \in \mathbb{R} \colon o \leftrightsquigarrow_t \infty\} \qquad \text{and} \qquad \Xi_\infty = \{t \in \mathbb{R} \colon X_o(t) \leftrightsquigarrow_t \infty\},$$

the events that the origin o, respectively the typical device, is part of the infinite cluster of $\mathcal{G}_r(X(t) \cup \{o\})$, respectively $\mathcal{G}_r(X(t))$. In words, in the regime of (relatively) dense infrastructure, the k-hop connection-interval measure approaches (in the spirit of a law of large numbers) a product measure that is given in terms of an expectation over interval lengths in which both, the typical device and at least one reachable infrastructure node, are part of the infinite cluster. On the other hand, for (relatively) sparse infrastructure, where $\alpha > d/2$, using the same definitions,

$$\tau_T(\mathrm{d}\ell, \mathrm{d}t) \xrightarrow{\mathrm{D}} \mathbb{E}[\delta_{I_o(N)}(\mathrm{d}\ell)|N]\mathrm{d}t.$$

Again in words, in this regime, there is less averaging, and the number of reachable infrastructure nodes remains random in the limit. Finally, in the critical regime $\alpha = d/2$, we see the emergence of a standard Brownian motion W_t, and

$$\tau_T(\mathrm{d}\ell, \mathrm{d}t) \xrightarrow{\mathrm{D}} \mathbb{E}[\delta_{I_o(Y'(B_{c'}(W_t)))}(\mathrm{d}\ell)|Y'(B_{c'}(W_t))]\mathrm{d}t,$$

where $c' = (c/|B_1(o)|)^{1/d}$, and Y' is a unit-intensity homogeneous Poisson point process. In this case, even the random number of reachable infrastructure nodes around the limiting trajectory of the typical random walker survives the limit.

Using various degrees of asymptotic decoupling in the highly detailed k-hop connection-interval measure τ_T, our results show that τ_T can be well approximated by much simpler connection-interval measures given in terms of expectations over percolation clusters.

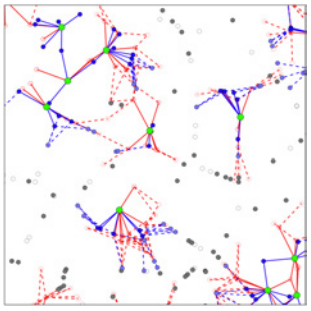


Fig. 6: *Realization of devices (transparent, grey, and blue) and infrastructure nodes (green). Devices at initial time (transparent) are either directly connected (solid red edges) or indirectly connected (dashed red edges) to infrastructure, or they are disconnected. At time 1, the devices have moved and their corresponding new locations offer either direct connections (solid blue edges) or indirect connections (dashed blue edges) to the infrastructure process, or no connections (grey).*

Malware propagation in random geometric graphs

Let us now revisit the static Poisson–Gilbert graph and consider first-passage percolation as introduced above. We are interested in the behavior of $\mathcal{H}_t = \mathcal{H}_t(q(o))$, where $q(o)$ is the closest point of the origin in the unique infinitely large connected component $\mathcal{C}$. The version of first-passage percolation in which the passage times are i.i.d. exponential random variables with parameter $\rho > 0$ is called the *Richardson model* (on the Poisson–Gilbert graph), and we write $\mathcal{H}_t^{\lambda,\rho}$ to indicate both, the intensity λ of the underlying Poisson point process as well as the parameter ρ. Our first result from [1] establishes weak convergence of the paths $\mathcal{H}_{[0,t]}^{\alpha\lambda,\rho/\alpha}$ (with respect to the

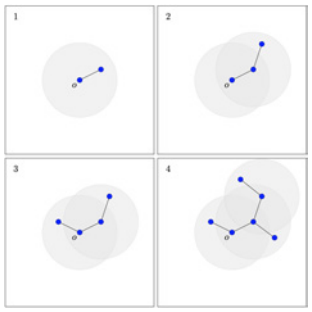


Fig. 7: *Illustration of $\mathcal{T}^{\lambda,\rho}$ at 4 increasing time steps. Gray disks indicate the area for possible offsprings.*

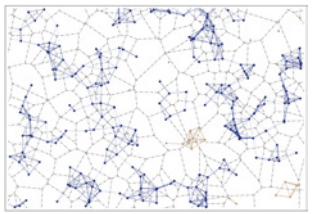


Fig. 8: *Realization of a Poisson–Voronoi tessellation with respect to the large connected component of a Poisson–Gilbert graph*

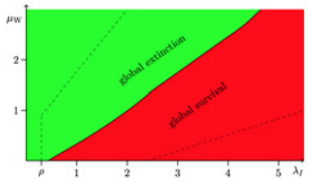


Fig. 9: *Phase diagram for global survival and extinction based on the infection rate λ_I and the white-knight intensity μ_W. The solid line is based on simulations, and the dashed lines indicate rigorous bounds. The constant ρ represents a threshold below which any positive white-knight intensity suffices to eliminate the malware on infinite clusters.*

Skorokhod topology based on the vague topology) towards a limiting branching process $\mathcal{T}^{\lambda,\rho}_{[0,t]}$, in the limit as α tends to infinity. This can be seen as high-density limit for devices with slow transitions. The limiting process $\mathcal{T}^{\lambda,\rho}_{[0,t]}$ has an initial device at the origin and then iteratively produces offsprings after independent exponential waiting times with parameter $|B_r(o)|\lambda\rho$. Here, the offsprings are uniformly distributed in the ball with radius r centered at the parent device; see Figure 7 for an illustration.

The main result in [1] is a *shape theorem* for $H_t = \bigcup_{x\in\mathcal{H}_t} V(x,\mathcal{C})$, the union of *Voronoi cells* $V(x,\mathcal{C})$ associated with points in $\mathcal{H}_t$, taken with respect to the infinite cluster $\mathcal{C}$; see Figure 8 for an illustration. The shape theorem can be understood as a spatial strong law of large numbers, i.e., almost surely,

$$\lim_{t\uparrow\infty} \frac{1}{t} H_t = B_\phi(o),$$

where $0 < \phi < \infty$ is a nontrivial speed constant. In words, the set of space points that are closest to a device that is reached at a time t by a message initially placed close to the origin, approaches a ball with radius given by $t\phi$. Note that, in order to avoid percolation already at time zero, it suffices to require that $\mathbb{P}(\tau = 0) < (\lambda|B_r(o)|)^{-1}$, the inverse of the expected degree of a typical node in the Poisson–Gilbert graph. On the other hand, in order to control fluctuations, we also have to assume that $\mathbb{E}[\tau^\eta] < \infty$ for some $\eta > 2d + 2$, but otherwise the distribution of τ is arbitrary; however, note that it influences the speed ϕ. The main ingredients in the proof are a good control on the length of shortest paths in the graph and subadditivity arguments.

Let us finally report also on results for the propagation of malware in the supercritical Poisson–Gilbert graph (and more refined *Cox–Gilbert graphs*, i.e., Poisson–Gilbert graphs in random environments) in the presence of a counter-measure, as presented in [2, 3]. We consider the Richardson model on the Poisson–Gilbert graph in which a typical device carries a malware at initial time. In addition to regular susceptible devices, at initial time, there is also an independent Poisson point process of special devices called *white knights* in the system. Now, white knights carry a patch that eliminates the malware, but this patch can only be transferred to devices that are infected (due to privacy regulations) and not to susceptible devices. Once patched, the device also becomes a white knight and, on the long-term run, we observe a competition between an escaping malware spreading and a chasing patch. Allowing for different transmission rates for the malware and the patch, we see various behavioral regimes depending on four parameters, the different rates and different initial intensities of susceptible devices and white knights. Our main findings in [2] (based on rigorous arguments) and in [3] (mainly based on simulations) concern phase transitions of global and local survival and extinction of the malware as exemplified in Figure 9. In a nutshell, sufficiently large white-knight intensities or patching rates lead to global extinction of the malware, whereas sufficiently large intensities of susceptible devices or infection rates guarantee positive probabilities of a global survival of the malware.

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1.2 Optimization and Uniform Point Sets on the Sphere

Holger Heitsch and René Henrion

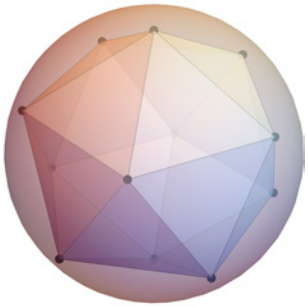

Fig. 1: *Icosahedron inscribed to a sphere such that its 12 vertices yield perfectly uniformly distributed points*

How to distribute points uniformly on a sphere may be considered as a question of mathematical interest even without having in mind any concrete application. A first idea could be related to perfectly regular point constellations as defined by the five platonic solids; see Figure 1. This idea, however, is limited to just a few number of points (4, 6, 8, 12, and 20), moreover, restricted to the classical two-dimensional sphere $\mathbb{S}^2$ in three-dimensional space. On the other hand, large samples of uniformly distributed points on spheres $\mathbb{S}^d$ of arbitrary dimension d (see Figure 2) are important in many problems of physics, chemistry, climate science, engineering and, not to the least, mathematics itself. The starting point for finding uniform point sets on the sphere is to define a criterion measuring uniformity. Such criterion is by no means uniquely defined and so, different criteria would produce different optimal point sets. Two prominent representatives are

$$\varphi_1(X) := \min_{1\le i<j\le N} \|x_i - x_j\|; \quad \varphi_2(X) := \sum_{i,j=1,\dots N, i\neq j} \frac{1}{\|x_i - x_j\|},$$

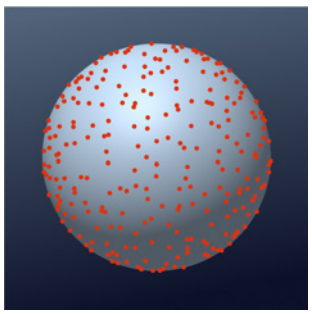

Fig. 2: *Low-discrepancy point set on the sphere*

where $X = \{x_1, \dots, x_N\}$ is a given set of points in $\mathbb{S}^d$. The first criterion measures the minimum pairwise distance of points, which increases with uniformity, while the second criterion is essentially the *Coulomb potential energy*. The latter is minimized by electrons located on the sphere and repulsing each other so that the result is a uniform constellation. In both cases, the relation with optimization is clear, the first criterion has to be maximized, the second one to be minimized over all point sets X on the sphere. The focus here shall be shifted to another measure of uniformity, the so-called *spherical cap discrepancy*, which plays an important role in bounding the integration error of spherical integrals (e.g., approximation of the global mean surface temperature on earth by an average of temperatures measured at finitely many points). Such integrals are important in optimization problems with probabilistic constraints, so that optimization benefits from point sets uniformly distributed on the sphere. On the other hand, contrary to φ_1 and φ_2, the discrepancy criterion is not directly computable by an explicit formula. It has been primarily used so far in the context of theoretical estimates, but not for direct evaluation of concrete samples. It is here that optimization in turn can help to provide an enumerative formula for numerical purposes. Both aspects of connecting optimization with uniform point sets on the sphere will be illustrated in the following.

The spherical cap discrepancy

While the criteria φ_1 and φ_2 mentioned above are based on geometrical or physical intuition about uniformity, the spherical cap discrepancy is related to probability measures by comparing the empirical distribution generated by the given point set with the uniform distribution (normalized surface measure) of $\mathbb{S}^d$. More precisely, for a fairly uniformly distributed collection of points it should hold true that for every hyperplane cutting the sphere, the relative share of points falling

into either of the two arising *spherical caps* is close to the surface measure of the respective cap divided by the surface measure of the whole sphere. In order to specify one out of the two possible caps, one defines a spherical cap as the intersection $\mathbb{S}^d \cap H(w,t)$ of the sphere with the closed half-space

$$H(w,t) := \{x \mid \langle w, x\rangle \geq t\} \quad (w \in \mathbb{S}^d,\ t \in [0,1]),$$

which is generated by a normal vector w and a level t. Figure 3 illustrates some spherical caps for $\mathbb{S}^1$ and $\mathbb{S}^2$.

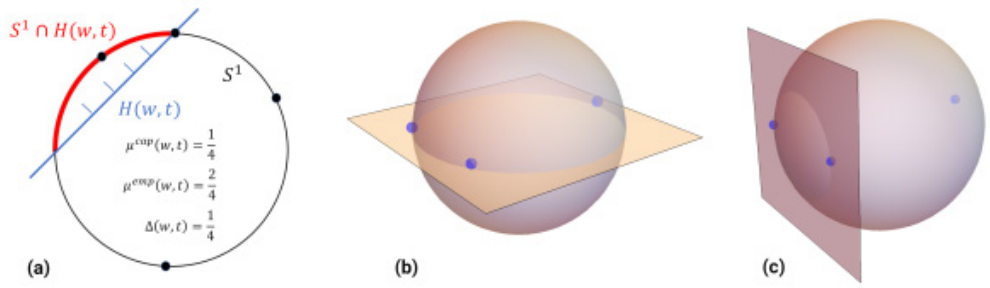

Fig. 3: *Some spherical caps for $\mathbb{S}^1$ and $\mathbb{S}^2$*

In this way, the family of spherical caps can be parameterized by $(w,t) \in \mathbb{S}^d \times [0,1]$, and each such cap can be assigned a *local discrepancy* $\Delta(w,t) := |\mu^{emp}(w,t) - \mu^{cap}(w,t)|$. Here, μ^{emp} is the empirical measure induced by the given point set on the sphere (counting the ratio of points inside the spherical cap or just inside the closed half-space), while μ^{cap} refers to the normalized surface measure providing the ratio between the area of the cap and that of the whole sphere; see Figure 3 (a) for an illustration of these notions. Both quantities, and, hence, $\Delta(w,t)$ are easy to determine. The overall (global) discrepancy between empirical and uniform distribution then results as the largest (supremum) of all the local discrepancies:

$$\Delta := \sup_{w \in \mathbb{S}^d, t \in [0,1]} \Delta(w,t).$$

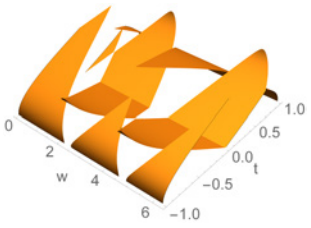

Fig. 4: *Local discrepancy for two points on $\mathbb{S}^1 \sim [0, 2\pi]$*

Unfortunately, $\Delta(w,t)$ is a highly irregular function (see Figure 4) and so, determining its largest value by applying some numerical optimization seems out of hope, much less a direct formula is evident. It is not even clear whether the supremum in the definition of Δ is attained, i.e., whether there exists some concrete spherical cap realizing this value. Indeed, despite the compactness of the set $\mathbb{S}^d \times [0,1]$, the application of the classical Weierstrass theorem fails due to $\Delta(w,t)$ not being upper semicontinuous. Nonetheless, one may show by independent arguments ([4, Prop. 1]) that there does exist a spherical cap realizing the largest value, i.e., $\Delta = \Delta(w^*,t^*)$ for some $(w^*,t^*) \in \mathbb{S}^d \times [0,1]$. Moreover, the boundary of the half-space $H(w^*,t^*)$ associated with this critical cap must contain at least one point of the given set, i.e., $\langle w^*, x^i\rangle = t^*$ for some $i \in \{1,\dots,N\}$. The computation of the global discrepancy drastically simplifies in the special case of the one-dimensional sphere $\mathbb{S}^1$ (circle). We already know that the straight line associated with the critical cap contains at least one point. If it does not contain any other point, then it has to be tangent to the circle because otherwise – after turning the straight line a bit while keeping the point on it – the discrepancy could be locally increased by locally increasing or decreasing μ^{cap} without changing μ^{emp} (see Figure 3 (a)). However, the larger of the two discrepancies defined by

a tangent through one point equals $1/N$, whereas the larger of the two discrepancies defined by a straight line passing through the two closest points on the circle is easily seen to be at least 1/N. Hence, there always exists a critical cap on $\mathbb{S}^1$ associated with a straight line passing through two distinct points. This fact allows one to enumerate the finite number of local discrepancies defined by couples of points in order to find the global discrepancy as their maximum value. Unfortunately, the idea of finding the critical cap as being defined among the finitely many hyperplanes related to maximal affinely independent subsets of $\{x_1, \dots, x_N\}$ fails for higher-dimensional spheres. This can be seen from Figure 3 (b), where a set of three points on the equator of $\mathbb{S}^2$ is given. The hyperplane passing through these points defines two spherical caps, each of which has local discrepancy $1/2$. On the other hand, the hyperplane passing through the two points on the left-hand side (see Figure 3 (c)) defines, in particular, a small cap to the left whose local discrepancy tends to $2/3$ when the two points converge to the "left pole" along the equator, whereas the previous hyperplane would still have local discrepancy $1/2$. Hence, the maximum discrepancy may not be realized by a hyperplane passing through a subset of $\{x_1, \dots, x_N\}$ with a maximum number (here: three) of affinely independent points.

An enumerative formula for the spherical cap discrepancy

The last observation means that a hyperplane defining a spherical cap with maximum local discrepancy may not be fixed by the set of points x^i it contains. Hence, there may remain a degree of freedom that prevents the global discrepancy Δ from being calculated via straightforward enumeration. This degree of freedom may be removed, however, by an argument from optimization. An essential observation in this direction is that a spherical cap realizing the maximum discrepancy always has an empirical measure not smaller than its normalized surface measure ([4, Cor. 1]). This fact allows one to get rid of the absolute value appearing in the local discrepancies and to write now

$$\Delta := \max_{w\in\mathbb{S}^d, t\in[0,1]} \Delta(w,t) = \max_{w\in\mathbb{S}^d, t\in[0,1]} \mu^{emp}(w,t) - \mu^{cap}(w,t).$$

Here, we already exploited that the supremum in the original definition of Δ is actually a maximum. Now, assume that (w^*, t^*) defines a critical cap ($\Delta = \Delta(w^*, t^*)$) and denote by $I := \{i | \langle w^*, x^i\rangle = t^*\}$ the index set of points x^i located on the hyperplane associated with this cap. Clearly, (w^*, t^*) must be a solution to the maximization problem

$$\max_{w\in\mathbb{S}^d, t\in[0,1]} \mu^{emp}(w,t) - \mu^{cap}(w,t) \quad \text{subject to} \quad \langle w, x^i\rangle = t \quad (i \in I),$$

because (w^*, t^*) itself satisfies the constraints of this problem. Evidently, for (w,t) satisfying these constraints and being close to (w^*, t^*), no additional points may enter the hyperplane, which implies that $\mu^{emp}(w^*, t^*) = \mu^{emp}(w,t)$ (empirical measure locally constant). Therefore, (w^*, t^*) must be a *local* solution to the maximization problem just for the negative spherical measure:

$$\max_{w\in\mathbb{S}^d, t\in[0,1]} -\mu^{cap}(w,t) \quad \text{subject to} \quad \langle w, x^i\rangle = t \quad (i \in I).$$

Observing that the surface measure μ^{cap} just depends on t (not on w) and actually is monotonically decreasing in t, one concludes that (w^*, t^*) must be a *local* solution to the problem

$$\max_{w\in\mathbb{S}^d, t\in[0,1]} t \quad \text{subject to} \quad \langle w, x^i\rangle = t \quad (i \in I). \tag{*}$$

This optimization problem (see Figure 5) is simple enough to identify its solutions from the necessary optimality conditions. More precisely, denote by X_I the matrix whose columns are generated by x^i for $i \in I$ and by $\tilde{X}_I := \begin{pmatrix} X_I \\ -\mathbf{1}^T \end{pmatrix}$ the extended matrix with $\mathbf{1} := (1, \dots, 1)^T$. Without loss of generality, we may assume that $\operatorname{rank} \tilde{X}_I = \#I$. Then, the critical cap is characterized explicitly by ([4, Lemma 3])

$$t^* = \left(\frac{1-\gamma_I}{\gamma_I}\right)^{1/2}, \quad w^* = \frac{1+(t^*)^2}{t^*} X_I \left(\tilde{X}_I^T \tilde{X}_I\right)^{-1} \mathbf{1} \quad (\gamma_I := \mathbf{1}^T \left(\tilde{X}_I^T \tilde{X}_I\right)^{-1} \mathbf{1}).$$

One may show that $0 < \gamma_I \le 1$. Clearly, the solution above is not defined for $\gamma_I = 1$, which is equivalent to $t^* = 0$. This corresponds to a hyperplane passing through the origin or a cap that is a hemisphere. This case is technically more delicate to treat. For randomly generated point sets as in Figure 6, one will have $t^* \neq 0$ with probability one, but for constructed sets as in Figure 2, this degenerate case may be relevant as well. Altogether, we arrive at the following explicit enumerative formula for the spherical cap discrepancy Δ ([4, Th. 1]) for which a MATLAB implementation is available at https://www.wias-berlin.de/people/heitsch/capdiscrepancy.

Keeping the notation introduced above, define

$$\begin{aligned} \Phi_1 &:= \left\{ I \subseteq \{1, \dots, N\} \,\middle|\, 1 \le \operatorname{rank} \tilde{X}_I = \#I \le \min\left\{n, \operatorname{rank} \tilde{X}\right\};\ \gamma_I < 1 \right\}, \\ \Phi_0 &:= \left\{ I \subseteq \{1, \dots, N\} \,\middle|\, \operatorname{rank} \tilde{X}_I = \#I = \min\left\{n, \operatorname{rank} \tilde{X}\right\};\ \gamma_I = 1 \right\}, \end{aligned}$$

$$t_I := \begin{cases} \left(\frac{1-\gamma_I}{\gamma_I}\right)^{1/2} & I \in \Phi_1 \\ 0 & I \in \Phi_0 \end{cases}, \quad w_I := \begin{cases} \frac{1+t_I^2}{t_I} X_I \left(\tilde{X}_I^T \tilde{X}_I\right)^{-1} \mathbf{1} & I \in \Phi_1 \\ \in \operatorname{Ker} X_I^T \cap \mathbb{S}^{n-1} & I \in \Phi_0 \end{cases},$$

where the selection of w_I in case of $I \in \Phi_0$ is arbitrary. Then, $\Delta = \max\{\Delta_1, \Delta_0\}$, where

$$\Delta_1 := \max_{I\in\Phi_1} \Delta(w_I, t_I), \quad \Delta_0 := \max_{I\in\Phi_0} \max\{\Delta(w_I, 0), \Delta(-w_I, 0)\}.$$

The formula may be exploited now in order to evaluate and compare point sets on spheres with respect to their uniformity. Figure 7 shows normalized Monte Carlo and quasi-Monte Carlo samples of a Gaussian distribution with independent components (yielding a uniform distribution on the sphere) as well as a low-discrepancy sequence using the Lambert transformation [2] on $\mathbb{S}^2$. Figure 8 plots the true discrepancies and a simple lower bound used in [2, p. 1005] for randomly generated samples on $\mathbb{S}^4$.

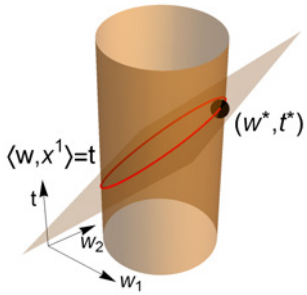

Fig. 5: *Optimization problem (*) in a trivial constellation ($\mathbb{S}^1$, $I = \{1\}$, $x^1 = (1, 0)$). The red curve represents the feasible set.*

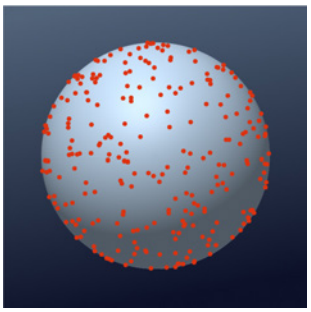

Fig. 6: *Set of randomly generated (Monte-Carlo) points on the sphere*

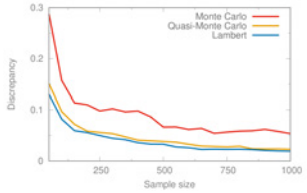

Fig. 7: *Discrepancies as functions of the sample size for three sampling methods on $\mathbb{S}^2$*

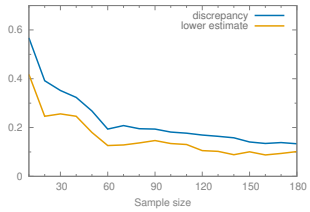

Fig. 8: *True discrepancies and simple lower estimates for randomly generated samples as functions of the sample size on* $\mathbb{S}^4$

Optimization under probabilistic constraints

Efficient samples of the uniform distribution on the sphere are in turn essential for the solution of optimization problems subject to probabilistic constraints

$$\text{minimize } f(x) \text{ subject to } \varphi(x) := \mathbb{P}(g_i(x,\xi) \geq 0 \ (i \in I)) \geq p, \qquad (**)$$

where x is a finite- or infinite-dimensional decision, f is some cost function, ξ is a random vector, and g represents some finite or infinite inequality system. Under such constraint, a decision x is declared to be feasible if the random inequality system is satisfied at least with a probability p. The essential ingredient of such optimization problems is the probability function φ whose values and gradients – needed in any numerical solution approach – are not given explicitly, but have to be approximated. In the case that ξ has an elliptically symmetric distribution, the probability can be represented as a spherical integral that promises a significant reduction of variance for the resulting estimate when compared to sampling "in space." For instance, if $\xi \sim \mathcal{N}(\mu, \Sigma)$ has a $d-$ dimensional normal distribution, then

$$\varphi(x) = \int_{\mathbb{S}^{d-1}} \alpha(z) d\nu^U(z); \quad \alpha(z) := \nu^\chi\{r \geq 0 \mid g_i(x, \mu + rLz) \geq 0 \ (i \in I)\},$$

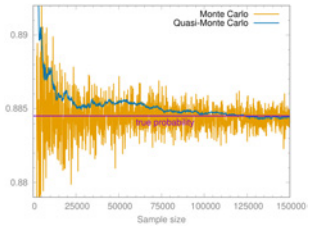

Fig. 9: *Probability estimated according to (***) (d=36) by Monte Carlo (Mersenne Twister) and quasi-Monte Carlo*

where $LL^T = \Sigma$, ν^U is the uniform distribution on $\mathbb{S}^{d-1}$, and ν^χ is the one-dimensional Chi-distribution with d degrees of freedom. Under suitable conditions on g (growth conditions, constraint qualifications), α can be shown to be differentiable [1], so that $\nabla\phi$ is obtained as a spherical integral as well by differentiating under the integral. For numerical purposes the spherical integral is approximated by the average over a finite number of points uniformly sampled over the sphere:

$$\varphi(x) \approx N^{-1} \sum_{i=1}^{N} \alpha(z^i) \quad (z^i \in \mathbb{S}^{d-1}). \qquad (***)$$

It is here that the mentioned relation between the spherical cap discrepancy and the integration error for spherical integrals comes into play (in particular, the latter tends to zero if the former does so). As a consequence, the difference in discrepancy between Monte Carlo and quasi-Monte Carlo sampling, which is visible in Figure 7, reflects also in the goodness of estimations of probabilities (and their gradients) as supported by Figure 9. Optimization problems with probabilistic constraints like (**) find a lot of applications in engineering, economics, power management, telecommunications, and other fields. Figures 10 and 11 illustrate two instances from optimal control under uncertainty. In the first application, an optimal Neumann boundary control of the vibrating string is considered under random initial conditions (random Fourier coefficients for initial position of the string) [3]. The aim is to find a cost-minimal control driving the terminal energy of the string close to zero (smaller than a given tolerance) with given probability.

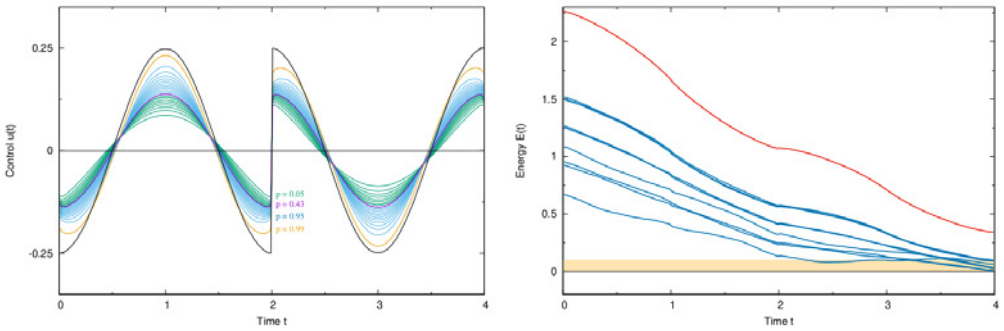

Fig. 10: Optimal control of the vibrating string under random initial condition and probabilistic constraint for terminal energy. The figure shows the optimal control functions (left) for different required probabilities $p \in (0,1)$ and the energy as function of time for $p = 0.9$ for ten generated scenarios of the initial condition (one instance not reaching the required small terminal energy).

The second application is the capacity maximization problem in gas networks under random loads. The network owner aims at documenting additional free capacity of the network for serving potential new clients under the constraint that the loads of new clients (arbitrary up to free capacity) plus the random loads of current clients (distribution estimated from historical data) can be served physically (here: respecting a lower pressure bound in pipes) with given high probability.

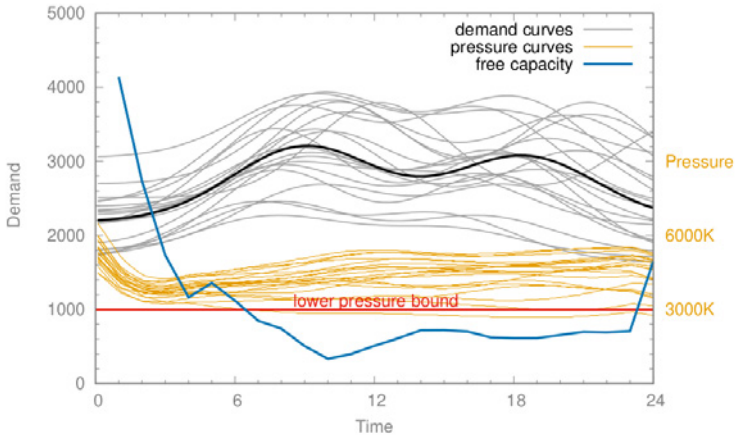

Fig. 11: Maximization of free capacity in gas networks. Mean (black) and simulated scenarios (gray) for load profiles of current clients. Resulting scenarios for pressure (yellow), most of which satisfy the lower bound.

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1.3 Multi-scale Chemical Reaction Systems

Artur Stephan

The mathematical description of complex processes in nature involves many challenging difficulties. These result from the fact that mathematical models are governed by the trade-off between accuracy and simplicity. A more accurate description, e.g., involving more physical states, provides richer information about the physical problem, which is desirable for a detailed understanding of the physical process. In contrast, a precise description involves many challenges affecting all branches of applied mathematics, namely modeling, analysis, and simulation: First, the validation of an applicable model requires precise measurements that become practically impossible if the state space is too large. Second, the analytic difficulties grow when increasing the complexity of the problem. Thirdly, good numerical algorithms may become too costly if the number of parameters and dimensions increases.

A procedure that reduces the complexity of a system is often called *coarse-graining*. It is a prominent research topic in all areas of natural sciences. These reductions or approximations are often physically motivated by scale separations of the problem and have the aim to derive an effective model that respects and reflects the most prominent features of the system. On different temporal or spatial scales, different processes may govern the physical system, resulting in different levels of description. The derivation of effective systems by reducing a system involving multiple scales to a smaller system with fewer scales, for example, only one distinguished scale, is an important task in applied mathematics and a prominent research area at WIAS. Usually, reductions are made on the level of the physical states. However, in recent years, it became more and more apparent that the intrinsic physical nature cannot be described by the physical states only. Desirably and as explained in the Annual Research Report of WIAS of 2014, a complete coarse-graining procedure should also take the global physical principles into account. Such a structural reduction procedure has many different advantages. First, the derived effective model automatically satisfies the desired physical principles, such as energy conservation and monotonicity of entropy production. Often, the additional information helps in the mathematical analysis of the equations. Moreover, errors in computer-based simulations may be reduced by preserving the physical structure.

Recently, theoretical progress was made for coarse-graining of multi-scale chemical reaction systems. Chemical reactions describe the transformation of species, molecules, or substances. Reaction systems are inevitable in modeling processes in biology, chemistry, physics, as well as social sciences, and economics. In many applications, the number of chemical species can be huge, and the reaction coefficients for the chemical reactions may vary in a large range. In such cases, not only the measurement of all necessary physical quantities, but also analytical or numerical treatment is out of reach. A natural simplification is made by the assumption that reactions can happen with different and distinguished magnitudes of speed. We will consider the case that slow and fast reactions are distinguished, namely the slow ones of order 1 and the fast ones of order $1/\varepsilon$ for a small parameter $\varepsilon > 0$. There are many instances for this kind of assumption in literature. As a biochemical example, we mention an mRNA-DNA system that can be modeled by a slow-fast reaction system (see Figure 1). There, proteins (monomers), synthesized by transcription of a gene, dimerize. Afterwards, they may bind to the gene. Dimerization is a fast reaction, as compared to

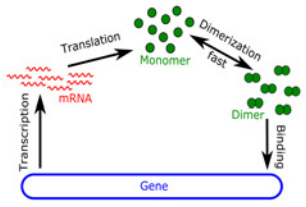

Fig. 1: *A simple model that describes the transcriptional regulatory system in gene production*

transcription, translation, mRNA and protein degradation, and protein binding.

Gradient structures and EDP-convergence

To include the physical structure, we focus on variational structures that define a gradient flow. Physically, they describe a closed physical system that is close to thermodynamic equilibrium. They provide an important modeling framework enjoying many applications in continuum mechanics, semiconductor physics, and also chemical processes. Gradient flows describe an evolution in the direction of the steepest descent of a driving functional, which is often given by the energy or entropy. Mathematically, gradient flow equations are evolution equations that are induced by a so-called *gradient system* $(Q, \mathcal{E}, \mathcal{R}^*)$, consisting of a state space Q (a subspace of a Banach space X), a driving (or energy) functional $\mathcal{E}$, and a geometric or dissipative structure in the form of a dissipation potential $\mathcal{R}$ that describes the geometry of the underlying state space Q (see [2]). Here, $\mathcal{R}$ is called a *dissipation potential* if $\mathcal{R}(q,\cdot) : X \to [0,\infty]$ is lower semicontinuous, convex, and satisfies $\mathcal{R}(q,0) = 0$. Then, $\mathcal{R}^*$ is the (partial) Legendre–Fenchel transform given by $\mathcal{R}^*(q,\xi) := \sup_{v\in X}\{\langle \xi, v\rangle - \mathcal{R}(q,v)\}$. The induced gradient flow equation is then defined by

$$\dot q = \mathrm{D}_\xi \mathcal{R}^*(q, -\mathrm{D}\mathcal{E}(q)) \quad \text{or equivalently} \quad 0 = \mathrm{D}_{\dot q}\mathcal{R}(q,\dot q) + \mathrm{D}\mathcal{E}(q). \tag{GFE}$$

The first equation is a rate equation in the state space $Q \subset X$. The second equation is a force balance, where the viscous force $\mathrm{D}_{\dot q}\mathcal{R}(q,\dot q)$ is balanced by the potential restoring force $-\mathrm{D}\mathcal{E}(q)$. Another equivalent formulation of the gradient flow equation (GFE) plays an important role. Introducing the total dissipation functional (also called the *De Giorgi functional*)

$$\mathfrak{D}(q) = \int_0^T \mathcal{R}(q,\dot q) + \mathcal{R}^*(q, -\mathrm{D}\mathcal{E}(q))\,\mathrm{d}t,$$

the gradient flow evolution can equivalently be described by the so-called *energy-dissipation balance*

$$\mathcal{E}(q(T)) + \mathfrak{D}(q) = \mathcal{E}(q(0)).$$

This energy-dissipation balance compares the energy at initial time $t = 0$ with the energy at final time $t = T$. The difference is given by the total dissipation functional $\mathfrak{D}(q)$, which has a particular form, consisting of the two terms $\mathcal{R}$ and $\mathcal{R}^*$. The energy-dissipation balance is a suitable starting point for multi-scale problems using Γ-convergence methods.

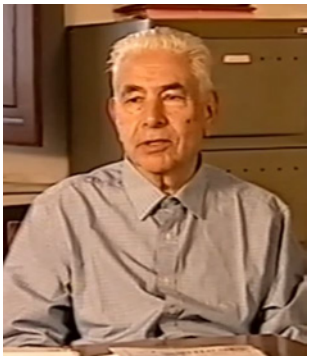

Fig. 2: *Italian mathematician Ennio De Giorgi during an interview in 1996, SNS Channel Mathematical and Natural Sciences, CC BY 3.0*

For families of gradient systems $(Q, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon^*)$, where $\varepsilon > 0$ is a small parameter featuring the multi-scale nature, a structural convergence, the so-called *EDP-convergence*, has been established in recent years [3]. Roughly speaking, EDP-convergence is defined by two Γ-convergences: for the energy functionals $\mathcal{E}_\varepsilon$, defined on the state space Q, and the dissipation functionals $\mathfrak{D}_\varepsilon$ given by

$$\mathfrak{D}_\varepsilon(q) = \int_0^T \mathcal{R}_\varepsilon(q,\dot q) + \mathcal{R}_\varepsilon^*(q, -\mathrm{D}\mathcal{E}_\varepsilon(q))\,\mathrm{d}t,$$

defined on the dynamic space of trajectories (in a suitable topology). The limit is again given by

$$\mathfrak{D}_0(q) = \int_0^T \mathcal{R}_{\mathrm{eff}}(q,\dot q) + \mathcal{R}_{\mathrm{eff}}^*(q, -\mathrm{D}\mathcal{E}_{\mathrm{eff}}(q))\,\mathrm{d}t.$$

The effective gradient system is, then, given by $(Q, \mathcal{E}_{\text{eff}}, \mathcal{R}^*_{\text{eff}})$. Physically, the convergence can be motivated from thermodynamics because it takes also fluctuations of solutions of the gradient flow equation (GFE) into account that have finite energy and dissipation.

An almost trivial consequence of EDP-convergence is that (under suitable technical assumptions) solutions with respect to the gradient system $(Q, \mathcal{E}_\varepsilon, \mathcal{R}^*_\varepsilon)$ converge to the solution of the effective gradient system $(Q, \mathcal{E}_{\text{eff}}, \mathcal{R}^*_{\text{eff}})$. The great advantage of EDP-convergence is that the limit gradient system is uniquely determined, and hence, the previously hidden physical principles of the effective evolution equation become evident; see Figure 3.

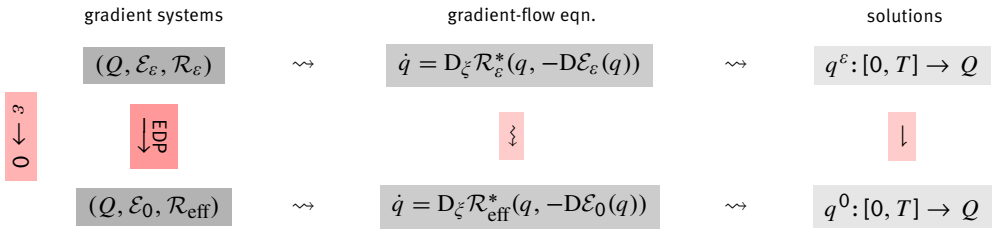

Fig. 3: *EDP-convergence leads to a commuting diagram. In particular, EDP-convergence generates the correct limit equation* $\dot q = \mathrm{D}_\xi \mathcal{R}^*_{\text{eff}}(q, -\mathrm{D}\mathcal{E}_0(q))$, *and the solutions* q^ε *converge to solutions* q^0 *of the limit equation. However,* $\mathcal{R}_{\text{eff}}$, *which is uniquely determined by EDP-convergence, provides information not contained in the limit equation.*

In this sense, EDP-convergence can be understood as a structural coarse-graining procedure that derives an effective system from a multi-scale system.

Fast-slow nonlinear reaction systems

In [4, 5, 6], the coarse-graining procedure was applied and extended to different fast-slow reaction and reaction-diffusion systems. We consider species X_i, $i \in I := \{1, \dots, i_*\}$, that undergo r_* forward-backward chemical reactions of mass-action type

$$\alpha_1^r X_1 + \cdots + \alpha_{i_*}^r X_{i_*} \quad \rightleftharpoons \quad \beta_1^r X_1 + \cdots + \beta_{i_*}^r X_{i_*}, \qquad r = 1, \dots, r_*,$$

where $\alpha^r = (\alpha_i^r)_{i\in I}$ and $\beta^r = (\beta_i^r)_{i\in I}$ are the stoichiometric vectors in $\mathbb{N}_0^{i_*}$. The fast-slow reaction-rate equation describing the evolution of densities $c \in \mathbf{C} = [0, \infty[^{i_*}$ of the species has the form

$$\dot c = \mathbf{R}_{\text{slow}}(c) + \frac{1}{\varepsilon}\mathbf{R}_{\text{fast}}(c) \text{ with } \mathbf{R}_{\text{xy}}(c) := -\sum_{r\in R_{\text{xy}}} \kappa_r \left(c_*^{\alpha^r} c_*^{\beta^r}\right)^{1/2} \left(\frac{c^{\alpha^r}}{c_*^{\alpha_r}} - \frac{c^{\beta^r}}{c_*^{\beta_r}}\right)(\alpha^r - \beta^r), \qquad \text{(RRE)}$$

for $\text{xy} \in \{\text{slow}, \text{fast}\}$, where $\kappa_r > 0$ are reaction rates, and $c_* = (c_i^*)_{i\in I} \in]0, \infty[^{i_*}$ is a positive concentration vector providing the detailed-balance equilibrium.

The fast-slow reaction-rate equation can be understood as a gradient flow equation of the cosh-type gradient structure $(\mathbf{C}, \mathcal{E}, \mathcal{R}^*_\varepsilon)$, where the ($\varepsilon$-independent) energy functional is the free energy

of Boltzmann type

$$\mathcal{E}(c) = \sum_{i=1}^{i_*} c_i^* E_{\mathrm{Bz}}(c_i/c_i^*), \quad E_{\mathrm{Bz}}(r) = r\log r - r + 1\,.$$

The dual dissipation potential $\mathcal{R}_\varepsilon^*$ consists of a slow part and a fast part and is given by

$$\mathcal{R}_\varepsilon^*(c,\xi) = \mathcal{R}_{\mathrm{slow}}^*(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}_{\mathrm{fast}}^*(c,\xi), \quad \mathcal{R}_{\mathrm{xy}}^*(c,\xi) = \sum_{r\in R_{\mathrm{xy}}} \kappa_r \big(c^{\alpha^r} c^{\beta^r}\big)^{1/2}\, \mathsf{C}^*\big((\alpha^r-\beta^r)\cdot\xi\big), \quad \text{(dDP)}$$

where the cosh function is given by $\mathsf{C}^*(r) = 4\cosh(r/2) - 4$. It follows that the reaction-rate equation (RRE) is indeed given by the gradient flow equation $\dot c = \mathrm{D}_\xi \mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c))$.

Heuristically, one expects that in the limit $\varepsilon \to 0$, an equilibration of the fast reactions occurs such that $\mathbf{R}_{\mathrm{fast}}(c(t)) \equiv 0$, which defines the slow manifold where the slow evolution takes place. This result can also be shown on the level of the gradient structure by proving EDP-convergence [4]. As it turns out, the gradient system $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon^*)$ converges to $(\mathbf{C}, \mathcal{E}_{\mathrm{eff}}, \mathcal{R}_{\mathrm{eff}}^*)$, where the effective gradient system is given by

$$\mathcal{E}_{\mathrm{eff}} = \mathcal{E}, \quad \mathcal{R}_{\mathrm{eff}}^* = \mathcal{R}_{\mathrm{slow}}^* + \chi_{\Gamma_{\mathrm{fast}}^\perp},$$

where $\chi_K(\xi) = 0$ for $\xi \in K$ and infinity, otherwise. The dissipation potential again consists of two parts: one part that captures the slow reactions and one part that restricts the evolution to the set of fast equilibria

$$\mathfrak{E}_{\mathrm{fast}} = \{c \in \mathbf{C} : \mathbf{R}_{\mathrm{fast}}(c) = 0\},$$

by forcing the chemical potentials to be transversal to the subspace of fast stoichiometric vectors $\Gamma_{\mathrm{fast}} = \mathrm{span}\{\alpha^r - \beta^r : r \text{ is fast}\}$. The important assumption is that the manifold of fast equilibria $\mathfrak{E}_{\mathrm{fast}}$ can be parametrized (by a function Ψ) in terms of adiabatic variables or, in other words, the conserved quantities of the fast reactions. These slow adiabatic variables are the natural variables of the coarse-grained systems and are given by $q \in \hat{\mathbf{C}} = Q_{\mathrm{fast}}\mathbf{C}$, where the matrix Q_{fast} satisfies $Q_{\mathrm{fast}}\Gamma_{\mathrm{fast}} = 0$. The effective system in its gradient structure can be equivalently expressed in these coarse-grained slow variables, where the state space is $\hat{\mathbf{C}} = Q_{\mathrm{fast}}\mathbf{C}$, and the energy functional and dissipation potential are given by

$$\hat{\mathcal{E}}(q) = \mathcal{E}(\Psi(q)), \quad \hat{\mathcal{R}}^*(q,\hat\xi) = \mathcal{R}_{\mathrm{slow}}^*(\Psi(q), Q_{\mathrm{fast}}^{\mathrm{T}}\hat\xi).$$

In particular, a new physical principle in terms of a yet undiscovered gradient structure is obtained because the coarse-grained driving functional is no longer of Boltzmann type. As an application, a structural reduction from two bimolecular chemical reactions to one trimolecular reaction can be performed; see Figure 4.

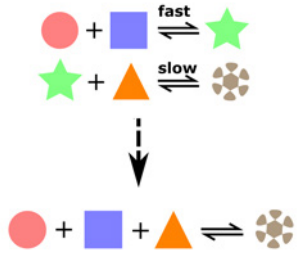

Fig. 4: *One fast and one slow bimolecular reaction coarse-grained to one trimolecular reaction*

Fast-slow linear reaction-diffusion system

Considering two species that, in addition to a fast linear reaction, also diffuse in a medium $\Omega \subset \mathbb{R}^d$, the evolution of their concentrations $c = (c_1, c_2)$ can be described by a linear reaction-

diffusion system (complemented by no-flux boundary conditions and initial conditions)

$$\dot{c_1} = \delta_1 \Delta c_1 - \frac{1}{\varepsilon}\left(\frac{c_1}{c_1^*} - \frac{c_2}{c_2^*}\right), \quad \dot{c_2} = \delta_2 \Delta c_2 + \frac{1}{\varepsilon}\left(\frac{c_1}{c_1^*} - \frac{c_2}{c_2^*}\right), \tag{RDS}$$

where $\delta_1, \delta_2 > 0$ are diffusion coefficients and $(c_1^*, c_2^*) > 0$ are the equilibrium concentrations, which define the reaction rates. These reaction-diffusion systems can again be written as a gradient-flow equation induced by a gradient system $(Q, \mathcal{E}, \mathcal{R}_\varepsilon^*)$, where the state space Q is now the infinite-dimensional manifold of probability measures $Q = \mathrm{Prob}(\Omega \times \{1,2\})$, and the driving functional is the free energy $\mathcal{E}(\mu) = \int_\Omega \sum_{j=1}^2 E_{\mathrm{Bz}}\left(\frac{c_j}{c_j^*}\right) c_j^* \,\mathrm{d}x$ for measures $\mu = c\,\mathrm{d}x$ and the stationary measure $c^* = (c_1^*, c_2^*)^{\mathrm{T}} \in Q$. Here, the dissipation potential $\mathcal{R}_\varepsilon^*$ is given by two parts $\mathcal{R}_\varepsilon^* = \mathcal{R}_{\mathrm{diff}}^* + \mathcal{R}_{\mathrm{react},\varepsilon}^*$, describing diffusion and reaction separately. The diffusion part $\mathcal{R}_{\mathrm{diff}}^*$ corresponds to the Wasserstein metric showing the connection to the theory of optimal transport. The reaction part $\mathcal{R}_{\mathrm{react},\varepsilon}^*$ is ε-dependent and defined by a straightforward generalization as in the space-independent situation (dDP). Together, they define a geometry on the space of probability measures that take transport and transformation into account. The reaction-diffusion system (RDS) can now formally be written as a gradient flow equation $\dot{\mu} = \mathrm{D}_\xi \mathcal{R}_\varepsilon^*(\mu, -\mathrm{D}\mathcal{E}(\mu))$.

In [5], EDP-convergence for the gradient systems was shown. In particular, the approach is robust to take also shifts (the so-called *tilts*) by a linear potential $V = (V_1, V_2)$ into account. On the level of the evolution equation, these additional energy shifts give rise to a linear reaction-drift diffusion system with space-dependent reaction coefficients

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \mathrm{div}\left(\begin{pmatrix} \delta_1 \nabla c_1 \\ \delta_2 \nabla c_2 \end{pmatrix} + \begin{pmatrix} \delta_1 c_1 \nabla V_1 \\ \delta_2 c_2 \nabla V_2 \end{pmatrix}\right) + \frac{1}{\varepsilon}\begin{pmatrix} -\frac{1}{c_1^*}\mathrm{e}^{\frac{V_1 - V_2}{2}} & \frac{1}{c_2^*}\mathrm{e}^{\frac{V_2 - V_1}{2}} \\ \frac{1}{c_1^*}\mathrm{e}^{\frac{V_1 - V_2}{2}} & -\frac{1}{c_2^*}\mathrm{e}^{\frac{V_2 - V_1}{2}} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$

where the new stationary solution is $c^{*,V} = (c_1^{*,V}, c_2^{*,V})$. In the potential-free situation (i.e. $V = \mathrm{const}$), we recover the reaction-diffusion system (RDS).

EDP-convergence provides an effective gradient system, where the effective dissipation potential consists again of two terms $\mathcal{R}_{\mathrm{eff}}^* = \mathcal{R}_{\mathrm{diff}}^* + \chi_{\{\xi_1 = \xi_2\}}$, where the first term describes the diffusion of the species, and the second term provides a coupling of the forces (or chemical potentials), which defines the linear slow manifold. Similar to the space-independent situation, the effective gradient system can also be equivalently described using coarse-grained slow variables $\hat{c} = c_1 + c_2$ such that $\Psi(\hat{c}) = (c_1, c_2)$, and the coarse-grained state space is given by $\hat{Q} = \mathrm{Prob}(\Omega)$. The coarse-grained energy functional and dissipation potential are defined by

$$\hat{\mathcal{R}}^*(\hat{\mu}, \hat{\xi}) = \frac{1}{2}\int_\Omega \hat{\delta}^V |\nabla \hat{\xi}|^2 \,\mathrm{d}\hat{\mu}, \qquad \hat{\mathcal{E}}(\hat{\mu}) = \int_\Omega \left(\log \hat{\mu} + \hat{V}\right) \mathrm{d}\hat{\mu},$$

where the mixed space-dependent diffusion coefficient and the mixed potential are given by

$$\hat{\delta}^V = \frac{\delta_1 c_1^{*,V} + \delta_2 c_2^{*,V}}{c_1^{*,V} + c_2^{*,V}}, \quad \hat{V} = -\log\left(c_1^* \mathrm{e}^{-V_1} + c_2^* \mathrm{e}^{-V_2}\right),$$

respectively. The coarse-grained evolution equation is a scalar drift-diffusion equation of the form

$$\dot{\hat{c}} = -\mathrm{div}\left(\hat{\delta}^V \hat{c}\,\nabla\left(-\frac{\delta\hat{\mathcal{E}}}{\delta\hat{\mu}}\right)\right) = \mathrm{div}\left(\hat{\delta}^V \nabla\hat{c} + \hat{\delta}^V \hat{c}\nabla\hat{V}\right).$$

In the potential-free case $V = \mathrm{const}$, we derive classical results for the PDE (partial differential equation) system [1]. In addition, EDP-convergence shows that the effective model can be derived in a consistent structural manner.

Conclusions and outlook

EDP-convergence provides a thermodynamical consistent way to derive effective gradient systems for multi-scale problems. Advantageously, the derived evolutionary systems satisfy the desired physical principles. Moreover, we have seen that previously unknown physical structures are uncovered. They provide theoretical insights in chemical reaction systems and, in this way, a better understanding of everyday chemical and biochemical processes. Mathematically, there are several interesting research directions. The geometry on the space of probability measures that is induced by a linear reaction diffusion system has to be explored. Moreover, the coupling to mechanical systems including explicit temperature dependence is interesting from the application point of view. Naturally, coarse-graining is connected to numerical simulations where continuous problems are approximated by discrete systems. Connection to discrete models will be further investigated in collaboration with the Collaborative Research Centre 1114 *Scaling Cascades in Complex Systems*, which also funded this research.

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1.4 Model-based Geometry Reconstruction of Quantum Dots from TEM

Anieza Maltsi, Thomas Koprucki, Karsten Tabelow, and Timo Streckenbach

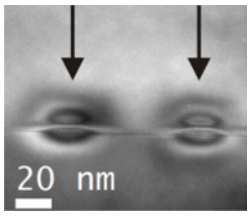

Fig. 1: *TEM image of InAs QDs recorded at TU Berlin showing a coffee-bean-like contrast*

The use of lenses to magnify the vision of objects dates back a couple of centuries. In the early seventeenth century the invention of the microscope really changed the way we may explore tiny objects that are otherwise not accessible to the human eye. Today, many areas of science and technology cannot be thought without different types of microscopes. While the first were based on light in the visible part of the spectrum and thus inherently limited in their spatial resolution due to the connection between the wavelength of the propagating waves and the minimal size of distinguishable objects, modern microscopes use other types of waves to image even tinier objects. One example is *transmission electron microscopy (TEM)* which uses the propagation of electron waves through magnetic lenses to create an image, see [1]. TEM allows imaging of the crystallographic structure of materials down to an atomic scale. As such, TEM has become an indispensable experimental tool to examine objects in life sciences or in material sciences at nanoscales. However, the creation of the image as well as its interpretation inherently require mathematical theory to solve the reconstruction problem for a single specimen and to allow for automated processing of bulks of them.

Model-based geometry reconstruction

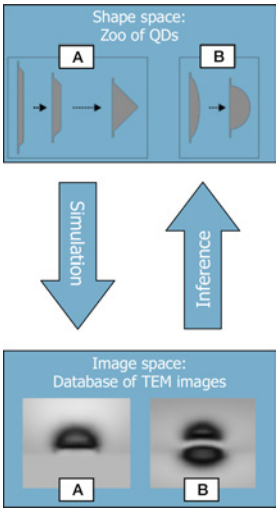

Fig. 2: *From shape space to image space by numerical simulation of TEM images and back by inference on the geometry of a single QD from a given TEM image*

Quantum dots (QD) are semiconductor nanostructures with interesting optoelectronic properties that are determined by their geometry and used in many different fields, such as lasers, quantum cryptography, and quantum metrology. The growth of semiconductor QDs with the desired electronic properties would highly benefit from an assessment of QD geometry, distribution, and strain profile in a feedback loop between epitaxial growth and analysis of their properties. In principle, TEM can be used to assist such an optimization loop of QDs. However, the reconstruction of the geometric properties of QDs from TEM images is a difficult problem due to the limited image resolution (0.5–1nm), the highly nonlinear behavior of the dynamic electron scattering, non-local effects due to strain, and strong stochastic influences resulting from uncertainties in the experiment. In contrast to what is common for images from light microscopy, for TEM imaging of QDs there is no simple one-to-one correspondence between the TEM image, which rather shows the so-called *coffee-bean contrast*, and the shape of the QD, see Figure 1 for an experimental example and Figure 2 for a simulated one.

Within the MATH+ project EF3-1 “Model-based geometry reconstruction from TEM images,” a novel concept was introduced for three-dimensional *model-based geometry reconstruction* (MBGR) of QDs from TEM imaging [2], see Figure 2: MBGR is based on a model for the QD configuration space that includes categorical variables, such as their shape (e.g., pyramidal or lense-shaped) and continuous parameters (e.g., size, height). By the numerical simulation of the imaging process, a database of simulated TEM images spanning the image space for a large number of possible QD configurations and image acquisition parameters can be generated. This simulated image space

can then be assigned to some explicit or implicit metrics and explored by means of statistical methodology, for example, by shape space methods, functional data analysis, or deep learning. Such methods can then be used for inferring the geometry of QDs from experimental TEM images. To realize the idea we combined expertise of the WIAS teams RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, RG 6 *Stochastic Algorithms and Nonparametric Statistics*, and of the *Electron Microscopy and Holography* work group of the *Institut für Optik und Atomare Physik* at Technische Universität Berlin. The work was funded by ECMath (OT7, 06/17–12/18) and MATH+ (EF3-1, 01/19–12/21).

Darwin–Howie–Whelan equations

For our first step in *model-based geometry reconstruction*, it is necessary to simulate TEM images by numerically solving the equations describing the electron propagation, namely the Darwin–Howie–Whelan (DHW) equations, see [4, Sec. 6.3]. The DHW equations can be derived from the Schrödinger equation

$$\Delta\Psi(\mathbf{r}) + (2\pi|\mathbf{k_0}|)^2\Psi(\mathbf{r}) = -4\pi^2 U(\mathbf{r})\Psi(\mathbf{r}), \tag{1}$$

where $\mathbf{k_0}$ is the wave vector of the monochromatic incoming beam, Ψ is the wave function of the electron beam propagating through the specimen, and U is the reduced electrostatic potential of the crystal, see [1]. For a perfect crystal, the specimen is described by a periodic lattice of atoms $\Lambda \subset \mathbb{R}^3$. We decomposed the spatial variable $\mathbf{r} = (x, y, z)$ into the transversal part (x, y) orthogonal to the thickness variable $z \in [0, z_*]$, see Figure 3.

The column approximation restricts the focus to solutions of (1) that are exactly periodic in (x, y) and are slow modulations in z of a highly-oscillatory function. This is due to the fact that in TEM the beam is formed by fast electrons with high energy, so they will not be scattered very far from the entrance point. Hence, we sought solutions in the form:

$$\Psi(\mathbf{r}) = \sum_{\mathbf{g}\in\Lambda^*} \psi_{\mathbf{g}}(z)\, e^{i\,2\pi\mathbf{k_0}\cdot\mathbf{r}}\, e^{i\,2\pi\mathbf{g}\cdot\mathbf{r}}, \tag{2}$$

where $\Lambda^* \subset \mathbb{R}^3$ denotes the dual lattice, and $\psi_{\mathbf{g}}$ are slowly varying envelope functions. Inserting the multi-beam ansatz (2) into (1), one obtains the DHW equations for infinitely many beams:

$$\frac{\rho_{\mathbf{g}}}{\pi}\frac{\mathrm{d}}{\mathrm{d}z}\psi_{\mathbf{g}}(z) = i\Big(\sigma_{\mathbf{g}}\psi_{\mathbf{g}}(z) + \sum_{\mathbf{h}\in\Lambda^*} U_{\mathbf{g}-\mathbf{h}}\psi_{\mathbf{h}}(z)\Big), \quad \psi_{\mathbf{g}}(0) = \delta_{0,\mathbf{g}}, \quad \text{for } \mathbf{g}\in\Lambda^*, \tag{3}$$

$$\text{where } \rho_{\mathbf{g}} = (\mathbf{k_0}+\mathbf{g})\cdot\nu \text{ and } \sigma_{\mathbf{g}} = |\mathbf{k_0}|^2 - |\mathbf{k_0}+\mathbf{g}|^2,$$

where $\nu = (0, 0, 1)^\top$ is the normal to the crystal surface and where $U_{\mathbf{g}}$ are the Fourier coefficients of the periodic potential U. This is an initial value problem for an infinite system of first-order ordinary differential equations describing the propagation of the electron beam through the specimen from $z = 0$ to the exit plane $z = z_*$. The incoming beam ($\mathbf{g} = 0$) is scattered in directions $\mathbf{k_0}+\mathbf{g}$.

One observation here is that the second derivative with respect to z has been dropped. This is due to the high energy of the electrons in the incoming beam. However, the coefficient of the first

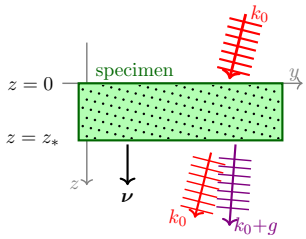

Fig. 3: *The incoming beam with wave vector $\mathbf{k_0}$ enters the specimen, is partially transmitted, and generates beams with nearby wave vectors $\mathbf{k_0}+\mathbf{g}$*

derivative $\rho_{\mathbf{g}}$ can change sign or even become 0 or arbitrarily close to 0 for some $\mathbf{g} \in \Lambda^*$. This means neglecting the second derivative for such $\mathbf{g}$'s makes the DHW equations (for *all* beams $\mathbf{g} \in \Lambda^*$) ill posed. Hence, the DHW equation (3) is only useful for a subset of beams $\mathbf{g}$ where $\rho_{\mathbf{g}}$ is close to $\rho_0 = \mathbf{k_0} \cdot \nu > 0$. The term ρ_0 corresponds to the incoming beam ($\mathbf{g} = 0$), which has to be included to satisfy the initial condition $\psi_{\mathbf{g}}(0) = \delta_{0,\mathbf{g}}$. But what do we mean by "close" and how many beams are needed to obtain a reliable approximation for the solution of the Schrödinger equation, in particular for high-energy electron beams?

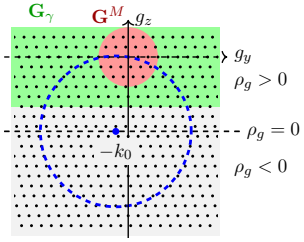

Fig. 4: *Dual lattice Λ^* (black dots) and admissible sets G_γ (green), G^M (red), and Ewald sphere (blue)*

We approached these questions by systematically investigating the dependence of the solutions $\psi^G = (\psi_{\mathbf{g}})_{\mathbf{g}\in G}$ on the chosen subset $G \subset \Lambda^*$ of the dual lattice. To do this, we first defined the subsets G that make the problem well posed. The condition to be satisfied is $\rho_0 > 0$, so that we can indeed drop the second derivative. For this, we introduced the set $G_\gamma := \{\mathbf{g} \in \Lambda^* \,|\, \rho_{\mathbf{g}} \geq \gamma \rho_0\}$ for $\gamma \in]0, 1[$, see Figure 4. On this set, the problem is well posed and it also satisfies the initial condition. Next, we defined the appropriate Hilbert space $\mathfrak{H}(G)$ and showed that the reduced DHW system for each $G \subset G_\gamma$ has a unique solution $\psi^G : \mathbb{R} \to \mathfrak{H}(G)$, see [3].

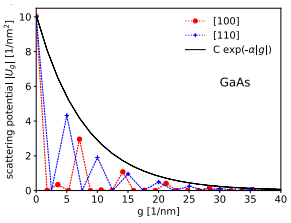

Fig. 5: *Fourier coefficients of the scattering potential for GaAs along different crystallographic directions (red, blue) showing an exponential decay (black)*

The set G_γ is still an infinite set. In numerical simulations of TEM images, only a finite number of beams $\mathbf{g}$ near the incoming beam $\mathbf{g} = 0$ is used, such as the two-beam or systematic row approximation, see [1, 2, 4]. We continued our investigation of the dependence of the solutions on finite subsets G of G_γ. For that purpose, we introduced the set $G^M := \{\mathbf{g} \in \Lambda^* \,|\, |\mathbf{g}| \leq M\}$, for $M > 0$, see Figure 4. This is important because the high-energy electrons are not scattered very far away from the incoming direction. We also assumed that the Fourier coefficients $U_{\mathbf{g}}$ of the scattering potential $\mathcal{U}$ decay exponentially:

$$|U_{\mathbf{g}}| \leq C_{\mathbb{U}}\, \mathrm{e}^{-\alpha_{\mathbb{U}}|\mathbf{g}|} \quad \text{for all } \mathbf{g} \in \Lambda^*. \tag{4}$$

This assumption is satisfied for a wide class of materials, see also Figure 5. Using these assumptions, we proved that the influence of the exact choice of the subsets G such that $G^M \subset G \subset G_\gamma$ is not important if we have enough modes around $\mathbf{g} = 0$. We provided explicit error bounds for the solutions in the finite subsets $G^M \subset G \subset G_\gamma$, which showed an exponential decay in dependence on the radius M.

We reduced the set of beams even further by restricting $\mathbf{g}$ into a neighborhood of the Ewald sphere

$$\mathbb{S}_{\mathrm{Ew}} := \{\mathbf{g} \in \mathbb{R}^3 \,|\, |\mathbf{k_0}|^2 - |\mathbf{k_0}+\mathbf{g}|^2 = 0\},$$

see Figure 4. Indeed, in TEM the incoming beam with wave vector $\mathbf{k_0}$ is chosen exactly in such a way that the intersection of the Ewald sphere $\mathbb{S}_{\mathrm{Ew}}$ with the dual lattice Λ^* contains, in addition to the incoming beam, a special number of other beams. An example is the so-called *Laue-zone approximation*, which is an approximation of a spherical cap of the Ewald sphere, see Figure 6. By using energy conservation, we provided error bounds for that choice. A similar error analysis was then carried out for both the two-beam and the systematic-row approximation, which are widely employed in TEM image simulation software such as PyTEM [5]. Finally, numerical simulations were done that underpin the quality of the error bounds and thus provide a justification of heuristic beam selection criteria often used in TEM simulation software. For more details on all the above-mentioned results; see [3].

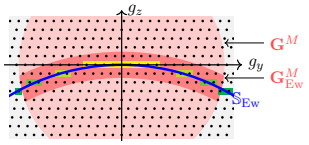

Fig. 6: *Ewald sphere (blue) and Laue zones from the lowest (yellow) to third order (green)*

Simulation of TEM images of QDs

In semiconductor nanostructures, such as QDs, the dynamical electron scattering as described above for perfect crystals, is additionally influenced by spatial variations in the material composition and by local deformations of the lattice due to elastic strain. In order to model the TEM images, we used elasticity theory to obtain the strain profile and coupled this profile with the DHW equations describing the electron propagation through the sample. We considered QDs composed of InGaAs inside a crystal matrix of GaAs, where the indium content is 80%. The influence of spatial variations in the indium content $c(\mathbf{r})$ and of the lattice deformations given by the displacement field $\mathbf{u}(\mathbf{r})$ can be approximated by the modification of the Fourier coefficients according to

$$U_{\mathbf{g}} \to U'_{\mathbf{g}}(\mathbf{r}) = \left[c(\mathbf{r})U_{\mathbf{g}}^{InAs} + (1 - c(\mathbf{r}))U_{\mathbf{g}}^{GaAs}\right] \times \exp(-2\pi i \mathbf{u}(\mathbf{r}) \cdot \mathbf{g}). \tag{5}$$

The projection of the displacement on the individual reciprocal lattice vector $\mathbf{g}$ enters the coupling as a phase factor. A simulated TEM image is created by propagating the beams through the specimen for every pixel (x_i, y_j), $i, j = 1, \ldots, N$. For the numerical simulation of the TEM images, the elasticity problem is solved with `WIAS-pdelib`, where we took as an input the geometry of the QD and computed the displacement field that enters the DHW-solver PyTEM [5], which computes the TEM image for the chosen excitation. An example of this toolchain for a pyramidal InGaAs QD and the influence of the excitation on the image contrast can be seen in Figure 7. For more details, see [2].

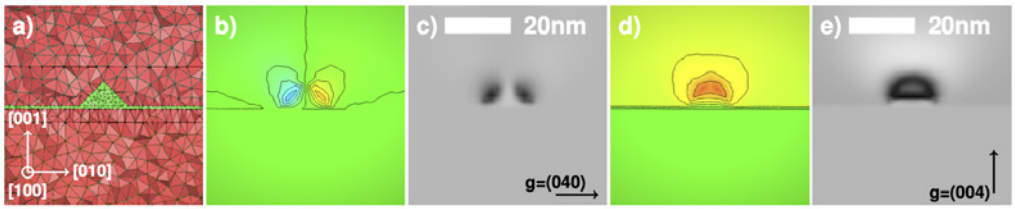

Fig. 7: *Simulation of TEM images: a) QD geometry, b) u_x component, and d) u_y component of displacement field. c) and e): corresponding TEM images for strong beam conditions.*

Database of TEM images of QDs

Using the toolchain described above, we generated a database of TEM images for initially two classes of geometries: pyramidal and lense-shaped QDs, see Figure 8. This database contains images for different QD geometry parameters (baselength, aspect-ratio, concentration, position) and excitation parameters (acceleration voltage, beam directions). A structured query language (SQL) database is used to store the metadata of the images including the actual values of the parameters, the numerical parameters controlling the solvers, and the file locations. The consistency of parameters and data across the toolchain is ensured by using portable metadata descriptions in JavaScript Object Notation (JSON).

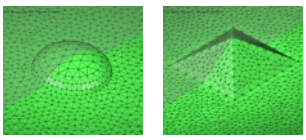

Fig. 8: *Three-dimensional geometry for lense-shaped and pyramidal QD*

Examples from the database are shown in Figure 9, where we have the TEM images for four geometries (flat and full lense-shaped, full and truncated pyramid) for two different excitations. An interesting first observation with the human eye by comparison with experimental data is that the

QD is lense shaped, while before it was considered to be a pyramidal one. For better and automated classification of QDs, we need methods like deep learning, which is an ongoing work in our project.

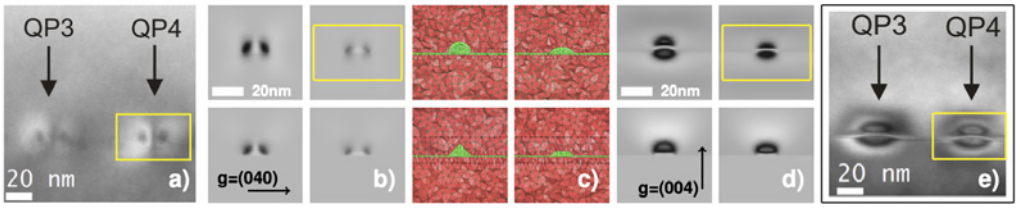

Fig. 9: *Comparison of experimental (a) and e)) and simulated (b) and d)) TEM images for geometries shown in c)*

Conclusions and outlook

We studied the mathematical structure of the DHW equations that led to a justification of heuristic beam selection criteria and explicit error bounds for different cases, including the widely used two-beam and systematic-row approximation, see [3]. The analysis is currently extended to the impact of strain in the system, which led to a mathematical underpinning of symmetries observed in TEM images; see, e.g., [6].

Together with Tore Niermann from Technische Universität Berlin, we developed a software for the simulation of TEM images for semiconductor QDs. Our toolchain was also applied to more general strained semiconductor nanostructures, as, for example, in [6] for quantum wells in tilted TEM lamellas. With this toolchain, we simulated a database of TEM images for different configurations, which will now be used for our last step in model-based geometry reconstruction, namely the classification of QDs and the analysis of the image space via methods like deep learning.

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1.5 Perovskite Models, Finite Volume Methods, and Painless Simulation

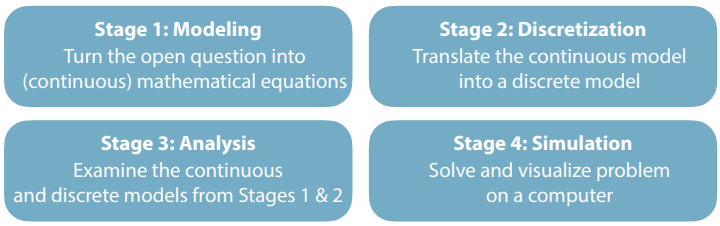
Dilara Abdel, Patricio Farrell, Jürgen Fuhrmann, and Petr Vágner

The four stages of turning crystal ions into math

In 2019, perovskite solar cells (PSCs) beat classical silicon solar cells. At least in terms of efficiency. With a sunlight-current conversion rate of over 25%, the novel PSCs can match the well-known light blue solar cells which cover roofs all over Germany. Although PSCs continue performing better and better, they do not last very long – the perovskite material degrades too fast. How can we improve PSC efficiency and simultaneously prevent their degradation?

Fig. 1: *A raw perovskite crystal named after the Russian mineralogist Lev Perovski (1792–1856)*
(c) K. Nash, CC-BY 3.0, wikipedia/Perowskit

Answering such a question – just as many other scientific open problems at the Weierstrass institute – involves at least four different stages, namely



Guided by this real-life question for perovskites as well as related charge transport problems, all four stages will be highlighted in the following article. But before we turn to the math, we will briefly explain the physical principles of semiconductors, solar cells, and PSCs.

In general, a semiconductor is a solid that conducts electric current better than an insulator but worse than a metal. The atoms in solids are densely packed, which creates a conduction band – a new space for electrons through which they can travel. Only the atom's outermost, valence electrons can enter the conduction band, and only if they are given an additional energy – the so-called *band-gap energy*. In the case of metals, the band-gap energy is negligible, whereas it is considerably large for insulators. The band gap of semiconductors lies between the two. Hence, where can an electron in a semiconductor get the energy to enter the conduction band? There are three main sources of energy: thermal, mechanical, and radiative. We will focus on a particular source of the radiation – photons emitted by the sun, summarized in a generation process denoted by G_{ph}.

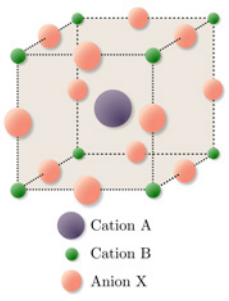


Fig. 2: *Perovskite ideal unit cell ABX_3. It consists of two cations A and B as well as an anion X; see [2]*

Roughly speaking, the core of a PSC consists of three parts: positively-doped semiconductor, perovskite, and negatively-doped semiconductor; see Figure 3. The doping in the semiconductors – artificially implanted positive or negative ions – alters the preference for holes and electrons. Therefore, the positively-doped semiconductor attracts electrons, whereas the negatively-doped semiconductor attracts holes. In between them, the perovskite, being also a semiconductor, generates the conduction electrons and valence holes. However, on top of those electrons and holes,

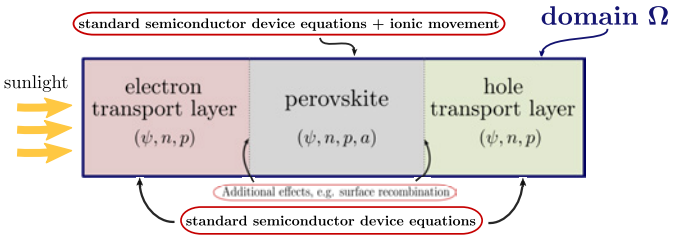


Fig. 3: *A three-layer device with the relevant charge carrier densities per area (n for electrons, p for holes, and a for anion vacancies) as well as the electric potential ψ*

the perovskite also contains charged vacancies, which are not fixed to the crystalline lattice, but migrate and affect the transport of the electrons and holes.

Perovskites form a class of crystalline solids with two cations and an anion – positively and negatively charged ions. Their idealized structure, visualized in Figure 2, is equivalent to the structure of a mineral with the same name discovered in the late 19th century. In reality, crystal defects occur that dynamically appear and reappear. They leave void spaces, called *vacancies*, within the crystal. For example, an ion next to a defect-caused vacancy can take advantage of the void space and occupy it, leaving a vacancy in its formerly occupied place. Even though the perovskites are solids, their microscopic behavior is similar to quicksands. This permanently changing crystalline structure affects the conduction electrons and valence holes like a dynamic doping, and it is not enough to consider only electrons and holes as carriers of charge. In perovskites, especially the movement of negatively charged anions influences the transport of charge that needs to be likewise captured by the model. We start with Stage 1 by turning the movement of crystal ions into mathematics.

Charge transport models for perovskites

Stage 1: Modeling

The interaction of electrons, holes, and electric potential in a semiconductor can be described by a system of partial differential equations introduced by van Roosbroeck in 1950; see [1]. We use this model to describe the doped transport layers; see Figure 3. As exposed in the Introduction, within PSCs, the moving anions in the perovskite influence the device behavior. To capture this influence, we describe the movement of anion vacancies – resulting in electrons n, holes p, and anion vacancies a as charge carriers. Their densities are denoted by n_α, $\alpha = n, p, a$. Within the perovskite layer, the semiconductor device equations (1a)–(1c) are extended by an additional equation (1d):

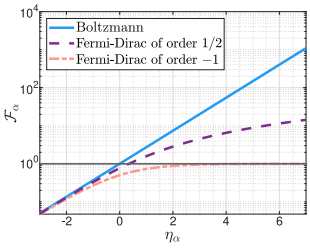


Fig. 4: *Statistics functions*

$$-\nabla \cdot (\varepsilon_s \nabla \psi) = q\Big(n_p - n_n + n_a - C\Big), \tag{1a}$$

$$\partial_t n_n - \frac{1}{q}\nabla \cdot \mathbf{j}_n = G_{\text{ph}} - R(n_n, n_p), \tag{1b}$$

$$\partial_t n_p + \frac{1}{q}\nabla \cdot \mathbf{j}_p = G_{\text{ph}} - R(n_n, n_p), \tag{1c}$$

$$\partial_t n_a + \frac{1}{q}\nabla \cdot \mathbf{j}_a = 0, \tag{1d}$$

$$\mathbf{j}_\alpha = -q z_\alpha \Big(D_\alpha \nabla n_\alpha + z_\alpha \mu_\alpha n_\alpha \nabla \psi\Big), \tag{1e}$$

where ε_s denotes the dielectric permittivity, q the elementary charge, and C a background charge due to cation vacancies of the perovskite. The right-hand sides of (1b), (1c) are given by a generation G_{ph}, portraying the illumination by the sun, and present recombination processes summarized in R. Within the electric current $\mathbf{j}_\alpha$, we have the charge number z_α, the diffusion coefficient D_α, and the mobility μ_α. The density of charge carriers can be related to the chemical potential η_α via [1]

$$n_\alpha = N_\alpha \mathcal{F}_\alpha(\eta_\alpha), \quad \alpha = n, p, a,$$

where N_α denotes the effective density of states, and $\mathcal{F}_\alpha$ a so-called *statistics function*. In many cases, we can choose the Fermi–Dirac integral of order one-half $F_{1/2}(\eta) = \frac{2}{\pi}\int_0^\infty \frac{\xi^{\frac{1}{2}}}{\exp(\xi-\eta)+1} d\xi$ for electrons and holes. As opposed to $F_{1/2}$ and its usual Boltzmann approximation $F_{\frac{1}{2}}(\eta) \approx \exp(\eta)$ valid for small η, the statistics function $F_{-1}(\eta) = \frac{1}{\exp(-\eta)+1}$ is always less than one; see Figure 4. Thus, it is well suited to the limited maximum concentration of the anion vacancies in perovskites.

As an extension, the charge transport model can be supplemented with further surface effects taking place between two different materials; see Figure 3.

Physics-preserving finite volume discretization

Stages 2 & 3: Discret. & Analysis

The continuous model (1) is analytically tractable only in special, simplified cases. Therefore, to simulate a realistic PSC, (1) will be approximated with a system of ordinary differential equations (ODEs), which we further solve using a computer. In particular, the ODEs are generated using the finite volume method [1] so that the system preserves physical properties of the PSC model. This method subdivides a computational domain $\Omega \subset \mathbb{R}^d, d = 1, 2, 3$, into a finite number N of control volumes ω_K, each associated with a node $\mathbf{x}_K \in \omega_K$; see Figure 5. For a given physical quantity, like, e.g., the electron density n_n, we use $n_{n,K}$, $n_{n,L}$, to denote its value at node $\mathbf{x}_K$, $\mathbf{x}_L$, respectively.

Furthermore, the system of partial differential equations is integrated over each control volume ω_K, using Gauss's theorem and one-point quadrature rules. For example, the discrete counterpart of the electron mass balance (1b) reads

$$|\omega_K|\partial_t n_{n,K} - \frac{1}{q}\sum_{\omega_L \in \mathcal{N}(\omega_K)} |\partial\omega_K \cap \partial\omega_L| j_{n;K,L} = |\omega_K|\Big(G_K - R(n_{n,K}, n_{p,K})\Big),$$

where $\mathcal{N}(\omega_K)$ denotes the set of control volumes neighboring ω_K. Here, $j_{n;K,L}$ approximates the projected flux $\mathbf{j}_n \cdot \nu_{K,L}$ across the interface $\partial\omega_K \cap \partial\omega_L$, with normal vector $\boldsymbol{\nu}_{K,L}$. This system of ODEs can be further discretized in time, e.g., by the implicit Euler method.

There are now several ways to adequately approximate the flux. For example, there exists the convenient excess chemical potential scheme [3, 4, 5], which extends the drift part in (1e) by the excess chemical potential, $\mu_\alpha^{ex} = \log \mathcal{F}_\alpha(\eta_\alpha) - \eta_\alpha$. The discrete flux reads

$$j_{\alpha;K,L} = -\frac{\mu_\alpha N_\alpha k_B T}{z_\alpha (x_L - x_K)}\Big(B(-Q_{\alpha;K,L})\mathcal{F}_\alpha\left(\eta_{\alpha;L}\right) - B\left(Q_{\alpha;K,L}\right)\mathcal{F}_\alpha\left(\eta_{\alpha;K}\right)\Big), \tag{2}$$

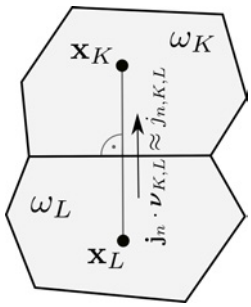


Fig. 5: *Two neighboring control volumes*

where $B(\xi) = \xi/(e^{\xi} - 1)$ is the Bernoulli function and

$$Q_{\alpha;K,L} = z_\alpha \frac{q(\psi_L - \psi_k)}{k_B T} + (\eta_{\alpha;L} - \eta_{\alpha,K}) - \log \frac{\mathcal{F}_\alpha(\eta_{\alpha;L})}{\mathcal{F}_\alpha(\eta_{\alpha;K})}.$$

Similar discretization schemes in the unipolar (single charged species with background charge) case and in the electrolyte case, where different charged quantities compete for the same space leading to a joint statistics distribution similar to the Fermi–Dirac integral of order -1 have been analyzed in [4, 5]. The discrete fluxes (2) lump the electrostatic force and the gradients of the excess chemical potential into a joint convective force. The resulting discrete system exactly conserves charge balances, both locally and globally. Moreover, the concentrations, given as the solution of the discrete system, will stay nonnegative during the evolution, and – in the case of statistics equal to Fermi–Dirac integral of order -1 – limited by the available amount of lattice sites. In addition, the discrete solutions relax to the steady state solution; see Figure 6. Results obtained for the special case of electrolytes with ion volume constraints [4, 5] suggest that also for the discrete perovskite model the relative free energy of the discrete solutions along a trajectory decays, and the solution of the discrete system is well defined, exists, and converges weakly to a solution of the continuous problem.

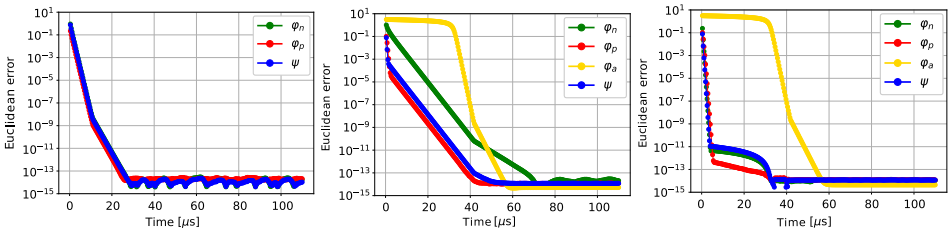


Fig. 6: *Approach towards the steady state solution for a three layer PSC device. The error between transient and steady state solution for three configurations are depicted: without mobile ions, with mobile ions & with mobile ions and surface recombination as further surface effect; see Figure 3.*

Stage 4: Simulation

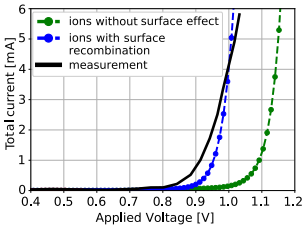


Fig. 7: *Simulation of a forward scan protocol of a PSC device with additional surface effects*

Painless simulation using automatic differentiation

In this section, we explain automatic differentiation and how we leverage it to solve the discrete systems. Solving a large system of nonlinear equations often relies on Newton's method, which in each of its iterations requires the assembly of the Jacobi matrix – the matrix of partial derivatives – of the nonlinear operator. Calculating the partial derivatives and implementing them into program code is a straightforward but tedious and error-prone task which can be automated.

Forward mode automatic differentiation allows to evaluate a nonlinear function such that both its value and its derivative are obtained at once. A straightforward implementation is based on dual numbers $\mathbb{D}$ defined by extending the set of real numbers $\mathbb{R}$. Similar to introducing the imaginary unit i with $i^2 = -1$ to define the complex numbers, one introduces a special number ε to define the set of dual numbers as $\mathbb{D} = \{a + b\varepsilon \mid a, b \in \mathbb{R}\}$. With positioning $\varepsilon^2 = 0$, the evaluation of a

polynomial $p(x) = \sum_{i=0}^{n} p_i x^i$ on a dual number $a + \varepsilon$ yields

$$p(a+\varepsilon) = \sum_{i=0}^{n} p_i a^i + \sum_{i=1}^{n} i p_i a^{i-1} \varepsilon = p(a) + p'(a)\varepsilon.$$

This fact can be generalized to differentiable functions of several variables and to multivariate dual numbers, allowing for the calculation of partial derivatives. The Julia computer language via the package `ForwardDiff.jl` provides an easily accessible implementation of dual number arithmetic helping to evaluate nonlinear functions along with their derivatives.

For implementing the Voronoi finite volume discretization as described above, we develop the Julia package `VoronoiFVM.jl`. It builds upon the experience available at WIAS on the implementation of the method [1]. It allows to describe discretizations of rather general nonlinear multiphysics reaction-diffusion-convection systems via reaction terms, flux functions like (2), and capacity terms. These constitutive functions are evaluated at discretization nodes and control volume interfaces using dual number arithmetic. The resulting local contributions are assembled into the residual vector of the discretized system and a sparse matrix representation of its Jacobi matrix. All computational results shown in this contribution and in refererences [2]–[6] have been obtained using this package.

Automatic calculation of Jacobians for discretized nonlinear systems of partial differential equations opens further computational possibilities. These include the utilization of efficient higher-order time discretization methods readily available in Julia via the package `DifferentialEquations.jl`. The Jacobi matrix evaluated at the steady state of a nonlinear system with an added frequency-dependent complex diagonal matrix can be used to obtain the phase shift and amplitude (related to the impedance) of the system response to a small periodic perturbation of this steady state. In [6], an implementation of a charge transport model for monocrystalline yttria-stabilized zirconia (YSZ)-based electrochemical cells in `VoronoiFVM.jl` has been used to fit measurements of cyclic voltammograms and impedance spectra to parameters of the model; see Figure 8.

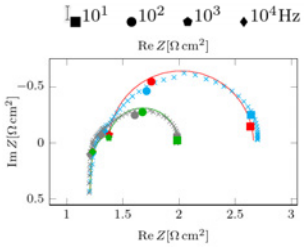


Fig. 8: *Experimental result (markers) and fitted numerical simulation (solid lines) of an impedance spectrum of an YSZ device at 850 °C [6]*

We envision to include derivatives with respect to problem parameters into the automatic differentiation approach that should benefit parameter identification and bifurcation analysis. Foremost, the introduction of ion concentration limitation and further model improvements are aimed at supporting the qualitative understanding of the performance and degradation issues of PSCs. Efficient and flexible numerical implementations matching experimental measurements can verify and calibrate the model, allowing to optimize geometry and materials of PSCs in future research.

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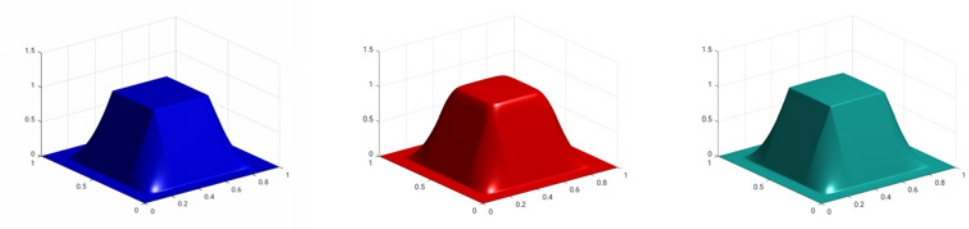
1.6 Quasi-Variational Inequalities and Optimal Control

Amal Alphonse and Michael Hintermüller

Introduction

A plethora of real-world applications involving nonlinear and non-smooth structures lead to a class of mathematical models called *quasi-variational inequalities* (QVIs). These are highly complex mathematical objects that have shown great versatility in their ability to be used to describe many phenomena in the applied and physical sciences such as game theory, solid mechanics, elasto-plasticity, superconductivity, and thermoforming. Our interests lie in studying the properties of QVIs, modeling of specific physical phenomena via QVIs, and using them as a base to study many aspects of what one calls *optimal control problems* where the aim is to find a control or action that most closely achieves some objective given that the underlying model is described by a QVI.

A large focus of our studies in QVIs is an application to thermoforming, which is the process where shapes (such as pots of yogurt or panels in cars) are mass-reproduced by heating up a plastic membrane to a high temperature and forcing it onto a mould shape (which is the desired shape to be reproduced), enabling it to take on the desired shape. Figure 1 shows the results of simulations based on a QVI model that describes such a thermoforming process. Indeed, Figure 1 (a) shows the (initial) mould shape that is to be reproduced, while Figure 1 (b) is the shape taken on by the membrane as a result of the thermoforming process. One sees that it is an accurate fit to the mould shape. In Figure 1 (c), we see the quasi-variational effect of the model in action: The mould shape has changed as a result of contact with the membrane.



(a) Mould shape (b) Membrane (c) Final mould shape

Fig. 1: *Computational results of thermoforming process*

Mathematical description

The defining feature of QVIs distinguishing them from variational inequalities (VIs) is that the constraint set in which the solution of the QVI is sought itself depends on the solution. Thus, QVIs are generalizations of VIs. The latter are simpler because the above-mentioned constraint sets are known *a priori* and are independent of the solution. This fundamental difference leads to considerable difficulties in the study of QVIs, requiring novel tools and methodologies.

The types of problems we are interested in are as follows. Given a constraint set $\mathbf{K}$ in some function space, VIs (of elliptic type) have the form

$$\text{Find } y \in \mathbf{K} : \langle Ay - f, y - v \rangle \leq 0 \quad \forall v \in \mathbf{K},$$

whereas QVIs take the form: given a set-valued map $\mathbf{K}(\cdot)$, consider

$$\text{Find } y \in \mathbf{K}(y) : \langle Ay - f, y - v \rangle \leq 0 \quad \forall v \in \mathbf{K}(y). \tag{1}$$

Note that the constraint set depends on the solution. We are primarily interested in inequalities of obstacle type, i.e.,

$$\mathbf{K}(y) := \{v \in V : v \leq \Phi(y)\},$$

where V is a reflexive Banach space which is also a vector lattice possessing an ordering $\leq$, $\Phi\colon V \to V$ is a given map, $f \in V^*$ is given data, and $A\colon V \to V^*$ is a linear elliptic operator. In the context of thermoforming, the inequality (1) could be the implicit obstacle problem where the membrane u lies below the mould shape $\Phi(u)$ and Φ could be the solution map of a partial differential equation (PDE) describing the relationship between the membrane and mould taking into account physical modeling assumptions. For full details, we refer the reader to [1, §6].

A fundamental pecularity of QVIs is that solutions of (1) are typically non-unique and in some cases they can be ordered with the existence of a smallest and largest solution.

We conducted extensive research on the following topics:

1. the analysis of the resulting QVIs of the above form: existence of solutions and properties [1, 2, 3],
2. directional differentiability of the solution map $\mathbf{Q}\colon V^* \rightrightarrows V$ that takes f into y and the solution maps related to smallest and largest solutions [1, 3],
3. optimal control problems with QVI constraints and stationarity conditions [2, 3].

The first two items relate directly to (1) whereas the third involves optimal control problems, which in this context looks like

$$\min_{\substack{u \in U_{ad} \\ y \in \mathbf{Q}(u)}} \frac{1}{2}\|y - y_d\|_H^2 + \frac{\nu}{2}\|u\|_H^2, \tag{2}$$

where H is a Hilbert space with $V \subset H$ and $U_{ad} \subset H$ is an admissible set of controls.

The motivation for this is the following: often in a QVI model there is an external quantity that influences the state (i.e., the solution of the QVI). We wish to control this external quantity so that the state satisfies some predefined performance criteria. The task of finding and characterizing such a control that maximizes our criteria is the optimal control problem. The specific objective functional appearing in (2) is known as a *tracking-type* objective and it models the case where we wish the state to be as close as possible to a desired state y_d whilst trying to minimize the control cost.

More details

Directional differentiability

We studied in [3, 1] the directional differentiability associated to (1), in particular, the directional differentiability of the multi-valued (or set-valued) mapping $\mathbf{Q}$ taking the source term f into the set of solutions y. It is important to know if the map is directionally differentiable and to characterize the derivative as it enables us to find out the effect that changes in the source term have on the solution (which can be useful in applications such as thermoforming), and it is a necessary step for obtaining useful first-order characterizations of the optimal control problem (2). Furthermore, it is an interesting problem in mathematical analysis and a fundamental question that deserves to be addressed.

Showing directional differentiability is completely non-trivial due to the nonsmooth nature of the inequality (which in addition contains a nonsmooth obstacle mapping Φ) as well as the multiplicity of solutions to the QVI that can be expected in general. This means that one needs to take care with multivalued solution concepts as well as conduct a fine and careful analysis of the ensuing subproblems. For full details, we refer to the aforementioned papers.

Let V be a reflexive Banach space, $\Phi\colon V \to V$ a Hadamard differentiable operator, and $A\colon V \to V^*$ an elliptic operator. Theorem 3.2 of [3] essentially states that under some assumptions, given $f \in V^*$ and $y \in \mathbf{Q}(f)$, there exists $y^s \in \mathbf{Q}(f + sd)$ and $\alpha = \alpha(d)$ such that

$$\lim_{s\to 0^+} \frac{y^s - y - s\alpha}{s} = 0 \text{ in } V\ ,$$

where α satisfies the QVI

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

and the constraint set appearing above is the *critical cone* defined by

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

This is a powerful result and it considerably improves our previous contribution [1] (which was the first result for the directional differentiability for QVIs in the infinite-dimensional setting) in which we needed further assumptions on the signs of the source and direction term. Let us also mention that directional differentiability of the minimal and maximal solution maps is studied in [4]; we refer the reader there for more details.

Optimal control

In [3, §4], we gave an existence result on the optimal points of the control problem (2), which we recall here:

$$\min_{\substack{u\in U_{ad}\\ y\in\mathbf{Q}(u)}} \frac{1}{2}\|y - y_d\|_H^2 + \frac{\nu}{2}\|u\|_H^2. \tag{2}$$

Furthermore, we also provided comprehensive first order characterizations of optimality in [3, §5]. Here, as mentioned above, U_{ad} is the so-called *admissible set of controls*, which is taken to be non-empty, closed, and convex.

These results were achieved by approximating the control problem (2) by

$$\min_{u\in U_{ad}} \frac{1}{2}\|y_\rho - y_d\|_H^2 + \frac{\nu}{2}\|u\|_H^2 \quad \text{where} \quad Ay_\rho + \frac{1}{\rho}m_\rho(y_\rho - \Phi(y_\rho)) = u, \tag{3}$$

deriving stationarity conditions for this problem (by standard constraint qualification) and then performing a delicate analysis in the passage to the limit in the parameter ρ under varying sets of assumptions. Here, for each $\rho > 0$, $m_\rho \colon V \to V^*$ is a C^1 map possessing certain properties that in some sense generalizes the positive part function $(\cdot)^+$. Thus, we have approximated the nonsmooth QVI by a sequence of more regular PDEs with penalization parameter ρ with the intention being to send $\rho \to 0$ and obtain results for the original problem.

The PDE in (3) is well posed in certain circumstances and solutions of (3) can be shown to converge to solutions of (2).

Stationarity systems are useful because they characterize optimal points and can often be easier to numerically solve than the original optimal control problem. There are a multitude of stationarity systems that can be derived depending on the hypotheses and structure of the problem.

Let us now describe the cascade of stationarity systems that we derived, in increasing order of the number of assumptions needed.

In the general vector lattice setting, we showed in [3, Theorem 5.5] the existence of multipliers $(p^*, \xi^*, \lambda^*) \in V \times V^* \times V^*$ satisfying what we call the *weak C-stationarity* system

$$y^* + (\mathrm{Id} - \Phi'(y^*))^*\lambda^* + A^*p^* = y_d, \tag{4a}$$
$$Ay^* - u^* + \xi^* = 0, \tag{4b}$$
$$\xi^* \geq 0 \text{ in } V^*, \quad y^* \leq \Phi(y^*), \quad \langle \xi^*, y^* - \Phi(y^*)\rangle = 0, \tag{4c}$$
$$u^* \in U_{ad} : (\nu u^* - p^*, u^* - v)_H \leq 0 \quad \forall v \in U_{ad}, \tag{4d}$$
$$\langle \lambda^*, p^*\rangle \geq 0. \tag{4e}$$

This is a system that lies in between the traditional notions of weak stationarity and C-stationarity, hence its name.

In case V is a Sobolev space over some domain $\Omega \subset \mathbb{R}^n$, we have at our disposal a specific family m_ρ that possesses enough regularity allowing us to improve the above system to an *$\mathcal{E}$-almost C-stationarity* system [3, Theorem 5.11] by additionally giving us the conditions

$$\langle \xi^*, (p^*)^+\rangle = \langle \xi^*, (p^*)^-\rangle = 0\,, \tag{5a}$$
$$\langle \lambda^*, y^* - \Phi(y^*)\rangle = 0, \tag{5b}$$
$$\forall \tau > 0, \exists E^\tau \subset \mathcal{I} \text{ with } |\mathcal{I} \setminus E^\tau| \leq \tau : \langle \lambda^*, v\rangle = 0 \quad \forall v \in V : v = 0 \text{ a.e. on } \Omega \setminus E^\tau. \tag{5c}$$

The final condition arises from an application of Egorov's theorem. Under an extra assumption of

continuity of $(\mathrm{Id} - \Phi)\colon V \to L^\infty(\Omega)$, we can strengthen the condition (5c) to

$$\langle \lambda^*, v\rangle = 0 \quad \forall v \in V : v = 0 \text{ a.e. on } \{y^* = \Phi(y^*)\}.$$

This is a fully *C-stationarity* system (with no need for the $\mathcal{E}$-almost damping).

By making further assumptions on the admissible set U_{ad}, we showed in [3, Theorem 5.16] that (y^*, u^*) is a *strong stationarity* point, i.e., the multipliers $(p^*, \xi^*, \lambda^*) \in V \times V^* \times V^*$ indeed satisfy

$$\begin{aligned}
y^* + (\mathrm{Id} - \Phi'(y^*)^*)\lambda^* + A^* p^* &= y_d,\\
Ay^* - u^* + \xi^* &= 0,\\
\xi^* \geq 0 \text{ in } V^*, \quad y^* \leq \Phi(y^*), \quad \langle \xi^*, y^* - \Phi(y^*)\rangle &= 0,\\
u^* \in U_{ad} : (\nu u^* - p^*, u^* - v) \leq 0 \quad &\forall v \in U_{ad},\\
p^* \geq 0 \quad &\text{q.e. on } \mathcal{B}(y^*) \text{ and } p^* = 0 \text{ q.e. on } \mathcal{A}_s(y^*),\\
\langle \lambda^*, v\rangle \geq 0 \quad &\forall v \in V : v \geq 0 \text{ q.e. on } \mathcal{B}(y^*), \text{ and}\\
&v = 0 \text{ q.e. on } \mathcal{A}_s(y^*).
\end{aligned}$$

Here, note that $\mathcal{A}_s(y^*) := \{\xi^* > 0\}$ is the *strongly active* set, and $\mathcal{B}(y^*) := \{y^* = \Phi(y^*)\} \cap \{\xi^* = 0\}$ is the *biactive* set. This is the strongest form of stationarity available; note in particular the pointwise q.e. (quasi everywhere) sign conditions on the adjoint p^* as well as a finer characterization of the multiplier λ^* in comparison to the previous systems.

Conclusions and outlook

As mentioned above, directional differentiability results for the minimal and maximal solution mappings do appear in our work [4], however, only for signed source and direction terms. The removal of these restrictions, as well as the obtainment of stationarity systems for optimal control problems with minimal/maximal control-to-state maps, are highly delicate and subjects of ongoing work.

As a final remark, we highlight that this work has been conducted within projects funded via the DFG SPP 1962 Priority Programme in collaboration with Carlos N. Rautenberg (George Mason University). A joint work [5] with José-Francisco Rodrigues (Lisbon University) has also been finished.

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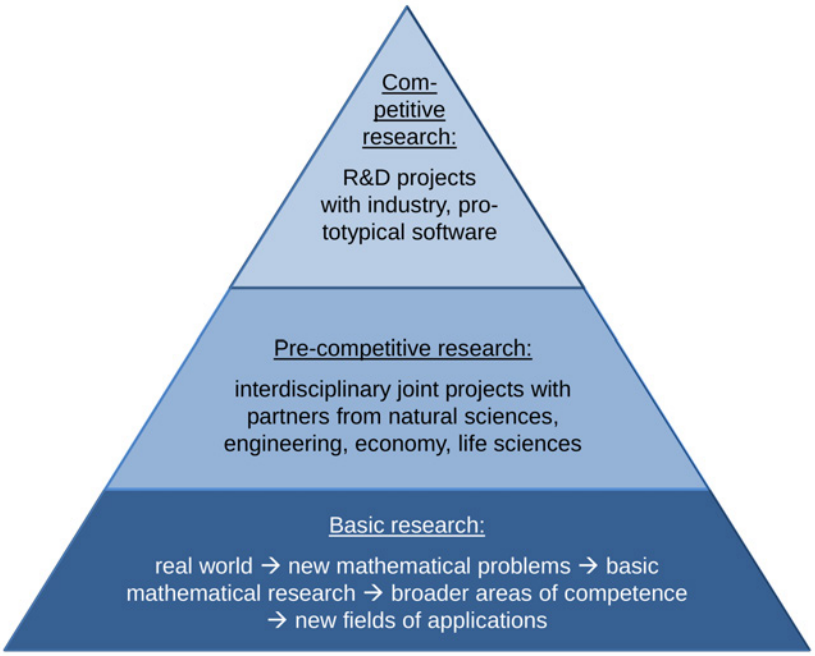
2 WIAS in 2021

- Profile
- Structure and Scientific Organization
- Equal Opportunity Activities
- 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 are individual members of the *Leibniz Association (WGL)*. The *Director of WIAS* is responsible for the scientific work at WIAS, the *Managing Director* of the *Common Administration of FVB* is in charge of its administrative business. The official German name of the institute is *Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e. V.*



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

A successful mathematical approach to complex applied problems necessitates a long-term 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 35 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. Unfortunately, the "Leibniz MMS Days 2021" could not take place due to the Corona crisis, but from August 23 to 27, 2021, the Leibniz MMS Summer School 2021 "Mathematical Methods for Machine Learning" took place at Schloss Dagstuhl – Leibniz-Zentrum für Informatik GmbH. Fundamental and advanced aspects of Machine Learning methods were presented to Ph.D. students from various Leibniz Institutes of the MMS network, with the aim to enable the participants to apply such methods to their specific research problems. On October 19, 2021, a Multiscale Simulation Day took place in the Leibniz-Institut für Verbundwerkstoffe online via Zoom.

WIAS is very proud to announce that a five-year period of funding of **the Mathematical Research Data Initiative (MaRDI)** (`http://www.mardi4nfdi.de/`) started on October 1, 2021. MaRDI is coordinated by WIAS as a leading institution within the German National Research Data Infrastructure (NFDI). WIAS is operating the MaRDI coordination office. Furthermore, in RG 6 *Stochastic Algorithms and Nonparametric Statistics*, two positions will work on workflows and software in statistics and the collaboration with the corresponding initiative for neuroscientific data within the task areas 3 and 4 of the consortium. Finally, a further position, in RG 1 *Partial Differential Equations*, will be dedicated to mathematical models that can be formulated in terms of (systems of) partial differential equations. There is a possibility of extension for another five years with the goal of building a sustainable, permanent 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 one of three co-speakers 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 2021, 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 60), 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:

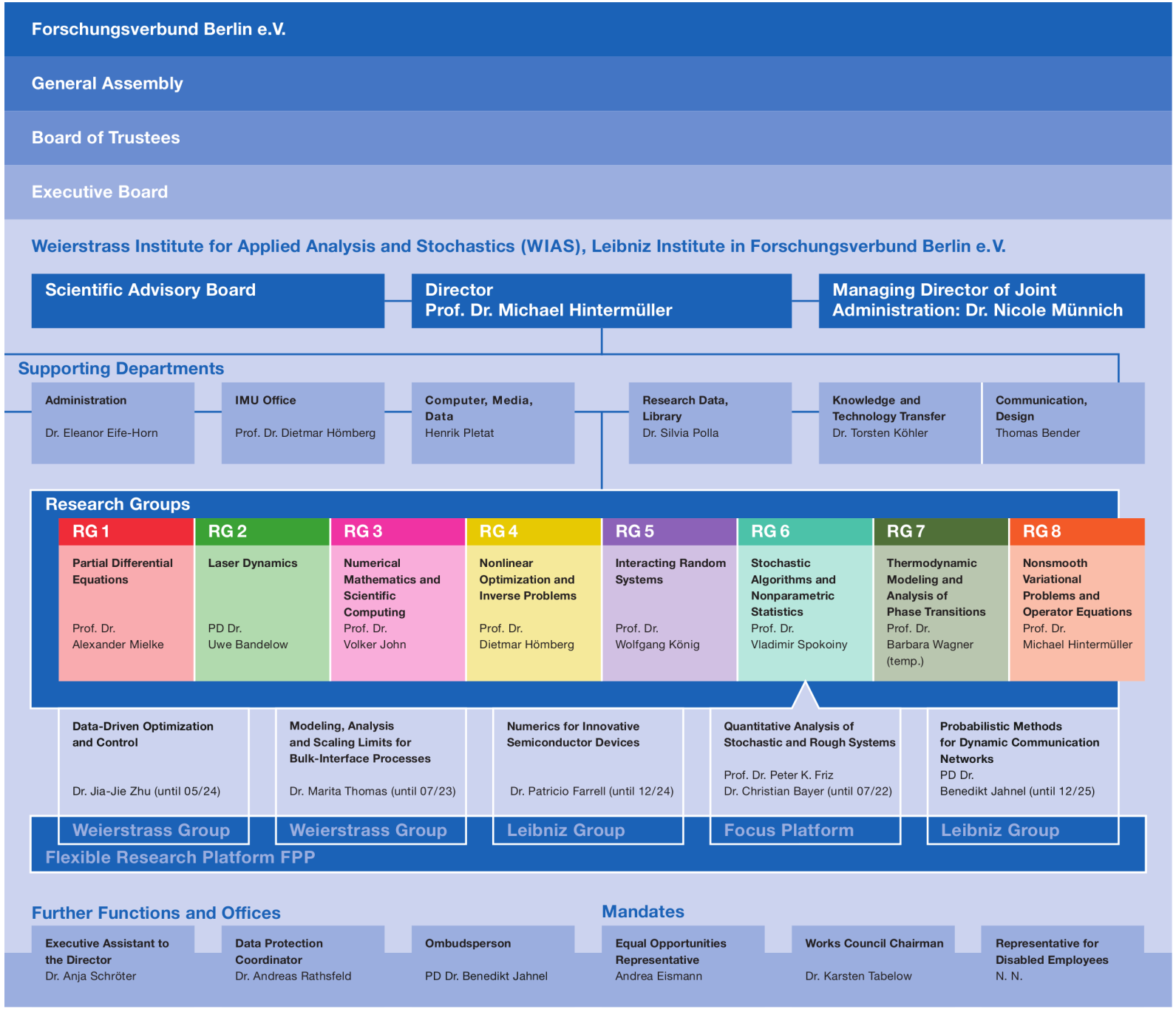
RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing
RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase 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 49 gives an overview of the organizational structure of WIAS in 2021.

[1] In the following, the terms "research group" will often be abbreviated by "RG," "Leibniz group" by "LG," Weierstrass group by "WG," and Focus Platform by "FP."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RG 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
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Equal Opportunities Representative
Andrea Eismann
Works Council Chairman
Dr. Karsten Tabelow
Representative for Disabled Employees
N. N.

2.2.2 Main Application Areas

The research at WIAS focused in 2021 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 2021 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 2021 within the general framework of the main application areas.

Conversion, Storage and Distribution of Energy

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

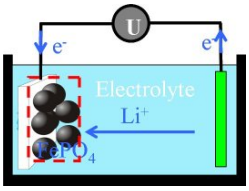


Fig. 1: *Sketch of a lithium-ion battery (LiFePO4)*

Core areas:

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

Flow and Transport

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

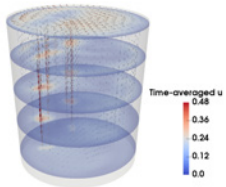


Fig. 2: *Time-averaged turbulent flow through a laddle*

Core areas:

- Thermodynamic models and numerical methods for electrochemical systems (in RG 1, RG 3, and RG 7)
- Development and analysis of physically consistent discretizations (in RG 3 and LG NUMSEMIC)
- Modeling and numerical methods for particle systems (in RG 1 and RG 5)
- Modeling of nanostructures of thin films (in RG 7)
- Computational hemodynamics (in RG 3 and RG 8)
- Scientific software platforms `ParMooN` and `pdelib` (in RG 3)
- Description of random message trajectories in spatial telecommunication models (in 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)

Materials Modeling

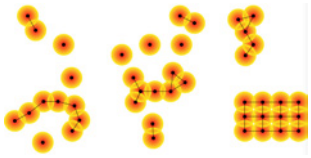


Fig. 3: *A realization of a many-body system showing a small crystal in the lower right corner*

Modern materials increasingly show multi-functional capabilities and require precise and systematically derived material models on many scaling regimes. To include theories from the atomistic to the continuum description, multi-scale techniques are at the core in the derivation of efficient models that enable the design of new materials and processes and drive the development of new technologies. Combining stochastic and continuum modeling with numerical methods and the rigor of mathematical analysis to address some of today's most challenging technological problems is a unique characteristic of WIAS.

Core areas:

- Homogenization and localization in random media (in RG 1, RG 5, and LG DYCOMNET)
- Models of condensation and crystallization in interacting many-particle systems (in RG 5, RG 6, 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.

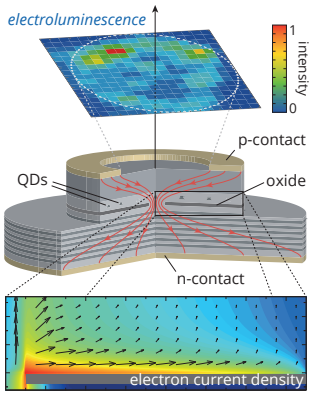


Fig. 4: *Simulated spreading of injection current density in a quantum-dot-based single photon emitter with Al-oxide aperture. An improved design was proposed on that base in:* M. Kantner, U. Bandelow, T. Koprucki, J.-H. Schulze, A. Strittmatter, H.-J. Wünsche, Efficient current injection into single 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 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

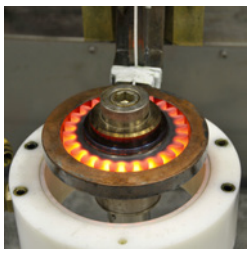


Fig. 5: *Induction heat treatment of a gear*

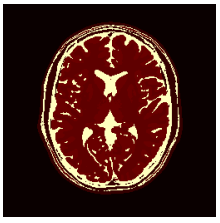
For planning and reconfiguration of complex production chains as they are considered in the Industry 4.0 paradigm as well as for innovative concepts combining economic market models and the underlying physical processes, e.g., in energy networks or telecommunication systems, modern methods of algorithmic 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.

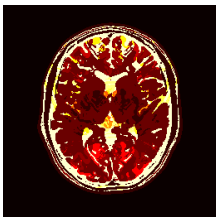
Applications may range from basic production processes such as welding and hardening to the design of diffractive structures and simulation tasks in process engineering industry to optimal decision in financial environments such as financial (energy) derivatives, energy production, and storage, and mobile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

Core areas:

- Simulation and control in process engineering (in RG 3, RG 4, and RG 6)
- Problems of optimal shape and topology design (in RG 4 and RG 8)
- Optimal control of 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)
- Optimal control of multiphase fluids and droplets (in RG 8)

Quantitative Biomedicine





Quantitative Biomedicine is concerned with the modeling, analysis, simulation, or optimization of various highly relevant processes in clinical practice. Not only the modeling of cellular, biochemical, and biomolecular processes, but also applications in medical engineering, such as the modeling, simulation, and optimization of prostheses or contributions to the area of imaging diagnostics, are major focus topics.

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

understanding of haemodynamic processes are developed, analyzed, and simulated. These models are then employed for the prognosis or optimization after medical interventions, using, e.g., model reduction and optimization techniques with partial differential equations. Other foci are the modeling and analysis of time-based systems, e.g., cartilage reconstruction, calcium release.

Core areas:

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

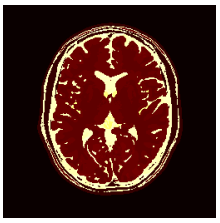


Fig. 6: *Quantitative MRI: Estimation of the T_2 relaxation times of matter leading to characterization of different types of tissue. (1) and (2) on previous page: (1) Ground truth, (2) State-of-the-art dictionary-based method (improved variant of Magnetic Resonance Fingerprinting-MRF), (3) Integrated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

2.3 Equal Opportunity Activities

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 officer's 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 for the period of one year. Barbara Wagner, acting head of Research Group 7 "Thermodynamic Modeling and Analysis of Phase Transitions" was designated as the person in charge in 2021. Andrea Eismann as the equal opportunities officer and Jutta Lohse as her deputy spend 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 November and December, the new central Equal Opportunities Officer of the Forschungsverbund Berlin (FVB), Marta Alirangues, organized with our support four online workshops about career planning for the female Ph.D. students of the FVB institutes. In 2021, five female master's degree candidates were recruited as student assistants at WIAS in the WIAS Female Master Students Program. In the report year, one of the former participants in this program became a WIAS Ph.D. student. On October 4–6, the "Junior Female Researchers in Probability" Workshop took place in a hybrid format, co-organized—jointly with other organizers of the International Research Training Group IRTG 2544 *Stochastic Analysis in Interaction*—by a former (Luisa Andreis (U Florence)) and a recent (Alexandra Quitmann) staff member of WIAS.

audit berufundfamilie. Since December 2013, WIAS has been certified and recertified 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. Although not all

measures envisaged 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" and the "Objective agreement for confirmation of the certificate for the *audit berufundfamilie*" 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 worked from home.

The *work and family* team, which monitors and supports the implementation of family-friendly policies at WIAS, comprised in 2021 Olaf Klein (project head of the *audit berufundfamilie*), Barbara Wagner (management), Jutta Lohse, and Veronica Bove, who is responsible for the team's internet presence. In 2021, the team informed the staff about relevant issues and events (announcements of webinars, online talks, and online events on dealing with the corona time, parenting, care for family members, stress coping, working from home and child care, etc.; distribution of information material related to these topics). On May 6, there was a presentation of the support services in cooperation with the employee service benefit@work, and on December 9, a presentation on resilience was organized.

On July 9, Olaf Klein and Barbara Wagner organized an executive strategy workshop on the compatibility of work and family and a family- and life-phase-conscious personnel policy for the management of the institute.

Instead of the annual Christmas party for the children of the collaborators, this year a Zoom event was offered. Several children were sent step-by-step instructions and the necessary material to create little apple men with walnut heads.

2.4 Grants

The raising of grants under scientific competition is one of the main indicators of scientific excellence and thus plays an important role in the efforts of WIAS. In this task, WIAS was very successful in 2021, having raised a total of 3.5 million euros, from which 51 additional researchers [2] (plus 12 outside WIAS; Dec. 31, 2021) were financed. In total in 2021, 25.2 percent of the total budget of WIAS and 44.74 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 133ff.

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

[2] Including scholarship holders.

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

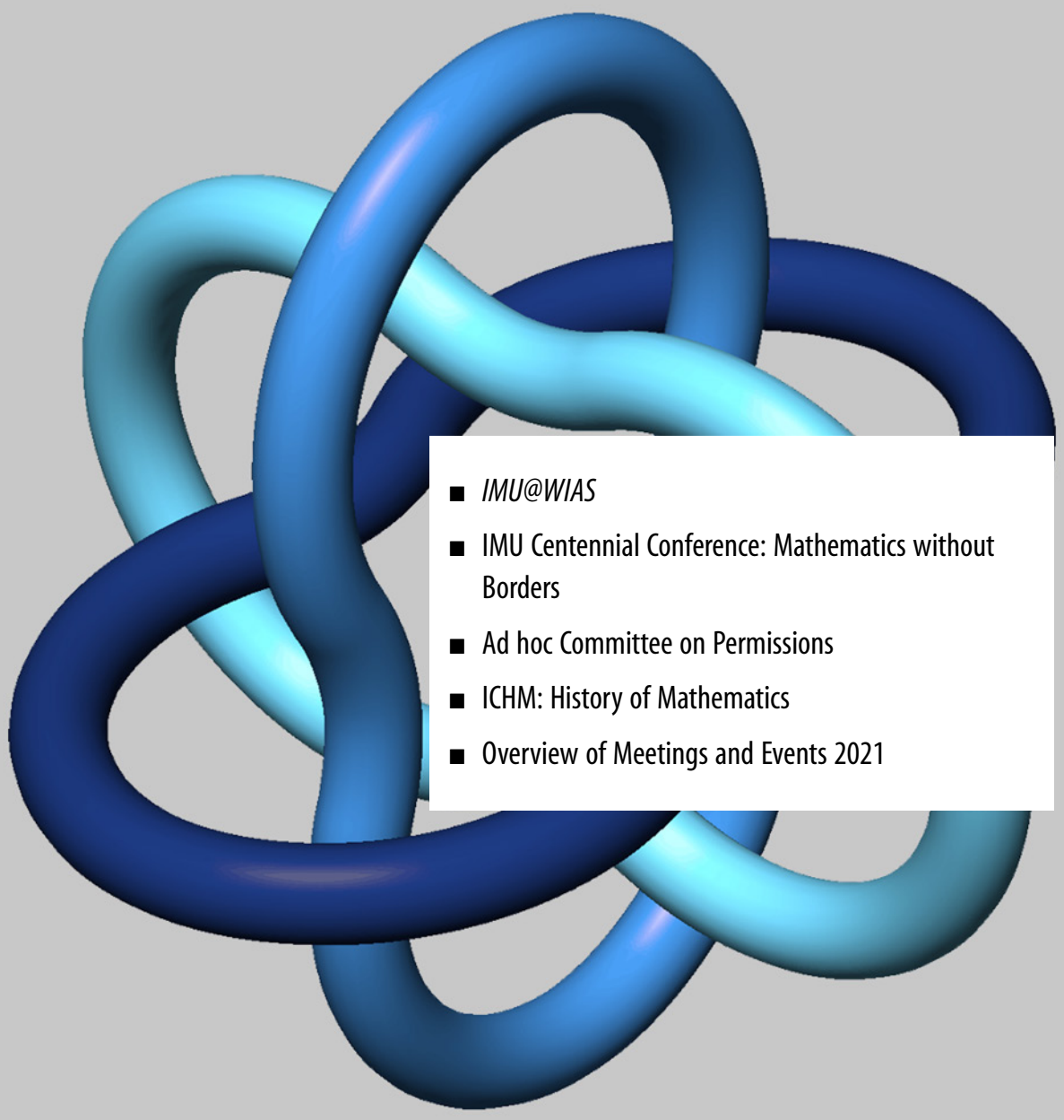
The main goal of DAEDALUS, based at the Technische Universität Berlin, consists in studying the interplay between data-based and differential equation-based modeling. DAEDALUS focuses on applications in life sciences as well as in fluid dynamics. A WIAS-supervised project (in RG 3) for a student from 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 189ff. for a list of software packages that WIAS makes available. Licensing models depend on the specifics of the corresponding projects. Codes are offered under open source and proprietary licenses as well as combinations thereof.

3 IMU@WIAS



3.1 The Secretariat of the International Mathematical Union

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, the Secretariat runs IMU's day-to-day business and provides support for many IMU operations, including administrative assistance for the International Commission on Mathematical Instruction (ICMI) and the Commission for Developing Countries (CDC) as well as mainly technical assistance for the Committee on Electronic Information and Communication (CEIC) and the Committee for Women in Mathematics (CWM). The IMU Secretariat also hosts the IMU Archive.

The collaboration of WIAS and 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 meeting.

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

Staff members

Dietmar Hömberg, *Head of the IMU Secretariat and IMU Treasurer*. D. Hömberg is a professor at Technische Universität Berlin, and head of Research Group 4 at WIAS. He has been Head of the Secretariat and IMU Treasurer since July 2020. In his function as the Head of the Secretariat, he is responsible for the IMU Secretariat as a separate unit within WIAS. As IMU Treasurer he reports to the IMU Executive Committee 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 IMU Executive Committee 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 the Commission for Developing Countries and the International Commission on Mathematical Instruction. This refers, in particular, to promoting the work of both commissions, managing their web presence – including public relations and communication – 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.

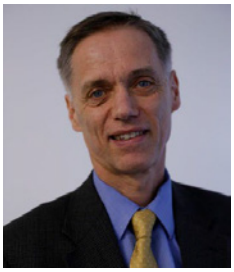
Birgit Seeliger, *IMU Archivist*. B. Seeliger is responsible for the IMU Archive and in charge of developing a strategy for preserving and making paper documents, photos, pictures, and IMU artifacts accessible, as well as supporting the decision process concerning the electronic archiving of the IMU's steadily increasing digital documentation. She also provided additional administrative support to CWM in 2021.

Frank Klöppel, *IT and Technical Support*. F. Klöppel is responsible for running the IT operations of the IMU Secretariat. This includes taking care of running the hardware and software infrastructure, in particular, the IMU server and mailing lists, and planning the extension of the IMU's IT services for its 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 is the IMU Secretary General. He holds a professorship at the Norwegian University of Science and Technology, Trondheim. He is in contact with the IMU Secretariat regularly via electronic communication and visits the office about once a month.



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

3.2 The IMU Centennial Conference: Mathematics without Borders

The IMU celebrated its belated centennial in Strasbourg on September 27–28, 2021, with the conference "Mathematics without Borders." The conference had originally been planned for September 2020 but had to be postponed by a year due to the COVID-19 pandemic. The IMU was officially founded on September 20, 1920, in Strasbourg, just prior to the International Congress of Mathematicians (ICM) being held there. The conference took place in the same building used for ICM

1920. We were delighted to welcome around 200 attendees to the conference on the day. The conference was also streamed live by the Université de Strasbourg. Among the speakers was Norbert Schappacher who gave an insight to his forthcoming monograph on the IMU's centennial with the talk "The Sinuous Road towards Global Mathematics."

To capture the occasion and for the benefit of those unable to attend, the talks were recorded and can be viewed on the Université de Strasbourg's web-channel. Additionally, the IMU engaged the science journalists Marianne Freiberger and Rachel Thomas from *Plus* magazine to write about the event. The resulting article can be found online

Fig. 1: *IMU 100 Group Photo: Catherine Schröder/Université de Strasbourg*

3.3 Ad hoc Committee on Permissions

Helge Holden, IMU Secretary General

As more and more journals are becoming digital – with several being exclusively available in digital format – it is increasingly important to establish viable means for ensuring free access to back issues of mathematical journals. For the mathematics community, it would be optimal to have the shortest possible window before open access. On the other hand, a short window would put financial pressure on learned societies and make it difficult to reach a broad agreement.

The IMU Executive Committee – on the advice of the IMU Committee on Electronic Information and Communication (CEIC) – has now created an ad hoc Committee on Permissions (CoP) to advise the IMU on a negotiating strategy regarding the window for open access.

Specifically, the task of the CoP is to report to the IMU Executive Committee regarding the following:

1. A recommendation for IMU policy on the time frame for making papers freely available after publication, together with technical details such as licenses.
2. A concrete proposal for how to implement this recommendation, for example, by outreach to publishers, with the particular goal of negotiating access to existing back issues.

3. Any additional considerations that may affect the availability of past papers, such as the demise of publishing companies or issues with archiving.

The first report of CoP will be considered by the IMU Executive Committee at its meeting in February 2022.

The committee has six members. The chair of CoP is Thomas Brennan (Harvard Law School, US).

3.4 ICHM: History of Mathematics

June Barrow-Green, ICHM Chair

The International Commission on the History of Mathematics (ICHM) is an inter-union commission joining the International Mathematical Union and the Division of the History of Science and Technology (DHST) of the International Union for the History and Philosophy of Science. It is composed of representatives of nations in which the history of mathematics is taught and/or actively researched. The core aims of the ICHM are to encourage the study of the history of mathematics, and to promote a high level of historically and mathematically sophisticated scholarship in the field. It sponsors, or co-sponsors, symposia at the quadrennial International Congresses of the History of Mathematics and of History of Science, and at other international conferences in the history of mathematics. It celebrates the excellence in the history of mathematics through the awarding of the Kenneth O. May Medal and the Montucla Prize.

Two members of the ICHM Executive Committee (EC) are elected by the IMU, the current IMU representatives being Isobel Falconer (UK) and Catherine Goldstein (France). Although the ICHM EC does not have an official DHST representative, one of our members, Michaela Malpangotto (France) was recently elected on to the Council of the DHST, having been proposed by the ICHM.

In common with other organizations, the ICHM's activities in 2021 were disrupted by COVID-19. In particular, we were affected by the move to online of the 26th International Congress of History of Science (ICHST), which was due to take place in July 2021 in Prague, Czech Republic. Although the move was unavoidable, this was especially disappointing for the ICHM since the ICHSTs are where we hold our Open Meetings and celebrate our prizewinners. Instead, we held an online Open Meeting during the Congress at which we announced our prizewinners, reported on our activities since the previous Congress, and had a discussion on ways in which the ICHM can help early-career scholars. This was also the occasion for the retirement of Niccolò Guicciardini (Italy) as Vice-Chair of the ICHM, a position he has held since 2017. Niccolò has played an invaluable role on the EC of the ICHM, being a constant source of wise advice, and the ICHM owes him a deep debt of gratitude. In his place we welcomed Clemency Montelle (New Zealand) who was elected as our new Vice-Chair. We also welcomed two newly elected members onto the EC: Adrian Rice (USA) and Seyyed Mohammad Mozaffari (Iran/China).

The main theme of the 26th ICHST was "Giants and Dwarfs in Science, Technology and Medicine," and we were very pleased to be able to sponsor three symposia at the Congress, with subjects ranging from the evolution of mathematics in China to collaborations and rivalries in history of

mathematics. Altogether these three symposia featured talks from 23 participants from 10 different countries.

Since our prizewinners were unable to receive their prizes in person at the ICHST, we are arranging for them to receive them and to give talks on their work at the ICHM symposium at the ICM2022 in St Petersburg. The May medalists are Sonja Brentjes (Germany) who works on Islamic mathematics and Christine Proust (France) who works on Mesopotamian mathematics; and the Montucla Prize winners are François Lê (France) and Brigitte Stenhouse (UK), both of whom work on 19th century European mathematics.

Fig. 2: *The Kenneth O. May Medal (mathunion.org/ichm/) The medal was designed by the Canadian sculptor Saulius Jaskus. Kenneth O. May (1915–1977), for whom the medal is named, was a Canadian historian of mathematics and the first chair of the ICHM, which was established as a result of his initiative.*

Supporting early-career scholars in history of mathematics is a priority for the ICHM, and in recent years we have regularly provided funding for the Novembertagung – the annual history of mathematics conference for post-graduate students and post-doctoral researchers – to help with participants' travel expenses. Since the conference had to be held online in both 2020 and 2021, we have been looking into other ways to support participants. To this end we have launched a grant scheme for early-career scholars whereby they can apply for funding to support individual projects. For example, the funding could cover the cost of the digitization of archive materials or online conference registration fees. For the 2021 Novembertagung, the theme of which was "Mathematics in Times of Crisis," we provided funding for technical support for online facilities and for covering the cost of childcare support for participants. In addition, we provided funding to pay for an online workshop "Creative Science Storytelling" to help participants develop external engagement skills.

We are keen to broaden our reach to help early-career scholars in the global south and are actively seeking contacts who can help us in this respect. In the past, we have been able to do only a little to help such scholars due to the costs involved in travel. However, the increase in accessibility afforded by meeting virtually has opened up new possibilities, such as combinations of online conferences with face-to-face satellite meetings, which we are currently exploring.

The ICHM would like to thank the IMU for their ongoing support, and especially for their help with banking matters and for hosting our website. We are particularly grateful to the IMU Secretariat whose ongoing assistance has been invaluable for the smooth running of our activities.

3.5 Overview of Meetings and Events 2021

Commission and Committee Meetings

Meeting of the IMU Executive Committee, March 19–21, 2021. The third annual meeting of the 2019–2022 IMU EC was held for the first time virtually due to travel restrictions resulting from the COVID-19 pandemic. A review of the progress made in planning the next ICM and General Assembly in 2022 was again one of the primary topics of the meeting alongside other recurring business. Hosted online by the IMU Secretariat.

Fig. 3: *IMU EC Virtual Meeting (Screenshot/Zoom)*

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, Dietmar Hömberg, Elisabetta Strickland, Scott Jung. Guests invited for particular agenda items: Martin Hairer, Stanislav Smirnov.

ICMI Executive Committee Meetings: January 4, February 16, April 15, May 31, July 18 (special meeting with invited guests (ICMI EC 2017–2020)), September 13, November 17, 2021 (held online). **Participants:** ICMI Executive Committee members, IMU EC liaison person, ICMI Administrative Manager.

ICME-15 International Program Committee (IPC) Meeting, September 24, 2021 (held online).

CDC Meeting, March 9–10, 2021 (held online). **Participants:** CDC members, invited guests, CDC Administrative Manager.

Conferences and Events

"Mathematics for a Better World." The International Day of Mathematics (IDM), March 14, 2021. "Mathematics for a Better World" was the theme for the IDM in 2021. The celebration consisted of liveblogging pictures and videos from IDM events worldwide, posters, announcements, and more. The main event was a series of short online talks for a general audience on mathematics and how it can make the world better, with three sessions in three different languages. The talks were streamed live through the IDM website. The theme for IDM 2022 will be "Mathematics Unites."

ICME–14. *International Congress on Mathematical Education*, Shanghai, China, July 11–18, 2021.

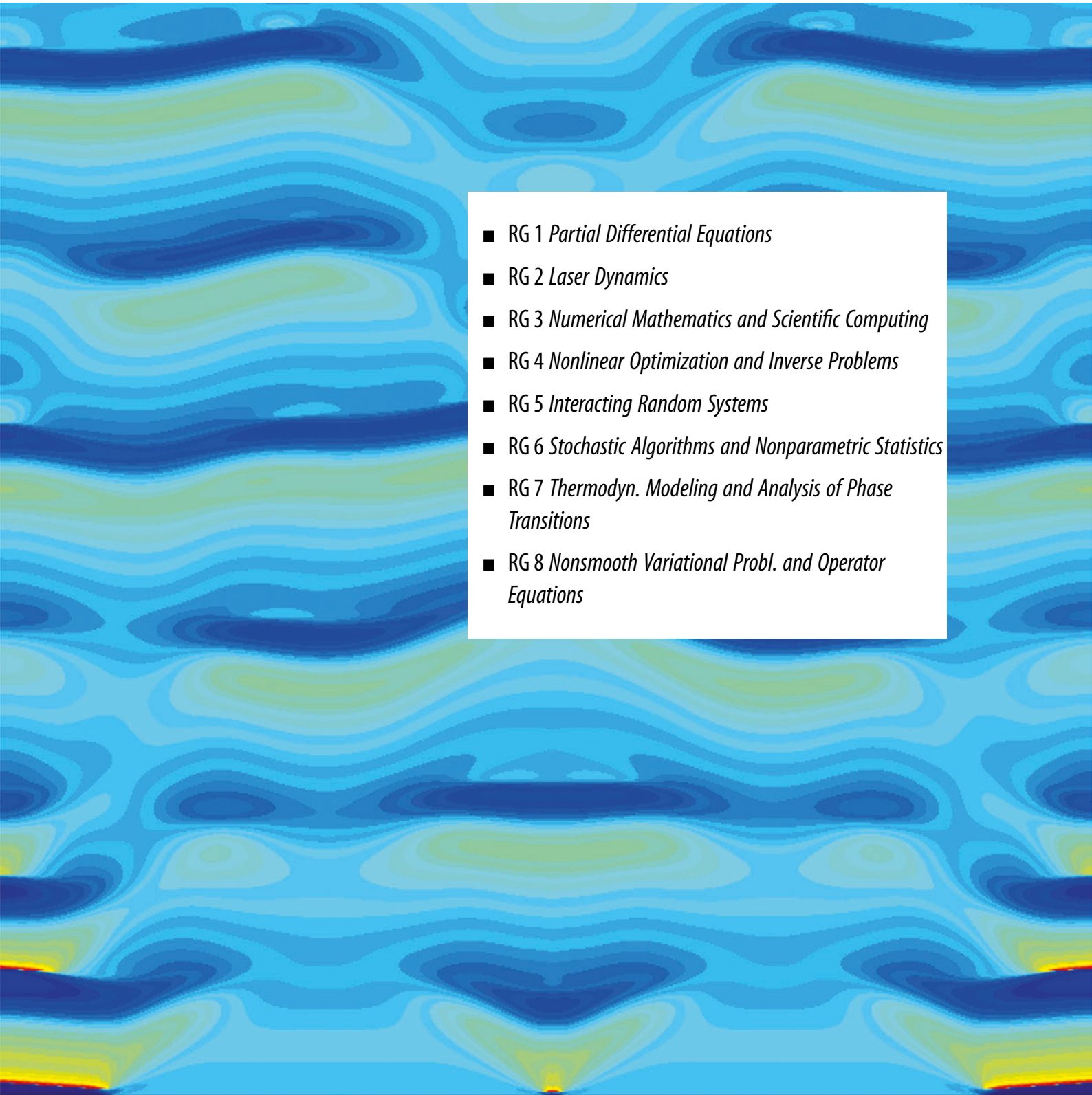
Mathematics without Borders. *The Centennial of the International Mathematical Union*, Strasbourg, France, September 27–28, 2021.

Guests and Visits at the IMU Secretariat

IMU Office Committee Visit. IMU Secretariat, Berlin, Germany, September 20, 2021. The IMU Office Committee is charged with monitoring the performance of the IMU Secretariat and assessing how the Secretariat enables the IMU to fulfill its goals to support and encourage mathematicians worldwide. The IMU Office Committee visit – postponed from 2020 – took place in September 2021. WIAS Director Prof. Dr. Michael Hintermüller welcomed the committee to WIAS at the start of its visit. The IMU Office Committee then met with the IMU Secretariat leadership and staff over the course of the day and will report its findings and recommendations to the IMU Executive Committee. **Participants:** IMU Office Committee: Ulrike Tillmann (chair), Luigi Ambrosio, Dipendra Prasad (virtually); Helge Holden, Dietmar Hömberg, Michael Hintermüller, IMU Secretariat staff.

Guests at the Secretariat. Historian Nobert Schappacher did research in the IMU Archive (July and September).

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. Hans-Christoph Kaiser Dr. Thomas Koprucki Anieza Maltsi Dr. Oliver Marquardt Arbi Moses Badlyan Dr. Grigor Nika Dr. Petr Pelech Dr. Joachim Rehberg Stefanie Schindler Dr. Artur Stephan Willem van Oosterhout
Secretary:	Andrea Eismann
Nonresident Members:	Prof. Dr. Jürgen Sprekels

In 2021, the Research Group RG 1 *Partial Differential Equations* continued its scientific work on the mathematical analysis of partial differential equations and their usage for modeling in sciences and engineering. The mathematical theory is developed in close connection to 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 partial differential equations (PDEs) provides a deeper understanding of the underlying processes and is decisive for the construction of efficient numerical and optimization algorithms.

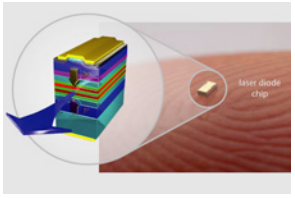


Fig. 1: *TU Berlin / Kremzo 3D sketch of laser diode, FBH / schurian.com (photo)*

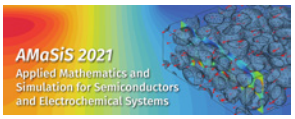
Despite the corona pandemic, the year 2021 had several highlights for RG 1:

The joint project "UV Lasers – From Modeling and Simulation to Technology (UVSimTech)," which is coordinated by group member Thomas Koprucki, successfully applied to the Leibniz Competition within the Leibniz Association and will be funded for three years with nearly one million euros. The UVSimTech consortium combines the multidisciplinary expertise of the Berlin Weierstrass Institute (WIAS) in mathematical modeling and simulation of complex semiconductor lasers and of the Institute of Optoelectronics of the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) with

materials science know-how, coming from the Berlin Leibniz-Institut für Kristallzüchtung (IKZ) and the Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik (FBH, also in Berlin), as well as from the experts in UV photonics at Technische Universität (TU) Berlin.

Artur Stephan successfully defended his Ph.D. thesis titled "Coarse-graining for gradient systems and Markov processes" at Humboldt-Universität zu Berlin. Some results of his thesis are summarized in his Scientific Highlights article, please see page 22.

Within the Leibniz Mentoring Program, Katharina Hopf was selected as a participant. The program supports highly qualified female post-doctorate researchers on their path to obtaining a professorship or some other leading position.



The AMaSiS 2021 Workshop "Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems," which dealt with the mathematical modeling, analysis, and simulation of semiconductors and electrochemical systems, took place September 6–9, 2021. It was organized jointly with Ansgar Jüngel from Vienna University of Technology, RG 2 *Laser Dynamics*, RG 3 *Numerical Mathematics and Scientific Computing*, and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*. The workshop was held online because of the pandemic. Moreover, the closing conference "Structures in Evolution: Theory and Applications" of the Thematic Einstein Semester "Energy-based Mathematical Methods for Reactive Multiphase Flows" funded by the Einstein Foundation Berlin was held February 23–25, 2021.

More detailed information on the group's achievements in 2021 is given below.

Effective models via homogenization

The derivation of effective models for problems with multiple scales is one of the central topics dealt with by RG 1 (see also the Scientific Highlights article on multi-scale chemical reaction systems on page 22). Novel and significant results were achieved in 2021, particularly in the derivation of homogenized models for systems with rapidly oscillating coefficients and random geometries.

Cosserat elasticity. The microstructure of engineered composites may introduce characteristic length scales giving rise to corresponding macroscopic properties that are vastly different from the underlying constitutive materials. When these characteristic length scales become comparable with the characteristic length of the microstructure, the classical theory of Cauchy continuum mechanics loses its accuracy in describing the mechanical behavior of such materials. A popular approach to study these size effects is to adopt a framework of generalized continuum mechanics, which naturally incorporates size effects through intrinsic length scale parameters. One of the earliest generalized continuum theories was that of the Cosserat brothers, who introduced the notion of couple stress. In [3], two different effective models from a heterogeneous Cosserat continuum are derived by taking into account the Cosserat intrinsic length of the constituents. The limit passage uses the theory of periodic unfolding, leading to a first rigorous proof of the results introduced in Forest, Pradel, and Sab, Int. J. Solids Struct., 2001. Depending on how different characteristic lengths of the domain scale with respect to the Cosserat intrinsic length, either effective Cosserat

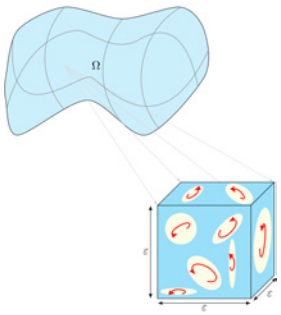


Fig. 2: *A Cosserat continuum characterized by a representative volume element of length* ε

or classical Cauchy continuum models are obtained. In the latter case, the effective moduli tensor depends on a standard set of local problems as in classical homogenization and on a set of local problems that contain the contribution of the rotations.

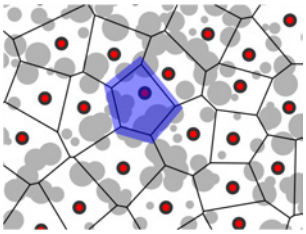


Fig. 3: *Cover of a stationary random open set (white) by Voronoi tessellation (black lines) with cell centers (red) inside the set. Cell centers have a positive minimal distance to the complement of the set (gray).*

Stochastic homogenization for random geometries. Real-world porous media typically exhibit a random geometry of the microscopic structure. In order to properly account for this, the development of stochastic homogenization methods has been a topic dealt with by RG 1 in the past years. Using newly developed techniques, it was possible to build up a framework to derive Poincaré and Korn inequalities for randomly perforated domains. Such inequalities are important tools for the analysis of PDEs as they allow proving compactness of the solutions in the homogenization limit. Furthermore, for the first time it was possible to provide a regularization technique in which a very irregular random geometry is approximated by a sequence of smoother random geometries that are easier to handle in homogenization limits. In a joint work with LG DYCOMNET *Probabilistic Methods for Dynamic Communication Networks*, it was proven that passing to the homogenization limit and afterwards passing to the limit in the regularization procedure leads to the expected homogenization behavior of PDEs, but it is ongoing work to show that the two limits permute.

Nano- and optoelectronic semiconductor devices

In this field, RG 1 cooperates with RG 2, RG 3, and LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*. In 2021, the incubator project "Electronic properties of gate-confined quantum dots in Si-Ge heterostructures for qubit generation" within the Berlin Mathematics Research Center MATH+ was approved.

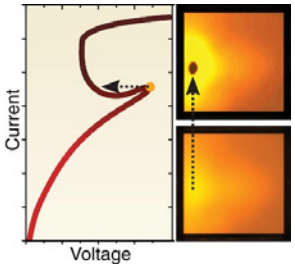


Fig. 4: *Tristability in the current-voltage relation of large-area organic LEDs and sudden burn-in due to self-heating effects*

Tristabilities in large-area organic LEDs. In cooperation with partners from experimental physics at Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, an undiscovered tristability in large-area lighting organic light-emitting diodes was identified. This tristability provokes switching processes and sudden burn-in phenomena in organic LEDs that cannot be prevented, neither by the current- nor by the voltage-controlled operation mode. By performing simulations of devices with a sufficiently large ratio of area to thickness, it could be demonstrated that there exist actually three stable operating branches for certain voltage ranges; see Figure 4. The description of the interplay of charge transport, Joule heating, and temperature activated electric conductivity is given via a $p(x)$ Laplace thermistor model that was established in a previous MATH$^+$ project.

Coupling atomistic and continuum models. Together with the Tyndall National Institute (Cork, Ireland), RG 3, and the Leibniz Group NUMSEMIC, a new theoretical multiscale framework was developed in [4] that connects atomistic effects, such as random alloy fluctuations, to macroscopic carrier transport in (InGa)N-based devices. In state-of-the-art transport calculations that account for alloy fluctuations, a combination of modified continuum-based models is used, which neglect to a large extent atomistic effects. The novel framework combines atomistic tight-binding theory and continuum-based drift-diffusion solvers, where quantum corrections are included via the localization landscape theory (LLT). In LLT, the stationary Schrödinger equation with single-band effective mass Hamiltonian and confining potential, e.g., from tight-binding calculations, is solved,

and an effective confining potential used in drift-diffusion simulations is extracted from its solution.

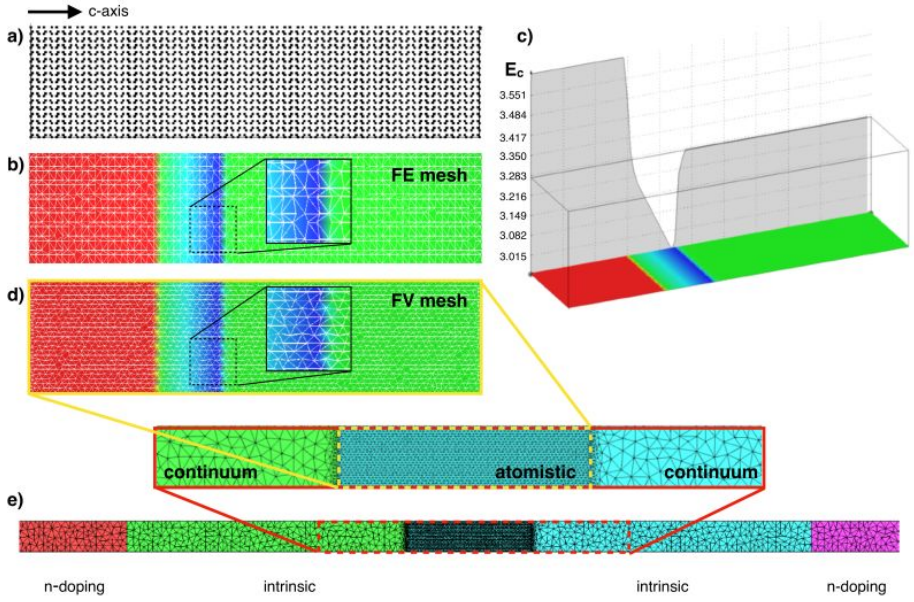


Fig. 5: *Transfer of local atomistic data to a larger finite-volume mesh for continuum-based drift–diffusion simulations*

Simulations reveal that both random alloy fluctuations and quantum corrections significantly affect the current-voltage characteristics of uni-polar electron transport in (In,Ga)N-based optoelectronic devices. The developed model and framework is flexible and will now help to guide the design of future energy efficient light emitters with new capabilities. The framework can be extended to ultraviolet wavelength emitters for biomedical applications or water purification.

Materials modeling

The research on this topic is done in cooperation with RG 4 *Nonlinear Optimization and Inverse Problems*, RG 5 *Interacting Random Systems*, and WG BIP *Modeling, Analysis and Scaling Limits for Bulk-Interface Processes* and is mainly driven by subprojects of the DFG Collaborative Research Center CRC 1114 *Scaling Cascades in Complex Systems* and the DFG Priority Program SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*.

Optimal control for tumor growth models. In recent years, the derivation of mathematical models to predict and control the evolution of malignant tumors in human tissue has drawn growing interest within the medical community. One important class of such models can be derived from the fact that all biological processes have to obey the universal principles of thermodynamics. Using as unknowns physical quantities like the chemical potential, the tumor fraction (which plays the role of an order parameter), and the nutrient extra-cellular water concentration, different thermodynamically consistent models for tumor growth have been devised. These models turn out to be strongly coupled systems of nonlinear partial differential equations that contain a so-called *Cahn–Hilliard structure* as a characteristic ingredient. In the past years, the Research Group has contributed numerous internationally leading papers to the study of such systems.

For the practical medical treatment of tumor patients, the solution of optimal control problems for such systems (e.g., optimal monitoring of the growth of the tumor fraction by supplying cytotoxic drugs in a chemotherapy) are of utmost importance. To avoid that the cancer cells develop a resistance against the drugs, it is desirable to apply them as seldom as possible. In [5], for the first time a related strategy of "time sparsity" was developed for an important class of tumor growth models.

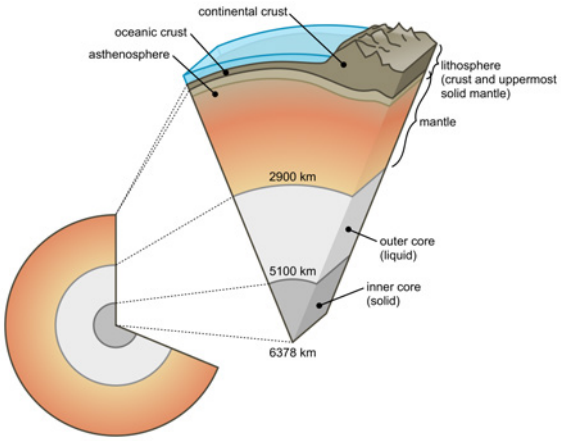


Fig. 6: *A schematic diagram of Earth's internal structure. The lithosphere consists of Earth's crust and the uppermost part of its solid mantle. In this region, rock deformation can be modeled as the flow of a viscoelastoplastic fluid.*

Viscoelastoplastic fluid models in geodynamics. Due to long time scales in geodynamics, the deformation of rocks in the lithosphere can be modeled as a fluid flow subject to viscoelastic and viscoplastic effects. In the context of subproject B01 of CRC 1114, the analytical study of such a viscoelastoplastic fluid model was initiated, where the stress tensor is transported along the flow with the Zaremba–Jaumann derivative and obeys a nonlinear and nonsmooth dissipation law. The latter is given in terms of a general dissipation potential and requires the introduction of a new solution concept composed of the classical weak formulation of the Navier–Stokes equations and a variational formulation of the stress evolution. The existence of such generalized solutions was shown globally in time in [2] under the assumption of stress diffusion, which ensured that the available a priori estimates were sufficient to treat the nonlinear terms. Moreover, the short-time existence of strong solutions as well as their uniqueness in the class of generalized solutions was shown together with RG 4 in the recent WIAS Preprint no. 2904, 2021 (T. Eiter, K. Hopf, R. Lasarzik: *Weak-strong uniqueness and energy-variational solutions for a class of viscoelastoplastic fluid models*). The underlying inequality for the relative energy also served as the basis for the definition of so-called *energy-variational solutions*, which are a generalization of the dissipative solutions introduced by P.-L. Lions for the Euler equations. In the framework of this solution concept, the a priori estimates are sufficient to pass to the limit of vanishing stress diffusion, which lead to global existence of energy-variational solutions also in this singular case.

Multicomponent fluid dynamics. New techniques were developed to handle the analysis of PDE models describing the transport of mass and the balance of momentum in homogeneous fluid mixtures. Moreover, important new results toward the justification of a thermodynamically consistent constitutive model for composite incompressible fluids were established. For an important part, these results were obtained in cooperation with the group of Dieter Bothe at the department

"Mathematische Modellierung und Analysis" of Technische Universität Darmstadt. In [1], it was shown that the basic equations of isothermal multicomponent fluid dynamics can be transformed into a system of mixed parabolic-hyperbolic type by an appropriate change of variables. We combine techniques used in compressible fluid dynamics with the theory of parabolic systems in the sense of Petrovski to show the local-in-time well-posedness of the PDE system in Sobolev spaces, yielding pointwise solutions. The general Maxwell–Stefan and Fick–Onsager forms of the diffusion fluxes are both included in the setting. In the recent WIAS Preprint no. 2869, 2021 (P.-E. Druet: *Maximal mixed parabolic-hyperbolic regularity for the full equations of multicomponent fluid dynamics*), these results are extended to the case of non-isothermal fluids. It is shown that solutions in the class of maximal regularity have strictly positive mass densities and bounded temperature as long as they exist.

The well-posedness for an isothermal model of multicomponent fluids subject to the volume constraint $\sum_{i=1}^{N} \rho_i/\rho_i^{\mathrm{ref}} = 1$ was established, where N is the number of species, $\rho_1, \dots, \rho_N$ are the partial mass densities of the species, and $\rho_1^{\mathrm{ref}}, \dots, \rho_N^{\mathrm{ref}}$ are the mass densities of the pure substances at reference temperature and pressure. This type of generalized incompressibility constraint was derived in a joint paper with RG 3 (WIAS Preprint no. 2825, 2021, D. Bothe, W. Dreyer, P.-E. Druet: *Multicomponent incompressible fluids – An asympotic study*, to appear in ZAMM) by performing the asymptotic limit in models for multicomponent fluids with small compressibility. Assuming that the variations $\partial_p v$ of the molar volume with respect to thermodynamic pressure tend to zero, the state of every composite incompressible fluid is subject to the linear constraint $\sum_{i=1}^{N} \rho_i v_i^{\mathrm{R}} = 1$. Interestingly, the Helmholtz free energy of the incompressible fluid is represented by a singular function of the main variables, and the free energies of the asymptotically approaching compressible systems tend to this singular limit in the sense of Γ-convergence.

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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 Lasse Ermoneit Alexander Gerdes Dr. Markus Kantner Lutz Mertenskötter 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 the RG 2 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, mainly in the field of *dynamical systems*. The research is mainly devoted to the application-oriented research topics *dynamics of semiconductor lasers* and *pulses in nonlinear optical media* and contributes to the WIAS core-expertise in *Modeling and Simulation of Semiconductor Devices*.

In 2021, external funding was received within the DFG Collaborative Research Center 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 the DFG-RSF projects (cooperation with Russia) "Underlying nonlinear science of hybrid SOA-fiber laser systems with feedback" and "Collective dynamics of heterogeneous networks of active elements." Furthermore, in 2021 we successfully completed a R&D project with the Ferdinand-Braun Institute for High-Frequency Technology (FBH) on numerical computation of the spectral linewidth of multi-section laser diodes [5]. With FBH, also a license agreement for the software BALaser (including support) concerning simulations of high-power broad-area semiconductor lasers, was extended for another two years. Further funding was granted for projects starting in 2022: The subproject AA2-13 "Data-driven stochastic modeling of semiconductor lasers" within the Cluster of Excellence MATH+ (until 2024, together with FBH and Technische Universität (TU) Berlin), the project *UV Lasers: From Modeling and Simulation to Technology (UVSimTec)* within the Leibniz competition (together with RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, TU Berlin, Universität Erlangen–Nürnberg, Leibniz-Institute for Crystal Growth, and FBH), and the DFG-ANR project (cooperation with France) "Hybrid chip-scale frequency combs combining III-V quantum-dash mode-locked lasers and high-Q silicon-nitride microresonators" (joint project with Karlsruher Institut für Technologie).

In summer 2021, the group organized the international workshop "Nonlinear Dynamics in Semiconductor Lasers" (NDSL 2021) which was held fully online. The program included 45 talks and

a poster session that covered a wide range of topics from theory and mathematical modeling to experiments and applications. The workshop attracted almost 100 registered participants from 16 countries. Furthermore, the group co-organized the workshop "Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems" (AMaSiS 2021) together with RG 1, RG 3 and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*.

In June 2021, Markus Kantner participated in the 70th Lindau Nobel Laureate Meeting (interdisciplinary) as a candidate of the Leibniz Association. The invitation to the meeting is an exceptional honor for selected young scientists, who have the opportunity to attend lectures by Nobel Laureates from all disciplines and to discuss with them in numerous networking meetings. Due to the pandemic situation, the event was held online, but accepted young scientists are invited to attend the next meeting of their specific discipline on site (73rd Lindau Nobel Laureate Meeting – Physics, 2024).

Fig. 1: *70th Lindau Nobel Laureate Meeting*

Dynamics of semiconductor lasers

Passive mode-locking. Passive mode-locking is a very powerful technique for generating high-quality picosecond and sub-picosecond pulses with fast repetition rates, and ongoing efforts are still devoted to the design of improved devices producing shorter and shorter pulses. A universally adopted model for pulse amplification and shaping in mode-locked (ML) lasers was developed in the 1970th by H.A. Haus, and since then different modifications of the Haus model assuming slow and fast gain recovery were developed. None of them, however, are able to simultaneously account for both the slow gain evolution from one round trip to the next and fast gain variations within a cavity round trip time. To fill this gap we derived a generalized Haus model from the delay-differential equation (DDE) model of a ML laser using a multiscale method. With the help of numerical simulations, it was shown that unlike the conventional class-B laser Haus models, the generalized model is able to describe not only the Q-switching instability of the fundamental ML regime, but also the pulse leading edge instability leading to harmonic ML regimes with the increase of the pump power (see Figure 2).

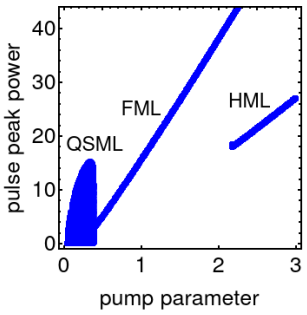

Fig. 2: *Bifurcation diagram illustrating dynamical regimes of the generalized class-B laser Haus model*

Nonlinear mirror ML lasers. Among different approaches to achieve mode-locking in lasers, a promising one relies on the use of the nonlinear optical mirror – nonlinear amplifying loop mirror (NOLM-NALM) principle, which contains a bidirectional loop with an asymmetrically located absorber or gain medium and a nonlinear element. We developed a DDE model of a NOLM-NALM ML laser [4] that takes into account finite relaxation rate of the gain medium and asymmetric beam splitting at the entrance of the nonlinear mirror loop. Using the DDE NOLM-NALM ML laser model, we investigated analytically the stability and bifurcations of continuous wave solutions in the limit of large delay. Numerical simulations revealed large domains of fundamental and harmonic ML regimes in the parameter space. It was shown that both the inversion relaxation rate and beam splitting ratio can strongly affect the dynamics of the system and the existence domains of stable ML regimes.

Fourier domain ML lasers. The dynamics of semiconductor lasers with a fiber-based unidirectional ring cavity that can be used as frequency-swept sources was investigated [3]. We studied the key factors behind the rich dynamical behavior of such lasers using state-of-the-art experimental and analytical methods. Using a DDE model, which can approximately describe a linear fiber delay line, it was demonstrated that the presence of chromatic dispersion can lead to a destabilization of the laser modes through modulational instability, resulting in undesirable chaotic emission. The instability threshold was characterized both theoretically and experimentally, and deterioration of the Fourier domain ML regime near the threshold was demonstrated.

High-power semiconductor lasers. The modeling, simulation, and analysis of high-power broad-area semiconductor lasers and coupled laser systems remains an important topic of our research. Together with the colleagues from FBH, we analyzed the performance of a broad-area laser containing a passive distributed Bragg reflector (DBR) at its rear facet and a longitudinal-lateral gain-loss-index modulation of the amplifying part of the device [6]. In experimental systems, modulation in both directions is achieved by alternating contacted and uncontacted regions and by additional etching of rectangular trenches beneath the uncontacted regions; see Figure 3 (a).

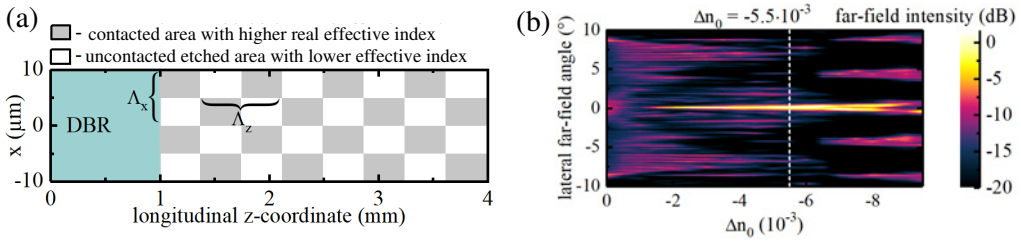

Fig. 3: Sketch of a periodically modulated broad-area laser (a) and its performance in dependence on the built-in refractive index difference Δ_{n0} (b)

The longitudinal and lateral periods Λ_z and Λ_x, see Figure 3 (a), are selected according to the Talbot-type condition $2\Lambda_x^2 n_{\mathrm{eff}}/\lambda_0 = \Lambda_z$, with n_{eff} and λ_0 denoting the effective refractive index and the central wavelength, respectively. This modulation utilizes the near-field diffraction properties and, for a proper refractive index difference induced by the trenches, see Figure 3 (b), allows diminishing the far-field divergence in simulations performed with our combined dynamical electro-optical-thermal solver `BALaser`.

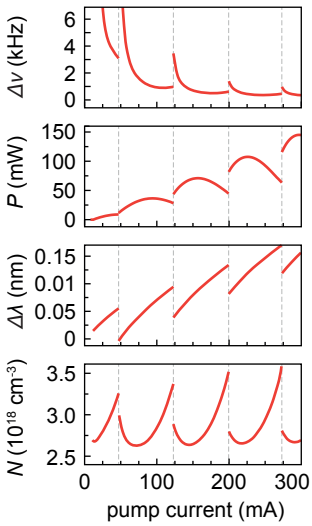

Fig. 4: Spectral linewidth, optical power, relative wavelength shift, and average carrier density in an ECDL vs. pump current [5]

Narrow-linewidth lasers are key elements of high-precision metrology systems including atom interferometers, optical atomic clocks, or gravitational wave detectors. These applications require sources of highly coherent laser light (and thus lasers with a narrow spectral linewidth), which is limited by numerous stochastic processes in the device (spontaneous emission into the laser mode, carrier recombination noise, pump current fluctuations, etc.). In the framework of the semi-classical laser theory, random fluctuations are described by Langevin equations, i.e., stochastic (partial) differential equations, where the noise correlation functions are derived from a quantum field theoretical treatment. We have reviewed the standard linewidth theory for semiconductor lasers with Markovian noise sources (white noise) and performed numerical computations of the linewidth (and several other critical lasing characteristics) for spatially-resolved multi-section laser diodes [5]. The numerical results were obtained using the software package `LDSL-tool`,

which simulates the dynamical traveling wave model. The software package was extended towards the computation of linewidth characteristics within the scope of an R&D project together with the FBH. In Figure 4 the spectral linewidth and further laser characteristics of a 4 mm long extended cavity diode laser (ECDL) are shown as a function of the pump current.

Further advancement of the current stochastic laser theory beyond the white noise limit requires the inclusion of non-Markovian noise sources (colored noise), which are known to cause a broadening of the laser linewidth. Such processes have become a limiting factor in laser interferometry applications and require better theoretical understanding. This problem is the subject of the new MATH+ project AA2-13 "Data-driven stochastic modeling of semiconductor lasers," which is a cross-institutional project between WIAS, FBH, and TU Berlin.

Pulses in nonlinear optical media

Optical microcavity solitons. Optical frequency combs generated by microcavities have revolutionized such fields of science and technology as high-precision spectroscopy, metrology, and photonic analog-to-digital conversion. In our research, a special attention was given to the frequency comb generation in the dissipative soliton (DS) regime when one or more short pulses circulate in the cavity. Being well separated from one another, two DSs can interact via their exponentially decaying tails. We derived an asymptotic equation governing the slow evolution of the coordinates of the interacting DSs in the Lugiato–Lefever equation with small forth-order dispersion and spectral filtering terms. It was shown that Cherenkov radiation due to the fourth-order dispersion can strongly enhance the DS interaction and lead to a formation of a large number of DS bound states. Finally, it was found that, in the case of a vanishing spectral filtering coefficient, DS bound states can undergo an oscillatory instability even when a single DS in the cavity is well below the Andronov–Hopf bifurcation threshold.

Additive splitting methods. The decomposition of an evolution operator into linear and nonlinear sub-operators followed by the application of a numerical splitting scheme, such as commonly known Strang or Yoshida splittings, is a popular method for simulations of pulses in nonlinear media. If the sub-operators turn out to be sufficiently simple, the resulting scheme is extremely efficient and can be calculated in parallel. On the other hand, the classical splitting methods have their limitations. Especially the one-dimensional Fourier transform, which is commonly used to simulate pulses in fibers, does not scale well with the number of available computer cores. We found a class of alternative additive splittings, which by construction can be calculated in parallel on a shared memory system for literally any splitting. One deals with a concurrent computation: The initial problem is divided into independent sub-tasks, and all available computer cores just go through these tasks one by one until a common synchronization point is reached. For a fixed time-discretization step τ, our additive schemes suffer from only a slight decrease in speed due to synchronization. In return, they offer a much better accuracy; see Figure 5.

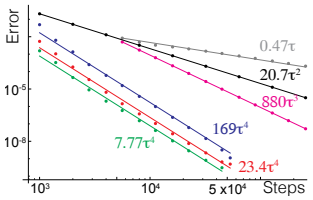

Fig. 5: *Errors of the new additive schemes (green and red lines) versus the classical multiplicative methods, [1]*

The first such scheme was found by trial and error using computer algebra, later on we discovered a general theory, which is based on the Baker–Campbell–Hausdorff formula. In addition, the new

schemes turn out to be more stable than the standard splittings; see Figure 6. The reasons of this welcome behavior remain to be found.

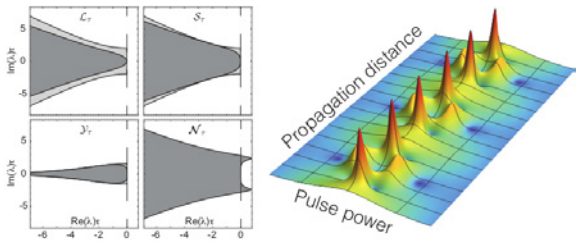

Fig. 6: *Left: Stability domains of different methods. The new scheme (bottom right) is the most stable one. Right: A typical calculation of a third-order soliton propagation, which was used to test numerical solutions, [1].*

Theory of dynamical systems

The mathematical research on Dynamical Systems provides the theoretical background for the applied topics in optoelectronics and nonlinear optics of RG 2. Ongoing work within the Collaborative Research Center 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application* is related to temporal dissipative solitons in delay-differential equations and collective dynamics in large coupled systems. An important result in the field of formation of coherence-incoherence patterns was obtained in [2], where for the first time a supercritical bifurcation for the emergence of such patterns was presented and a relation to the classical Turing instability was demonstrated.

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4.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

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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. Some research topics of the group are briefly described below. A further topic, partially covered in the Scientific Highlights articles "Perovskite Models, Finite Volume Methods and Painless Simulation" on page 33 and "Model-based Geometry Reconstruction of Quantum Dots from TEM" on page 28, is the modeling of processes in semiconductor devices and electrochemical systems as well as numerical methods for performing simulations based on these models.

Gradient-robust discretizations for computational fluid dynamics

Gradient-robust discretizations have been an ongoing research topic in RG 3 for several years. They aim to repair the incorrect balancing of irrotational and divergence-free forces in the discrete momentum balance of the Navier–Stokes equations to avoid possibly large discretization errors. Gradient-robustness extends the initial research on pressure-robustness in the incompressible case to well-balanced schemes for compressible fluids at low Mach numbers. In the recent year, the focus was on incompressible model problems to investigate new tools for efficient convec-

tion stabilization and to guarantee a posteriori error control suitable for divergence-free or other pressure-robust methods.

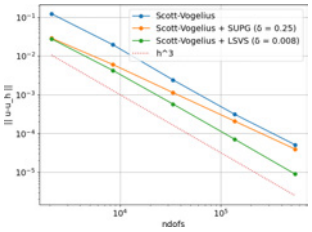

Fig. 1: *Convergence history of the velocity error of the Scott–Vogelius FEM with novel LSVS (green), classical SUPG (orange), or no (blue) stabilization in a planar lattice flow test problem*

Based on the observation that the velocity field is only steered by the vorticity, a novel convection stabilization was suggested in [1] that involves a volume term based on the residual of the (pressure-free) vorticity equation and an additional penalty term on the jump of convective gradients over element faces. It was shown that this approach yields optimal velocity error estimates for several divergence-free pressure-robust schemes for a class of generalized Oseen problems. Figure 1 shows a comparison of the novel stabilization versus a classical streamline-upwind Petrov–Galerkin (SUPG) stabilization or the Galerkin discretization without any stabilization for the divergence-free Scott–Vogelius finite element method on a series of unstructured meshes in a manufactured Oseen test problem for the planar lattice flow $\mathbf{u}(x,y) = (\sin(2\pi x)\sin(2\pi y), \cos(2\pi x)\cos(2\pi y))$ and viscosity $\mu = 10^{-5}$.

Efficient guaranteed error control allows for sharp stopping criteria and adaptive mesh refinement and can be achieved by constructing equilibrated fluxes of the mixed stress, here the gradient of the velocity. For pressure-robust discretizations in the incompressible Stokes setting, these fluxes have to satisfy a certain carefully discretized equilibrium constraint to imply pressure-robust guaranteed upper velocity error bounds. For this approach, a general framework was derived in [5], and novel global and local designs of such equilibrated fluxes were suggested. They are based on a recently developed mass-conservative mixed stress method, and the so obtained upper bounds are shown to be efficient, independently of the exact pressure.

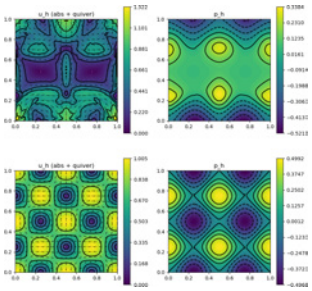

Fig. 2: *Classical (top) and p-robustly modified (bottom) Bernardi–Raugel FEM solutions for a planar lattice flow with $\mu = 2 \cdot 10^{-4}$ (steady Navier–Stokes equations)*

The Julia package `GradientRobustMultiPhysics.jl` focusing on gradient-robust schemes, like a modified Bernardi–Raugel method as in Figure 2, and multi-physics applications was further matured and is or will be used in several external and internal cooperation projects. A recently started project with Winnifried Wollner (TU Darmstadt) investigates gradient-robust schemes for reducing the influence of irrotational data errors in optimal flow control problems. A DFG-granted project conducted together with Sebastian Matera (Fritz-Haber Institute, Berlin) starting 2022 will employ gradient-robust schemes as part of a multi-scale simulation of heterogeneous catalysis in in-situ surface characterization experiments involving stationary low Mach number gas flows.

`GradientRobustMultiPhysics.jl` is also used in internal collaborations beyond the scope of gradient-robust schemes. An ongoing collaboration with RG 4 *Nonlinear Optimization and Inverse Problems* aims at the analysis and development of adaptive stochastic Galerkin finite element methods, e.g., for the lognormal Darcy equation for groundwater flow modeling. This research comprises an efficient sparse implementation as well as efficient a posteriori error control. In the ongoing collaboration with LG NUMSEMIC *Numerical Methods for Innovative Semiconductor Devices*, this code supports the electro-mechanical simulation and study of bending nanowires. Here, in particular the automatic differentiation features come in handy to avoid hand-written Jacobians.

Numerical methods for cardiovascular and tissue modeling

Medical imaging is a pillar of clinical diagnostics, as it allows to obtain, in vivo and non-invasively, important anatomical and functional information related to biological flows and tissues. These

data, in connection with mathematical and computational models able to describe the underlying physics and biology, can be used to correlate the observations with biomarkers that can characterize the presence or the stage of pathologies, such as cancer, fibrosis, or cardiovascular anomalies.

The resulting data assimilation problem, i.e., the incorporation of available data into a mathematical model, requires the combination of efficient and robust schemes for the solution of PDEs describing the forward problems (e.g., flow or tissue mechanics), with techniques for model-order reduction and numerical methods for the solution of inverse problems. From the practical point of view, the major challenges are represented by the availability and quality of data, as well as by the resolution, which is typically coarser than the scale of the physical model considered.

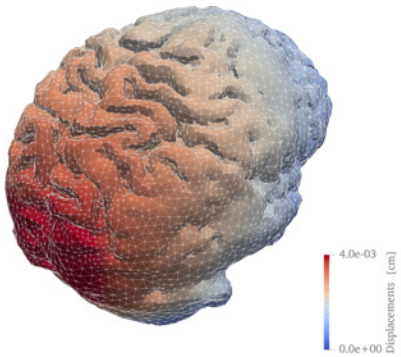

Fig. 3: *Numerical simulation of brain tissue displacement during a magnetic resonance elastography examination*

One application, which is currently subject of an interdisciplinary collaboration, together with RG 6 *Stochastic Algorithms and Nonparametric Statistics* and the Institute of Radiology of the Charité (Ingolf Sack), concerns the reconstruction of full three-dimensional displacement images of brain tissues from partial elastography data (Figure 3).

Inverse problems (such as data assimilation) typically require several numerical solutions of underlying forward problems. In order to reduce the overall computational cost, it is therefore important to consider reduced-order models that, constructed by using the geometrical or physical properties, allow to efficiently recover selected quantities of interest with satisfactory accuracy.

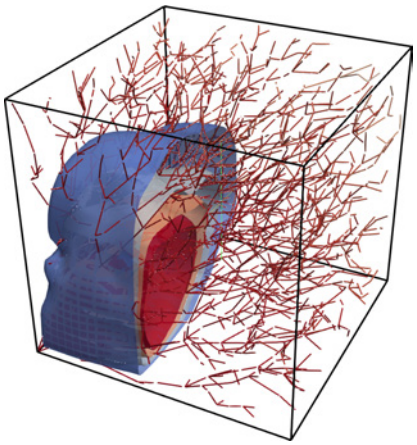

Fig. 4: *Simulation of elastic displacement (iso-surfaces) in a tissue sample induced by a pressure pulse in the vasculature (red segments)*

One example is the numerical simulation of vascularized tissues, where, due to the scale and the complexity of micro- and mesovasculature, full three-dimensional models describing separately

fluid vessels and tissue are computationally infeasible. To address this issue, a multiscale (3D-1D) immersed method was proposed in [3], in which the effect of a network of thin vessels (vasculature) inside a tissue sample can be approximated by a sum of hyper-singular terms located along the centerlines of the vessels. The method was validated on a synthetic tissue benchmark (Figure 4), and will be extended to more general cases in upcoming work.

The interplay of different scales in inverse problems was investigated from a theoretical perspective in [2], considering the problem of estimating microscale parameters from coarse scale data. The proposed approach is based on the numerical homogenization technique. In particular, it is shown how to reconstruct a discrete (finite element) model that can account for microstructures without explicitly resolving them in the geometrical discretization.

A SUPG-POD-ROM method for convection-diffusion equations

The goal of reduced-order models (ROMs) consists in performing very efficient simulations of time-dependent problems. To this end, a finite element simulation is performed as a pre-processing step, whose results are utilized for computing a basis of the ROM via a proper orthogonal decomposition (POD). This basis, consisting only of very few functions, contains already information on the solution. It can be used for simulating problems that are in some sense close to the problem from the pre-processing step, e.g., having slightly different data.

For convection-dominated problems, so-called *stabilized discretizations* have to be applied. The streamline-upwind Petrov–Galerkin (SUPG) method is among the most popular ones. In [4], an error analysis of a SUPG-POD-ROM is presented. Robust estimates for the error of the SUPG-POD-ROM solution with respect to the weak solution of the equation are derived, i.e., the constants in the error bounds do not blow up as the diffusion coefficient tends to zero. It is the first time that this kind of bounds is proved for POD-ROM models. An essential feature of the method is that the set of snapshots does not only contain the functions at the time instants but also approximations of the temporal derivative. The analysis is based on an appropriate decomposition of the error, involving the projection of the finite element solution onto the POD space.

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4.4 Research Group 4 "Nonlinear Optimization and Inverse Problems"

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Deputy Head:	Priv.-Doz. Dr. René Henrion
Team:	Dr. Ingo Bremer Moritz Ebeling-Rump Priv.-Doz. Dr. Martin Eigel Robert Gruhlke Dr. Holger Heitsch Dr. Robert Lasarzik 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.

In the reporting period, the group was successful in raising third-party funds in cooperation with European and German partners. An ANR-DFG French-German collaborative project together with Antony Nouy (Nantes) on compositional functions networks will start in March 2022. As a part of the "European Metrology Program for Innovation and Research" (EMPIR) in collaboration with Physikalisch-Technische Bundesanstalt and under the umbrella of the joint initiative of Berlin's non-university research institutions BR50, a Ph.D. project on "Machine learning for inverse problems with continuous normalizing flows" will be launched. Moreover, the group succeeded in acquiring a project in the newly started Priority Programm SPP 2298 *Theoretical Foundations of Deep Learning* and a new Berlin Mathematics Research Center MATH+ project on the control and optimal design of minigrids for rural Africa.

In the following, selected scientific achievements of the research group in 2021 are detailed.

Stochastic and nonsmooth optimization

As in previous years, the research on stochastic and nonsmooth optimization was mainly driven by projects within the programs DFG Transregio (TRR) 154, MATH+, and Gaspard Monge Program for Optimization (PGMO) funded by Fondation Mathématique Jacques Hadamard. The PGMO project – whose funding has been renewed for another year – is devoted now to the derivation of necessary optimality conditions for and the numerical solution of optimal control problems under probabilistic endpoint constraints. Within MATH+, work on the running project was continued and a new project could be acquired for the next funding period. Its topic is the optimal control of

weakly coupled mini-grids under consideration of uncertainties (renewables, local demand, outages of main grid). The aim is to control the probability of successful islanding (survival of local net in case of an outage of the main grid). Current work focuses on modeling aspects. Regarding the Transregio TRR 154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks*, the main concern was the successful termination of the second and preparation of a possible third funding period. The research here turned around probabilistic equilibrium problems as they arise in gas markets (Figure 1, left). The earlier introduced class of probust (probabilistic/robust) optimization problems (see [1]) was applied to new problems in gas network optimization, such as capacity maximization under transient flow and probabilistic demand satisfaction). The main numerical instrument in dealing with probabilistic constraints requires the computation of spheric integrals in order to evaluate multivariate probabilities (and their sensitivities) of elliptically symmetric distributions. The need for efficient uniform sampling schemes on the sphere leads to the notion of spherical cap discrepancy. In the Scientific Highlights article on page 16, an explicit enumerative formula for this well-known measure of quality was provided and applied to different sampling methods (see Figure 1, right). Apart from the project-driven research, a new cooperation with Abderrahim Jourani (Dijon) and Boris Mordukhovich (Detroit) was initiated on the topic of optimal control of polyhedral sweeping processes.

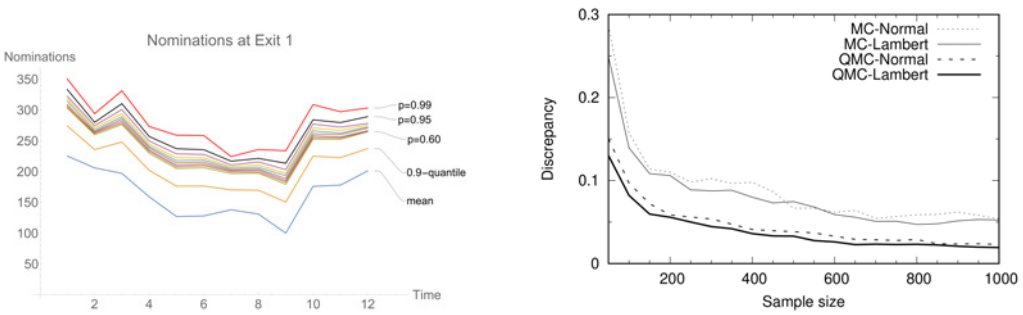

Fig. 1: *Left: Nominations for an exit of a gas network at market equilibrium under increasing probabilities of load coverage. Right: Spherical cap discrepancy for different uniform sampling schemes on the sphere.*

Inverse problems for stochastic data and reconstruction of stochastic surfaces

Several new methods based on modern hierarchical tensor compression were developed. Using an empirical tensor regression, an adaptive non-intrusive Galerkin method was devised. The analysis and control of stochastic errors hinges on previous results for the Variational Monte Carlo method, relying on statistical learning theory. It is one of the few methods that allow reliable error estimates and adaptivity with non-affine data, i.e. in particular, models with lognormal coefficients.

In collaboration with RG 6 *Stochastic Algorithms and Nonparametric Statistics*, an efficient compression technique for popular option pricing methods was developed [2]. It was shown that the "curse of dimensionality" can be alleviated for the computation of Bermudan option prices with the Monte Carlo least-squares approach as well as the dual martingale method, both using high-dimensional tensorized polynomial expansions.

A novel method for nonlinear optimal control problems was developed that yields a true feedback controller and has greatly reduced computational cost compared to current state-of-the-art

methods [5]. The method is based on policy iteration, linearizing the Hamilton–Jacobi–Bellman equation and a modification of the Dirac–Frenkel variational principle. On a challenging benchmark task, this method was shown to achieve similar performance as state-of-the-art methods (see Figure 2) with computation time reduced by an order of magnitude.

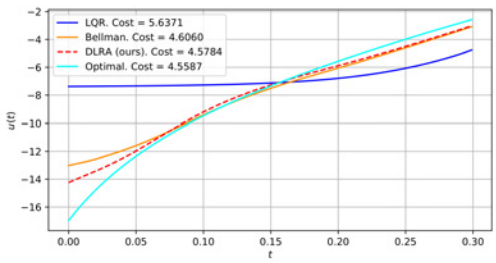

Fig. 2: *Comparison of different controllers $u(t)$ on a 12-dimensional semi-discretized heat equation with unstable reaction term. The dynamical low-rank approximation (DLRA) method outperforms (i.e., achieves lower cost than) the linear quadratic regulator (LQR) as well as the state-of-the-art Bellman method, while requiring less computation time.*

Possibilistic and probabilistic tools for the assimilation, description, and propagation of material imperfections were studied [4]. A fuzzy-set approach was developed in cooperation with Dieter Moser (Aachen) for the description of the interface design of matrix composite materials; see Figure 3. For this, a high-dimensional parametric effective material forecast was realized with low-rank tensor train compression, which led to efficient acceleration and emulation for the underlying optimization tasks necessary for the propagation of fuzzy sets.

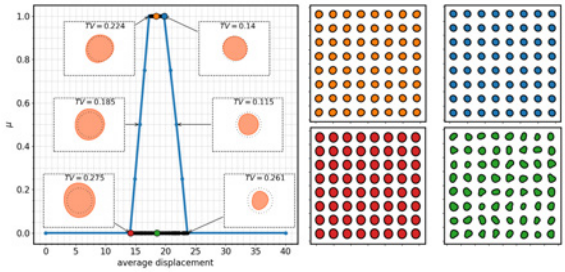

Fig. 3: *Result of the possibilistic propagation based on fuzzy sets. A best-worst case analysis was performed to bound the effect of the average displacement of upscaled composite material based on variable shapes of the underlying composite structure.*

The detection of irregularities close to surfaces is an important issue with applications from searching for minerals in geology to the analysis of defects of micro- and nanostructures. Non-destructive methods utilize the response of different kinds of waves for the localization and shape reconstruction of such irregularities.

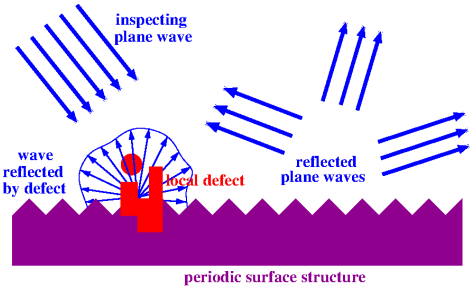

Fig. 4: *Scheme of scattering by surface with local defect: Total wave is superposition of incoming plane wave, plane waves reflected by ideal surface structure, and extra field due to defect*

In cooperation with Xiuchen Yu and Wangtao Lu (Tianjin) and Guanghui Hu (Hangzhou) (cf. [7]), a model of a periodic background geometry and of time-harmonic acoustic and electro-magnetic inspecting waves with sound-soft and perfectly conducting boundary conditions, respectively, was investigated. A finite element method (FEM) solver was designed. The domain of the wave equation is the half space bounded by a periodic surface with a local perturbation, and the solution, satisfying the Sommerfeld half-space radiation condition, is either the total wave for point source illumination or the deviation from the solution of the ideally periodic case for plane wave incidence (cf. Figure 4). Introducing a finite layer over the boundary together with a small perfectly matched layer (PML) above it and requiring a homogeneous boundary condition at the upper end of the PML reduces the FEM domain to a layer. In a second step, the layer of infinite extent is reduced to a finite domain containing the non-periodic irregularities by imposing lateral boundary conditions with Neumann–to–Dirichlet operators (NtD).

Optimal control of multifield and multiscale problems

One focus of this year's research was on introducing techniques from optimization into the existence theory of nonlinear evolutionary partial differential equations (PDEs). By introducing energy-variational solutions in the context of incompressible fluid dynamics, it was possible to show that these solutions enjoy different desirable properties. Beside the fact that the solution set is convex and weakly* closed, it depends continuously on the given data in a set-valued sense. Additionally, concatenations and restrictions of these solutions are solutions again. Interestingly, minimizing the energy over the set of energy-variational solutions gives a unique solution, which turns out to be a weak solution again and thus enjoys additional regularity. This implies that some compactness is achieved via optimization, which hopefully is a new insight for the analysis of PDEs in general [6]. A similar concept was used in a collaboration with RG 1 *Partial Differential Equations*, where energy-variational solutions were used to prove the existence of solutions to a viscoelasto-plastic model appearing in geodynamics. This model includes dissipation from a nonsmooth potential, which gives rise to the plastic behavior. This nonsmooth convex potential together with the non-standard objective derivatives is difficult to treat analytically. By combining the energy-variational formulation with an evolutionary variational inequality, a promising solvability concept is introduced and analyzed. This approach paves the way for future collaborations with RG 1 on generalized solution concepts for nonlinear evolutionary PDEs.

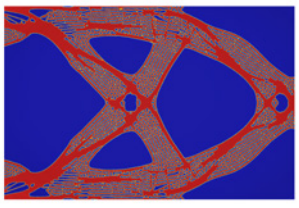

Fig. 5: *Structure with local volume constraint, where the allowed local material percentage depends on the local stress values*

Another focus of last year's work was topology optimization for additive manufacturing. There, the creation of porous infill structures is desirable in order to increase the surface to volume ratio of the structure, which leads to better thermal or acoustic isolation and can improve the stability with respect to buckling. In the recent preprint [3], a novel two-scale topology optimization approach was introduced, which relies on a minimization problem with global and local volume constraint, where the local volume constraint depends on the stress of the associated mechanical problem. A calculated structure can be seen in Figure 5.

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4.5 Research Group 5 "Interacting Random Systems"

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Secretary:	Christina van de Sand

During 2021, the Research Group RG 5 *Interacting Random Systems* continued its research efforts on large systems with complex interactions and random effects in spatial environments. Most of this work focused on large collections of particles that interact with each other where either the interaction or the environment exhibits randomness. The applications and motivations for the research can generally be found in questions arising in materials science, chemistry, and physics.

In 2021, there have been a lot of changes in the composition of the group members: an outsourcing of the topic "mobile communication" into a newly founded group, a loss of a member to an assistant professor position in Italy, and an enhancement by three new members, two of which in projects funded by the German Science Foundation priority program *Random Geometric Systems (SPP 2265)* and led by members of the group. These changes implied a stronger focus on spatially oriented models and introduced new topics to the group, like random graphs and continuous-space Gibbs measures on point processes with marks.

The group further seeks to apply its knowledge to questions arising in other fields. In recent years, the most prominent example of this was a very productive program modeling mobile communication networks with large numbers of connected devices. This research was so successful that an extra group, the LG DYCOMNET *Probabilistic Methods for Dynamic Communication Networks* is funded by the Leibniz Association and led by Benedikt Jahnel, the senior scientist who was previously coordinating this topic within the RG 5. He also put a highlight in early 2021 by finishing his habilitation procedure at Technische Universität Berlin; a milestone that had been prepared for entirely during his time within the RG 5. The LG DYCOMNET began its independent work this year and reports separately on it. Certainly, the RG 5 and LG DYCOMNET have worked closely together. The group is also occasionally involved in research on interacting random systems that arise in numerical or computational settings; the most recent example of this kind is discussed below under the heading "Asymptotics of the Stein variational gradient descent."

It is a pleasure to report that Luisa Andreis has become an assistant professor in Florence. She continues to work with the RG 5 on ongoing projects, in particular, in the context of SPP 2265 project

"P01: Spatial coagulation and gelation." This project and the other one in this SPP, "P04: The statistical mechanics of the Brownian interlacement process," ultimately focus on the emergence of macroscopic features in systems of spatially distributed microscopic particles, more precisely, the gelation of coagulating particles and Bose–Einstein condensation of random structures with unbounded sizes, respectively. They provide additional impetus to work of the research group on questions regarding the interplay between randomness, geometry, and position.

The year 2021 saw comparatively little physical travel and conference organization in the group reflecting the public health situation. At the same time, online and hybrid formats continued to establish themselves as methods for the presentation of results although video conferencing does not seem to be a good substitute for informal and exploratory scientific discussions in person. One member of the RG 5 was part of the organizing committee for the hybrid workshop "Junior Female Researchers in Probability," which took place with around sixty participants on site and further colleagues listening online.

An overview of three achievements by members of theRG 5 covering topics from random graphs, stochastic numerics, and self-repellent random walks in random medium is given below. Further topics studied in the group during 2021 include large deviations and variational representations of the limiting dynamics for interacting particle systems of chemical reaction type, large deviations for the entire cluster structure of a random inhomogeneous Erdős–Rényi graph, condensation phenomena of Bose–Einstein type, and the gelation phase transition in models of coagulating particles.

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 subjects. Some of the members also did this independently. A further member of the group gave a lecture course at Freie Universität Berlin.

Asymptotics of the Stein variational gradient descent

When analyzing or learning from large data sets as well as when simulating complex physical models, one often needs to analyze probability distributions on $\mathbb{R}^d$ of the form $\pi(\mathrm{d}x) = \mathrm{e}^{V(x)}\,\mathrm{d}x/Z$, where Z is a normalization constant and V some given potential. In particular, calculating the partition function Z efficiently is a hard task. This problem becomes very difficult and computationally intensive in practically relevant settings where d is large. Two families of methods that aim to strike a balance between cost and quality are available: First, *variational inference*, where one averages over a large family of N particles, and second, *Markov Chain Monte Carlo*, where one averages the behavior of a cleverly designed Markov process over a long period of time of length T. These methods are designed in such a way that as N, respectively T, becomes large, the averages become increasingly good approximations of the target distribution π.

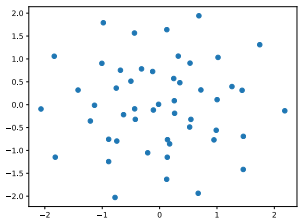

Fig. 1: *Stein approximation of a measure in two dimensions using a Gauss kernel*

The recently developed *stochastic Stein variational gradient descent* combines these two approaches by considering a system of coupled stochastic differential equations (SDEs) describing the random movement of N interacting particle positions in $\mathbb{R}^d$ on a large time interval of length T. The dynamics of the particles are chosen in such a way that both in the limit $N \to \infty$ and in the limit $T \to \infty$ the time average over $[0, T]$ of the mean of the N particle positions converges to π.

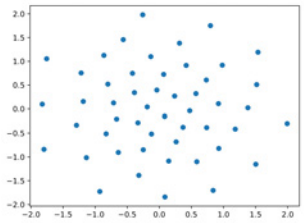

Fig. 2: *Stein approximation of a measure in two dimensions using a Matern kernel*

In the paper [1], the exponential speed of this convergence was studied by a member of the group via large-deviation principles, a technique used widely in the RG 5. The first result showed that for fixed T as $N \to \infty$, the paths of the N-particle averages (mean field) are in distribution exponentially attracted to some particular path on $[0, T]$ with an explicit formula for the exponential rate of the probabilities of deviations from it. This result showed a crucial connection to the known non-stochastic Stein variational gradient descent. In the second result, it was shown by Γ-convergence that the above-mentioned exponential rate as $T \to \infty$ is proportional to some explicit functional that can be interpreted as a *Fisher information*. As the used SDEs depend on the choice of a sufficiently regular kernel, faster rates of convergence are expected for kernels for which this functional is larger. This claim is vaguely supported by some preliminary simulations. Compare Figure 1 and Figure 2, where one sees a less regular distribution of points obtained using a Gauss kernel $\exp(-|x-y|^2)$ (low Fisher information) than with a Matern kernel $\exp(-|x-y|)$ (high Fisher information).

Condensation phenomena in evolving networks

Networks that emerge from complex systems of interactions, such as the internet or other systems in sociology or biology, are often *scale free*, which refers to the fact that the number of nodes with degree (the number of edges ending at the node) k scales like $k^{-\tau}$ for a critical exponent $\tau \in [2, 3]$. One consequence of this fact is that the network displays the *small-world phenomenon* with diameter and typical distances growing very slowly with network size (logarithmic or even slower).

Fig. 3: *An example of a complex network; a graph illustrating a social network of members of the International Committee on Intellectual Cooperation, by Martin Grandjean, La connaissance est un réseau; Les Cahiers du Numérique 10 (3): 37-54. DOI:10.3166/LCN.10.3.37-54., CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=29364647*

The simplest mathematical models for network growth do not reproduce the scale-free property; however, the *preferential attachment model* overcomes this limitation. In this model, nodes arrive in the network one at a time and connect to previous nodes with probability proportional to their degree. An extension of this model, which seeks to capture the inherent inhomogeneities of real-world networks, assigns positive "weights" to each node, so that new nodes attach to existing nodes with probability proportional to either the product or the sum of their weight and their degree. In the product case, a condensation phenomenon can occur; heuristically, this means that nodes of weight that are closer to the maximal possible value have a disproportionately larger number of connections in the network than otherwise.

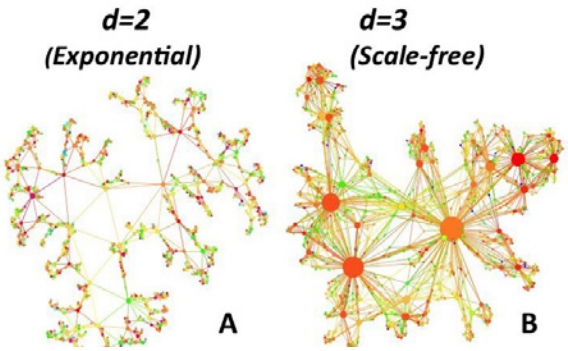

Fig. 4: *The model of evolving simplicial complexes studied in [4], which displays a scale-free degree distribution when $d > 2$ (as we proved in [2]). Illustration obtained from [4], reproduced under the CC BY 4.0 license.*

With colleagues we are investigating preferential attachment models incorporating higher-dimensional interactions: Newly arriving vertices take into account the weights of multiple vertices, and may connect to one or more vertices upon arrival. In [2], we studied a preferential attachment model of simplicial complexes. We found a limiting formula for the degree distribution and, in the process, rigorously confirmed conjectures from physics in regard to the scale-free nature of the degree distributions for a class of these models with interaction dimension $d > 2$.

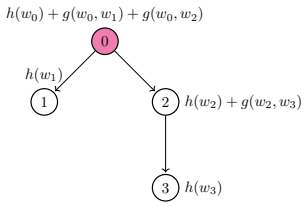

Fig. 5: *An illustration of the evolution of the preferential attachment with neighborhood influence model. A node (in this case 0) is selected at each time step with probability proportional to a function of its own weight and the weights of its neighbors, and connects to a newly arriving node.*

Moreover, in [3], we studied a model of preferential attachment trees where newly arriving vertices connect to existing vertices according to a function of the weight of the existing vertex, *and* the weights of its neighbors. In this model, we managed to generalize the known condensation phenomena observed in the preferential attachment model with multiplicative fitness. Currently, more work is being done to obtain a deeper understanding of this condensation phenomenon, including investigating whether this occurs in the model of random simplicial complexes and other probabilistic models, such as so called *time-dependent (Crump–Mode–Jagers (CMJ)) branching processes* with more complex dependency structures.

Weakly self-avoiding walk in a Pareto-distributed potential

On very fine scales, the properties of materials display significant disorder and randomness even when robust structures are present. This disorder has important consequences for the transmission of energy through the material whether by light, electric current, or in the form of heat. In studying such problems, one is led to consider random motions in random media, and these pose many challenging questions to mathematicians. One particular type of such models is called the *random walk in random potential* and is intrinsically connected with the parabolic Anderson model (PAM). The spectral properties of the corresponding Anderson operator (the Laplace operator with

random potential) are a realistic model for optical properties of glasses with impurities and for the electrical conductance properties of alloys of metals.

The decisive phenomenon when analyzing the spectrum of the Anderson operator is *Anderson localization*. Localization is the confinement of the random walk for an extended period of time to small randomly located islands (called *intermittent islands*). For heavy-tailed distributions of the random potentials (those which have a comparatively large probability of yielding extremely large values), particularly Pareto-distributed potentials, it is known that the attraction to just *one* intermittent island dominates the behavior of the walk.

Members of this group and colleagues overseas are now jointly considering a self-repelling random walk in a random potential as a first step to understanding the behavior of long chain molecules. Self-repulsion means that the random walk additionally has a deterministic self-repellent interaction that makes it unfavorable to stay in the same region for a long amount of time. More concretely, the probability of seeing a path X increases with the Hamiltonian

$$H_t(X) = \int_0^t \xi(X_s)\,\mathrm{d}\,s - \beta_t \int_0^t \int_0^t \mathbf{1}_{\{X_s = X_u\}}\,\mathrm{d}\,s\,\mathrm{d}\,u,$$

where $(\xi(z))_{z\in\mathbb{Z}^d}$ are i.i.d. α*-Pareto-distributed* random potential values (with parameter $\alpha > d$) and $\beta_t > 0$. We call this model the *weakly self-avoiding random walk in a random potential*.

For this walk we derive a limiting free energy and show that, contrary to the PAM mentioned above, subsequent multiple visits to several intermittent islands dominate the behavior of the walk and determine the spectrum of the operator. Moreover, we show that the random number of such islands is almost surely finite.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

Head:	Prof. Dr. Vladimir Spokoiny
Deputy Head:	Priv.-Doz. Dr. John Schoenmakers
Team:	Dr. Valeriy Avanesov Dr. Christian Bayer Franz Besold Heather Bielert (WIAS Female Master Students Program) Simon Breneis Dr. Oleg Butkovsky Darina Dvinskikh Dr. Pavel Dvurechensky Prof. Dr. Peter Friz Dr. Vaios Laschos Dr. Jörg Polzehl Dr. Alexandra Suvorikova Dr. Karsten Tabelow Dr. Nikolas Esteban Tapia Muñoz
Secretary:	Christine Schneider

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

Members of the research group participated in the 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 2021:

- Darina Dvinskikh successfully defended her dissertation "Decentralized Algorithms for Wasserstein Barycenters" with predicate summa cum laude at the Humboldt-Universität zu Berlin (under the supervison of Vladimir Spokoiny).
- The paper "On a combination of alternating minimization and Nesterov's momentum" by Sergey Guminov, Pavel Dvurechensky (RG 6), Nazarii Tupitsa, and Alexander Gasnikov was presented at the 38th International Conference on Machine Learning (ICML 2021; WIAS Preprint no. 2695).
- The paper "Newton method over networks is fast up to the statistical precision" by Amir Daneshmand, Gesualdo Scutari, Pavel Dvurechensky (RG 6), and Alexander Gasnikov was presented at the 38th International Conference on Machine Learning (ICML 2021).
- The new *MATH*$^+$ project EF3-11 "Quantitative tissue pressure imaging via PDE-informed assimilation of MR data" (PIs: Alfonso Caiazzo (RG 3 *Numerical Mathematics and Scientific Computing*), Karsten Tabelow (RG 6), Ingolf Sack (Charité Berlin)) was approved for funding.
- Within the Mathematical Research Data Initiative *MaRDI*, one position in the task area 3 "Statistics and Machine Learning" and one position in the task area 4 "Collaboration with other disciplines" (PI: Karsten Tabelow) were approved.

In 2021, the members of the group made some significant contributions to statistical literature.

A new method of manifold learning is proposed and studied in Puchkin and Spokoiny (arXiv:1906.05014; to appear in J. Machine Learning Research, 2021). The results claim that the method of structural adaptation yields rate optimal manifold recovery with an 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 introduced in [1] 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 threedimensional multidimensional scaling 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 which developmental stage is not known.

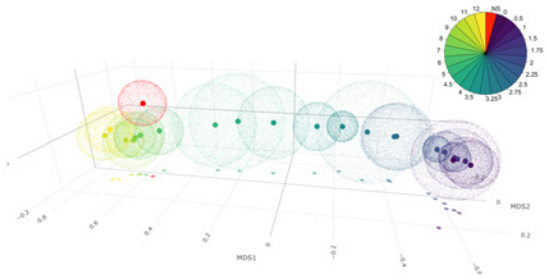

Fig. 1: *The gradual transition of the barycenters of the cells from 0 to 12 hours can be observed in the 3D space*

Within the MATH$^+$ project EF3-8 "Analysis of brain signals by Bayesian optimal transport" (jointly with Technische Universität (TU) 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 posterior density and use it for a sampling procedure. Then, by sampling from the posterior, the idea is to estimate the posterior mean and update the prior. This iterative procedure is studied theoretically and numerically to obtain convergence to the population Wasserstein barycenter. In the broader sense, this procedure is planned to be applied for general optimization problems, mimicking gradient- and Hessian-free second-order optimization procedures. We also developed an alternative approach for the population Wasserstein barycenter problem based on its reformulation as a stochastic saddle-point problem, see Tiapkin, Gasnikov, and Dvurechensky (arXiv:2006.06763; to appear in Optim. Letters, 2021). In particular, we propose a Kernel Mirror Descent algorithm for this problem in the semi-infinite formulation and estimate its complexity. This line of research is continued in collaboration with the newly established Leibniz group LG DOC *Data-driven Optimization and Control* at WIAS.

In 2021, we continued studying computational aspects of the optimal transport problems and the Wasserstein barycenter problem. Within the project "Optimal transport for imaging" (jointly with RG 8 *Nonsmooth Variational Problems and Operator Equations*) funded by the Cluster of Excellence *Berlin Mathematics Research Center* MATH$^+$, we investigated a function-space-based framework for image segmentation via optimal transport distances used as a data-fitting term in an inverse problem. The approach is based on constructing the predual problem and applying a semi-smooth Newton's method for its solution. We also proposed a general accelerated alternating minimization algorithm that is adaptive to the smoothness and convexity of the problem and has optimal convergence rates both for convex and non-convex classes of smooth problems. We applied this algorithm to the optimal transport problem (resulting in accelerated Sinkhorn's algorithm) and to the Wasserstein barycenter problem (resulting in the accelerated Iterative Bregman Projections algorithm). We showed experimentally the superiority of the algorithm compared to existing algorithms. The results were published in the proceedings of the 38th International Conference on Machine Learning (ICML 2021) [2].

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 2021, we developed a non-accelerated Newton's method for the decentralized setting, focusing on optimization up to statistical precision. The result is published in the proceedings of the International Conference on Machine Learning 2021. Further, we proposed a second-order accelerated method for the centralized setting and a first-order accelerated method for the decentralized setting, both for stochastic convex optimization problems. The results are published in the proceedings of the 60th IEEE Conference on Decision and Control (CDC 2021).

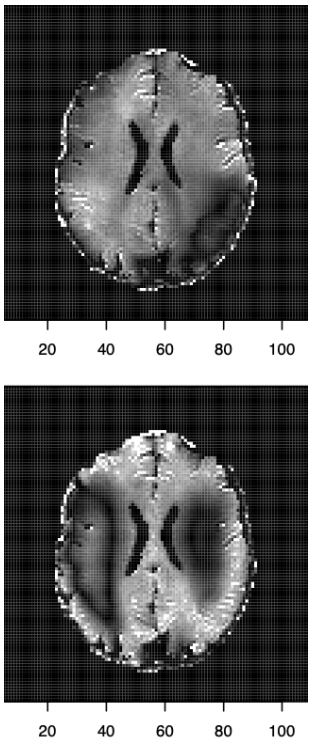

Fig. 2: *Estimated displacement field from magnetic resonance elastography data*

The research group contributes to the WIAS main application area *Quantitative Biomedicine*, especially for (quantitative) imaging problems and in neuroscientific applications. We developed new biophysical models for magnetic resonance (MR) imaging data and statistical methods for estimation of parameters and their error bounds therein (Mohammadi et al., bioRxiv preprint no. 2022.01.11.475846, 2022). Furthermore, we established a new anatomically informed procedure to solve the multiple comparison problem in function MR imaging (Neumann et al., WIAS Preprint no. 2806, 2021). The group also contributed to corresponding research software.

Together with RG 3, we worked on the MATH$^+$ project EF3-9 "Mathematical framework for MR poroelastography," a short-term project to establish a new mathematical framework for inference of mechanical properties of tissue especially in the human brain that takes its porosity into account. We analyzed an approach that requires additional MR measurements to find porosity maps that can then be used for an improved numerical model of the brain tissue and the propagation of mechanical waves. With this research, we laid the foundation for a new MATH$^+$ project EF3-11 "Quantitative tissue pressure imaging via PDE-informed assimilation of MR data," the goal of which is to infer on in-vivo information of the pressure in brain tissue.

In 2021, we finished the work within the MATH$^+$ project EF3-1 "Model-based geometry reconstruction from TEM images" that started in 2017 with the ECMath project OT-7 in collaboration with RG 1 *Partial Differential Equations*, RG 3 and TU Berlin. The project aimed at the reconstruction of geometric parameters of quantum dot nano structures from low resolution images from transmission electron microscopy (TEM) using our suggested model-based geometry reconstruction approach (MBGR). By establishing a virtual microscope, we were able to create a database of simulated TEM images for nano structures. The spanned image space will then be used to infer on the geometry also in experimental images. The simulation relies on extensive theory on electronic scattering. In 2021, we established the mathematical foundations of the utilized approximations, see also the Scientific Highlights article "Model-based Geometry Reconstruction of Quantum Dots from TEM" on page 28.

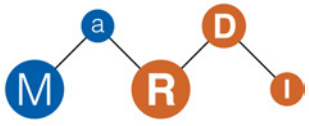

Fig. 3: *The Mathematical Research Data Initiative will be funded 2021–2026*

2021 also saw the starting of a five-year period of funding of the Mathematical Research Data Initiative (MaRDI) (`http://www.mardi4nfdi.de/`) coordinated by WIAS as a leading institution within the German National Research Data Inititiative (NFDI); see also page 47. As such WIAS is hosting the MaRDI coordination office. Furthermore, in RG 6 two positions will work on workflows and software in statistics and the collaboration with the corresponding initiative for neuroscientific data within the task areas 3 and 4 of the consortium. Finally, a further position, in RG 1, will be dedicated to mathematical models that can be formulated in terms of (systems of) partial differential equations.

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 2021:

- The *MATH*$^+$ project AA4-2 "Optimal control in energy markets using rough analysis and deep networks" (PIs: Christian Bayer, Peter Friz, John Schoenmakers, Vladimir Spokoiny) was successfully completed, and a continuation grant for three more years was approved for funding.
- 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) was approved for funding.
- The article [3] on "Randomized optimal stopping algorithms and their convergence analysis" was published in SIAM J. Financial Math., the article on "Pricing options under rough volatility with backward SPDEs" by Christian Bayer, Jinniao Qiu, and Yao Yao (University of Calgary) was accepted for publication in the same journal.
- The article "Short-dated smile under rough volatility: Asymptotics and numerics," numerical companion paper to an Ann. Appl. Probab. paper from last year, by Peter Friz, Paul Gassiat, and former WIAS postdoc Paolo Pigato forthcoming in Quant. Fin.
- The concluding article [5] of an interdisciplinary WIAS project on battery modelling, ran by Clemens Guhlke, Wolfgang Dreyer (former head of RG 7), and Peter Friz (RG 6) was accepted in SIAM J. Math. Anal.
- The article "Forests, cumulants, martingales" by Peter Friz with Jim Gatheral (recipient of the 2021 Risk Award) was accepted in Annal. Probab.
- The article [4] by Oleg Butkovsky (RG 6), Konstantinos Dareiotis, and Máté Gerencser on "Approximation of SDEs: A stochastic sewing approach" was published in Probab. Theory Related Fields.

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. In the year under report, the focus was on singular McKean–Vlasov equations that turn up in the smile calibration problem for plain vanilla options, for instance. 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, we regularize the singular MV stochastic differential equation (SDE) by replacing the conditional expectation by a functional that depends on

the unknown distribution in a Lipschitz continuous way and arbitrarily closely approximates the conditional expectation. This approach leads to a particle method where the approximate conditional expectation is obtained via cross-sectional ridge regression in a *reproducing kernel Hilbert space*. This quite challenging study will be continued in the subsequent year.

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 the WIAS Preprint no. 2810, both weakly and surely optimal martingales are completely characterized for the optimal stopping problem. In a subsequent study, WIAS Preprint no. 2884, we present and analyze a randomized empirical dual optimization procedure that sorts out such undesirable "weak" martingales, and which can be implemented as a linear program.

New numerical quadrature methods for solutions of stochastic differential equations were developed based on numerical smoothing of discontinuous target functionals. These methods exhibit considerably faster convergence speeds to the true expectation especially for financial options (with non-smooth payoffs) or calculations of probabilities of events or even densities. Smoothing techniques were analyzed in conjunction with adaptive sparse grids, quasi-Monte Carlo (see WIAS Preprint no. 2917), and even multilevel Monte Carlo.

Focus Platform *Quantitative Analysis of Rough and Stochastic Systems*

The investigation of rough volatility models continued. The numerical benefits of the theory developed in a paper published in 2021 in the Annals of Applied Probability were studied. Implied volatility expansions also led to a fundamental work on our understanding of cumulants in generic stochastic models, to paper [6] that is to appear in the Annals of Probability. Our works on extremely rough volatility models based on log-modulation of the fractional kernel was completed and published as C. Bayer, F. Harang, P. Pigato, *Log-modulated rough stochastic volatility model*, SIAM J. Financial Math., **12**:3, (2021), pp. 1257–1284.

Markovian approximations to rough volatility models were studied. Previously known approximations of that kind required using very high-dimensional (say $d \gg 100$) Markov processes to achieve satisfactory results. However, by improving the choice of the parameters in the Markovian approximations, it was shown that 6 to 8-dimensional Markov processes already yield good approximations. These lower-dimensional approximations may prove useful for the pricing of American options under rough volatility. The findings are documented in the WIAS Preprint no. 2868.

The weak error of Euler-type approximations of the stock price process in rough volatility models was analyzed. The analysis is based on standard error representation for the Markovian approximations discussed above. By uniformly bounding the errors associated with the Markovian approximations, error bounds for the underlying non-Markovian model are obtained. This analysis

leads to convergence rates $H + 1/2$ for the weak error, in contrast to the strong error rate H, an enormous improvement given that $H \ll 1/2$, see WIAS Preprint no. 2917.

The Log-ODE method is a family of methods for numerically solving rough differential equations in which the (complicated) driving rough path is replaced by a sequence of (simpler) rough paths leading to a sequence of ordinary differential equations (ODEs) that can be solved with well-known methods. The simpler rough paths can be chosen to approximate the original rough path up to an arbitrary degree of accuracy. Higher degree approximations yield better convergence rates, but may be more inefficient in practice. The optimal choice of the degree of approximation was studied both theoretically and numerically.

Further research focused on leveraging the framework of iterated-sums signatures introduced in Diehl, Ebrahimi-Fard, Tapia (*Time-warping invariants of multidimensional time series*, Acta Appl. Math. 171 (2021)) in order to develop numerical schemes for rough (partial) differential equations and general analysis of discrete dynamical systems; see also WIAS Preprint no. 2732. Additional work was done to apply rough analysis methods to similar problems in continuous time resulting in two publications focusing on transport and continuity equations with (very) rough noise as well as extending the concept of signature cumulants and introducing a new, generalized Magnus expansion. Further research was done on applications of Hopf algebra techniques to the study of Wick polynomials in non-commutative probability.

The mathematical analysis of numerical methods for solving general stochastic differential equations (SDEs)driven by various types of noise was another main aspect of the research of the focus platform. The optimal strong rates of convergence of the Euler–Maruyama scheme for SDEs driven by multiplicative Brownian or fractional Brownian noise with non-regular drift were obtained in [4]. Contrary to the results available in the literature, it is shown that the rate of convergence does not go to 0 as the drift becomes less regular. A key tool to obtain this result was the extension of the stochastic sewing lemma.

Another research direction was the analysis of the Schramm–Loewner evolution (SLE). This is a family of random planar fractal curves that describe scaling limits of a number of crucial models in statistical physics. The law of the SLE tip was obtained and its properties were studied by a combination of methods from the theory of parabolic partial differential equations and ergodic theory.

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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 Erhardt Dr. Manuel Landstorfer 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

Liquid-liquid phase separation of intrinsically disordered proteins. Protein condensation driven by liquid-liquid phase separation (LLPS) is a powerful concept to understand the mesoscale organization of cells. It provides a simple mechanism to form non-membrane bound organelles that separate from the nucleo- and cytosol. Intrinsically disordered proteins are the drivers of cellular liquid-liquid phase separation. However, it remains a challenge to directly predict the phase behavior of a protein based on its primary sequence, and under physiological conditions.

We use machine-learning methods to determine the intrinsically disordered regions (IDRs) of phase separating proteins. We present a random-phase approximation that allows for variable salt concentration and thus accounts for salt partitioning of the phase-separated regions. We use this approach to link the sequence of the disordered regions with the behavior of the complete protein through direct comparisons to *in vitro* phase-separation assays in collaboration with experimentalists Anatol Fritsch and Juan Iglesias at the Hyman Lab of the Max-Planck-Institute for Molecuar Cell Biology and Genetics and Simone Reber at IRI Life Sciences, Humboldt-Universität zu Berlin. In particular, for the protein fused in sarcoma (FUS) we determine the exact region responsible for LLPS, settling a long-standing debate; see Figure 1. Our work Meca-Fritsch-Iglesias-Artola-Reber-Wagner

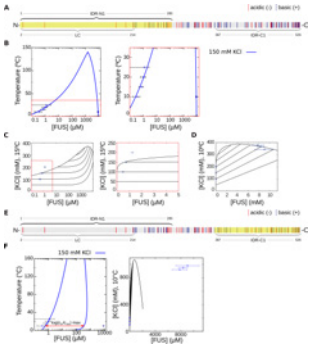

Fig. 1: *Intrinsically disordered regions and comparisons of phase diagrams*

(2021), [1], provides a powerful theoretical tool that can easily be adapted to systematically assess the phase behavior and salt partitioning of other structurally complex proteins.

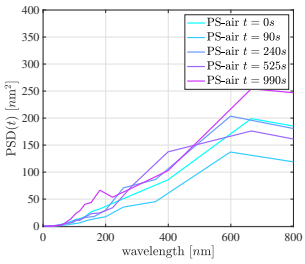

Fig. 2: *Power spectral densities of polystyrene (PS)-air interface*

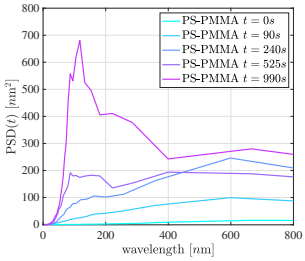

Fig. 3: *... and of PS-poly(methyl methacrylate) (PMMA) interface*

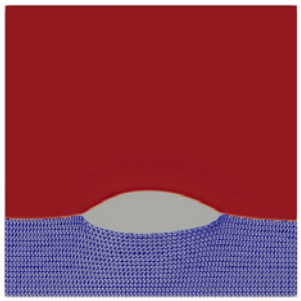

Fig. 4: *Equilibrium PS-drop on polydimethylsiloxane (PDMS) gel*

Dewetting dynamics and morphology of liquid polymers on hydrogels. Dewetting is the hydrodynamic process where a uniform layer of liquid destabilizes and decays into distinct patterns of stationary droplets by virtue of interfacial and intermolecular energies. In collaboration with the group of Ralf Seemann (Experimental Physics at Universität des Saarlandes), Leonie Schmeller (RG 7), Barbara Wagner (RG 7), and Dirk Peschka (WG BIP) showed a surprising discrepancy of the predictions of stability theory and experimental results, both for spinodal wavelength and rupture times for a liquid-liquid polymer system. The key factor for this discrepancy is the altered mode selection process due to the initial surface roughness of the liquid-air and liquid-liquid interfaces perturbed by partially correlated colored noise in the linearly unstable region. The strong impact of noise on the mode selection and on the rupture time is clearly demonstrated through long-time numerical solutions of the full nonlinear model when compared to experimental results. These results suggest that thermal fluctuations have a major impact on liquid-liquid dewetting, necessitating new strategies for incorporating thermal fluctuations into mathematical models for the dewetting of liquids from soft substrates [2].

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. Together with the group of Ralf Seemann, we addressed fundamental open questions regarding morphology and dynamics of a liquid layer on soft gels; see Figure 4.

Mathematical modeling of cellular self-organization on stimuli responsive extracellular matrix (ECM). In the interdisciplinary MATH+ project AA1-12 headed by Sara Checa and Ansgar Petersen (both at Charité), Barbara Wagner and André Erhardt (both RG 7), we developed a model that couples a model for a hydrogel with an agent-based model for the collective movement of cells while they excert a traction force on the hydrogel. We developed a two-dimensional numerical code based on the one developed for the hydrogel. The numerical simulations for different initial cell configurations resolve the long-time mechanically drive cellular organization. We plan to compare this to *in vitro* experimental results carried out in the group of Ansgar Petersen.

Eventually, biologically more realistic models for the ECM will include additional physically cross-linked networks to address remodeling processes during cellular organization. In addition, features of polyelectrolyte gels, where dependence on concentrations of surrounding salt solution and electrostatic interactions will be taken account of; see [3].

Mathematical models of cardiac dynamics and its analysis. The mathematical investigation of complex dynamics in cardiology gains in importance for the study of diseases like cardiac arrhythmia. In this line of research, in collaboration with Susanne Solem (Norwegian University of Life

Science), cardiac cell models and their extension on macroscale level were optimized to address the analysis of cardiac dynamics early after depolarization and chaotic dynamics [4, 5]. Bifurcation analysis and stability theory were used to decode cardiac dynamics. In Figure 5 and 6, we show a simulation of the one-dimensional heart model for different diffusion parameters.

Further, self-organizing electrophysiological patterns occurring in the heart like spiral waves and wave break-ups were numerically investigated. In particular, the synchronization of cardiac cells and the potential spreading of cardiac arrhythmia to the tissue depend on the number of affected cells and is highly sensitive to changes in the tissue-specific parameter of the diffusivity, cf. Figures 4 and 5.

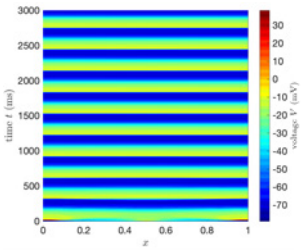

Fig. 5: *Diffusion parameter* 0.0028 *mS*

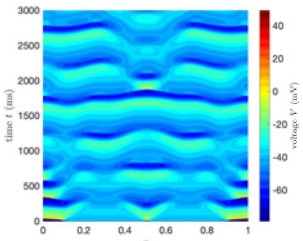

Fig. 6: *Diffusion parameter* 0.00005 *mS*

Mathematical models and theory of electrochemical processes

MATH+ AA2-6: "Modeling and simulation of multi-material electrocatalysis" (MultECat). This project headed by Manuel Landstorfer (RG 7) and Jürgen Fuhrmann (RG 3 *Numerical Mathematics and Scientific Computing*) aims at continuum models for electrocatalysis at multi-material electrodes on a nm– μm scale. The modeled processes couple reactions on catalytic interfaces, reactant transport in electrolytes, and charge transport in catalyst substrates. Multi-material electrocatalytic surfaces, as well as polycristalline electrode surfaces, induce complex boundary layers in an adjacent electrolyte. There, the electric field strength can rise from almost zero in the bulk to $10^9\ Vm^{-1}$, cf. Figure 7 and in this range, the dependence of the dielectric susceptibility χ on the field strength is not directly accessible to experiments. The project analyzes the impact of non-constant dielectric susceptibility on the boundary layer as the environment of electrocatalytic reactions. As shown in Figure 8, the dielectric saturation due to strong electric fields considerably narrows the boundary layers and, thereby, further increases the local electric field strength [8]. 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; see Figure 9 on page 104. To analyze the dependence of electrocatalytic reactions on the crystallographic orientation of surfaces, formal asymptotic methods are employed. They show the compatibility of our model with macroscopic Butler–Volmer equations for the reaction rates even at polycristalline surfaces.

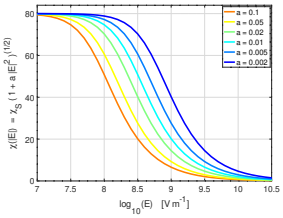

Fig. 7: *Dependence of the dielectric susceptibility χ of water on the electric field strength $|E|$*

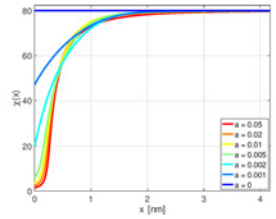

Fig. 8: *Profiles of the dielectric susceptibility χ in the boundary layer of the electrolyte*

Mathematical modeling of lithium-ion batteries. The year 2021 was the final year of the BMBF compound project MALLi^2 (Model-based assessment of the life span of aged Li batteries for second-life use for stationary energy storage), headed by Manuel Landstorfer of RG 7, as well as the initial year of the MATH+ project AA4-8 "Recovery of battery ageing dynamics with multiple timescales," headed by Martin Eigel of RG 4 *Nonlinear Optimization and Inverse Problems*, Martin Heida of RG 1 *Partial Differential Equations*, and Manuel Landstorfer of RG 7, with Alireza Selahi working as a Ph.D. student on the project.

Mathematical modeling of lithium-ion batteries (LIBs) continues to be an important pillar of the RG 7 research plan. Various aspects of modeling and simulation of LIBs are addressed within RG 7, among others the derivation of homogenized equations for porous electrodes [6] (see Figure 10 on page 104), investigations of phase-separating materials [7], numerical implementations of a flex-

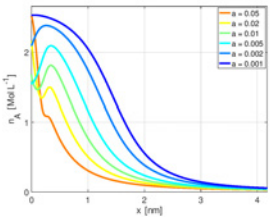

Fig. 9: Profiles of the counter-ion density for various applied voltages

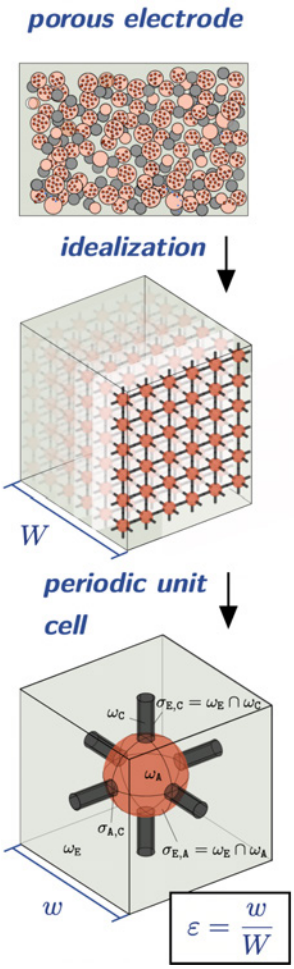

Fig. 10: Sketch of a porous electrode and its idealization as periodic repetition of unit cells which allows for homogenization techniques

ible battery model framework, mesh generation for porous media, modeling of ageing and degradation effects, as well as material modeling for different components of LIBs.

Within the project MALLi [2], a complete *model framework* for a general LIB cell was derived and validated at experimental data [6]. This model was fully implemented and allows for time-dependent charge and discharge simulations of general LIBs. The model and its numerical implementation are extremely flexible regarding the materials of a specific LIB. In an object oriented manner, a specific LIB, for instance consisting of a graphite anode, a $LiCoO_2$ cathode, and a 1M $LiPF_6$ (DMC) electrolyte, is initiated as an object of a general LIB class. This result is achieved by strictly separating the general transport equations for a LIB (e.g., expressed in general chemical potential functions) from the material-specific quantities (i.e., explicit equilibrium and non-equilibrium parameters as well as functions) and the underlying micro-structure of the electrode. This *model framework* is widely applicable and is being further developed with respect to various physico-chemical phenomena, for instance, deformation and crack formation, side reactions, and gas evaporation, as well as solid electrolyte interphase (SEI) growth, and is used in the subsequent projects such as AA4-8 of MATH+.

Further, a methodology was developed to systematically incorporate degradation effects in the model framework to enable model-based lifetime estimations for LIBs. Our project partners from Universität Stuttgart (Peter Birke, Alexander Ridder) produced 10 specific cells with raw materials of industrial standard (from our project partner VARTA). These were cycled to 90%, 80%, 60%, and 40% of their original capacity, at two different discharge rates, and the electrochemical data of the whole time series was recorded. This data serves to calibrate the mathematical model, more precisely, the degradation in terms of cycle number-dependent parameters. The variation of specific parameters yields a unique fingerprint in the resulting electrochemical characteristic, i.e., the voltage status of charge relation. This approach can be exploited to identify a specific parameter from an inverse problem on the measured data. To achieve this result numerically effectively, reduced-order methods were employed [6] by our project partners of Westfälische Wilhelms-Universität Münster (Mario Ohlberger).

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 using the software package UQLab (Marelli–Sudret (2014), see https://www.uqlab.com/).

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

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Team:	Dr. Amal Alphonse Jo Andrea Brüggemann Dr. Marcelo Bongarti Dr. Guozhi Dong Sarah Essadi Dr. Caroline Geiersbach Dr. Axel Kröner Dr. Jonathan Leake Hong Nguyen Dr. Kostas Papafitsoros Clemens Sirotenko Steven-Marian Stengl Kathrin Völkner (WIAS Female Master Students Program)
Guests:	Prof. Dr. Juan Carlos De los Reyes Jonas Holley Dr. Olivier Huber
Secretary:	Patricia Rouland
Nonresident Members:	Prof. Dr. Martin Brokate

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

Three new members joined the group during 2021: Dr. Marcelo Bongarti is a new postdoc from the University of Memphis, USA, with expertise in partial differential equations (PDE) via semigroup theory. Juan Carlos De los Reyes, Professor of Optimization and Control at the Escuela Politécnica Nacional, Ecuador, is spending his sabbatical as a special guest of the MATH+ Thematic Einstein Semester on "Mathematics of Imaging in Real-World Challenges." Finally, Dr. Jonathan Leake joined the group as a Berlin Mathematical School (BMS) Dirichlet Postdoctoral Fellow, a joint position with Technische Universität Berlin.

General relevance of the scientific topics considered by the RG

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

In order to tackle such problems, there are two main approaches: The first approach is to regularize the nonsmoothness in order to use existing results and perform some limiting analysis. The second approach is to develop theories that can directly handle specific types of nonsmoothness. For instance, in the variational models in image processing, where nonsmooth objectives have a crucial role in preserving discontinuities (image edges), nonsmoothness can be tackled via convex duality theory. On the other hand, in the context of noncooperative games, the characterization of Nash equilibrium can be done by considering the collection of first-order conditions for all game participants. This characterization leads to a (quasi-)variational inequality, for which existence results and numerical schemes are available. In the context of stochastic optimization, stochastic approximation has proven to be an effective tool for solving problems with nonsmoothness. This class of algorithms includes random iterative schemes such as the proximal stochastic gradient method and has been applied to optimization problems in infinite dimensions. Finally, nonsmoothness also typically appears in optimization problems associated with deep learning, especially with regards to nonsmooth neural network training, stemming from the use of nonsmooth activation functions, e.g., the rectified linear unit (ReLU).

Selected research results

Generalized Nash equilibrium problems (GNEP). The topic of GNEP continues to be part of the group's research efforts. In [2], the concept of Γ-convergence is extended to a class of equilibrium problems. The latter subsumes, e.g., GNEPs and many instances of quasi-variational inequalities (QVI). The abstract results are used to derive convergence of GNEPs with penalized state constraints.

In [3], a stylized model for the gas market is investigated. The latter combines features from economical modeling along with a PDE model for the gas flow. For a given time horizon $[0, T]$, on a single pipe, the problem for player k has the following structure:

$$\begin{aligned} \text{maximize} \quad & \int_0^T \pi(t, \sum_j q_j^{\text{out}}(t)) q_k^{\text{out}}(t) - c_k(t) q_k^{\text{in}}(t)\, \mathrm{d}t + g_k(u_k) \\ \text{subject to} \quad & (p_k^{\text{in}}, p_k^{\text{out}}, q_k^{\text{in}}, q_k^{\text{out}}) =: u_k \in U_k^{\text{ad}}, \\ & S(u_k, u_{-k}) \in B, \end{aligned} \tag{1}$$

where $(p_k^{\text{in}}, q_k^{\text{in}})$, respectively $(p_k^{\text{out}}, q_k^{\text{out}})$, is the pair of pressure and mass flow at the input, respectively output, node. The cost of procuring gas is c_k and the (selling) price of gas is modeled by the inverse demand function π. The set U_k^{ad} captures the private constraints of each player. The notation u_{-k} denotes the decision variables of all players except k. The mapping S is the control-to-state operator associated with the evolution equation for the gas flow in $(0, T)$. The

pointwise box constraints on the state are modeled by the set B. The last inclusion in (1) is the shared constraint among players. Whenever each player's problem is convex, this gives rise to a jointly convex GNEP. The solution concept of variational equilibrium (VE) is considered. The main result is the existence under mild conditions of such solution. In the case of a symmetric game, a VE can be constructed from the solution to an optimization problem. The use of an evolution equation enables the assessment of linepacking, that is the use of pipelines as temporary storage device. Numerical results illustrate the impact of this phenomenon on the decisions of the producers. Future research directions include tackling different gas flow models and incorporating uncertainties in both the economical and physical data.

Stochastic optimization on function spaces. The group continued its research in characterizing optimality for convex stochastic optimization problems with almost sure state constraints in the function space setting. This study was essential in handling applications in PDE-constrained optimization under uncertainty, where the states of the PDE are subject to additional constraints. The problem class under investigation was of the following form:

$$\begin{aligned} \text{minimize} \quad & \mathcal{R}[J_2(u, y, \cdot)] + J_1(u) && \text{over } (u, y) \in U \times L^\infty(\Omega, Y) \\ \text{subject to} \quad & u \in U_{\text{ad}} \subset U, \quad e(u, y(\omega), \omega) = 0 && \text{almost surely (a.s.)}, \\ & i(u, y(\omega), \omega) \in K && \text{a.s.} \end{aligned} \tag{2}$$

Here, $\mathcal{R}$ is a risk measure, Ω is a sample space corresponding to a probability space, and e and i are linear and K-convex constraints, respectively, defined on separable and reflexive Banach spaces U and Y.

Building on prior work as well as classical finite-dimensional theory from two-stage stochastic optimization, the results in [1] provided necessary and sufficient first-order optimality conditions for risk-averse problems of the form (2). The work was a significant theoretical advancement in the handling of problems not satisfying the assumption of relatively complete recourse; this assumption is commonly used in the stochastic optimization literature but is rarely satisfied in the setting of state-constrained PDE-constrained optimization problems under uncertainty. The main contributions included: constructive conditions under which saddle points to the associated Lagrange function exist; necessary and sufficient first-order optimality conditions with and without the assumption of relatively complete recourse; and a consistency analysis for the Moreau–Yosida regularization of state constraints. Future research will involve developing stochastic algorithms to solve PDE-constrained optimization with almost sure-type state constraints and other applications in the context of generalized Nash equilibrium problems.

Optimal control of learning-informed nonsmooth PDEs. The group continued its activities on optimal control of learning-informed PDEs which has started with the recently published work [4], cf. also the relevant Scientific Highlights article on *Learning-enriched Differential Equation Models in Optimal Control and Inverse Problems* of the WIAS Annual Research Report 2020. The term refers to PDEs which have nonlinear constituents that are in principle unknown but nevertheless they

are accessible though data, making them suitable to be learned by artificial neural networks. This framework can be applied when the precise formulation of a (part of) physical law that governs a process of interest is missing but can be learned by available data. RG 8 has identified key applications, especially in quantitative imaging, in which the need to learn unknown physical laws arises, with targeted research carried out in the recently completed project EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization" in the frame of the Center of Excellence MATH+. In a series of papers to be completed soon, cf. also the relevant master thesis [5], nonsmooth learning-informed PDEs were considered.

More specifically, the following optimization problem received special attention:

$$\begin{aligned} &\text{minimize} \quad J(y,u) := \frac{1}{2}\|y-g\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)}, \quad \text{over } (y,u) \in H^1_0(\Omega) \times L^2(\Omega), \\ &\text{subject to} \begin{cases} -\Delta y + \mathcal{N}(\cdot, y) = u, & \text{in } \Omega \\ y = 0, & \text{on } \partial\Omega \end{cases}, \quad \text{and} \quad u \in \mathcal{C}_{ad}. \end{aligned} \tag{$P_{\mathcal{N}}$}$$

The term that makes the above problem non-standard is the function $\mathcal{N} : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$, a constituent of the PDE acting as a constraint for the minimization problem. Here, $\mathcal{N}$ is considered to be a ReLU artificial neural network, that is, a neural network that has the ReLU $\sigma(t) := \max(t, 0)$ as an activation function. In that case, the PDE in $(P_{\mathcal{N}})$ contains the term $\mathcal{N}$, which is non-differentiable in the classical sense, making the overall optimal control problem not treatable with standard methods. In the aforementioned works, the optimal control problem itself was studied in full generality and several stationary conditions were established based on generalized differentiability concepts. Furthermore, based on approximation capabilities of ReLU networks, fundamental questions regarding approximating properties of the learning-informed control-to-state map were addressed. Finally, a numerical algorithm that treats directly the nonsmooth optimal control problem was proposed and analyzed. The latter was achieved by employing a descent algorithm inspired from a bundle-free method. The concept of learning-informed physical laws is also a central topic in the recently approved MATH+ project EF3-12 "Integrated learning and variational methods for quantitative dynamic imaging," where in combination with data-driven regularization, novel methods for spatio-temporal qualitative and quantitative imaging will be developed.

Further highlights in 2021

Despite the challenges posed by the ongoing Covid-19 pandemic, RG 8 continued to be quite active in the organization of scientific events. The "15th International Conference on Free Boundary Problems" FBP 2021 took place from September 13–17, 2021, after having been originally planned for September 2020. Michael Hintermüller was the Chair of the Organizing Committee with several members of the group being in the Local Support Team.

The Thematic Einstein Semester on "Mathematics of Imaging in Real-World Challenges" of the Berlin Mathematics Research Center MATH+ is taking place in Berlin from October 2021 – March 2022 and is co-organized by RG 8. It consists of a kick-off workshop, three plenary tandem talks, three tutorials, a hackathon event and it will conclude with the SIAM Conference on Imaging Science, March 2022. Furthermore, the group had one MATH+ project that concluded in 2021, AA4-3

"Equilibria for energy markets with transport," and one currently running, AA4-7 "Decision-making for energy network dynamics," while the projects EF3-3 "Optimal transport for imaging" and EF3-5 "Direct reconstruction of biophysical parameters using dictionary learning and robust regularization," were extended until June and September 2022, respectively. Three new projects were approved in the latest MATH+ call and will start in 2022: EF1-15 "Robust multilevel training for artificial neural networks," EF1-17 "Data-driven robust model predictive control under distribution shift," and EF3-12 "Integrated learning and variational methods for quantitative dynamic imaging." Additionally, Michael Hintermüller is in the executive board of the center and a scientist-in-charge of the MATH+ Emerging Field 3 (EF3) Model-Based Imaging.

The SPP 1962 *Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization* continues to run successfully with a large number of preprints, and the annual meeting was held virtually in March 2021. Furthermore, a special issue book collecting the research achievements of the first 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.

Several members of RG 8 contributed to proposal writing for the project "Multicriteria optimization subject to equilibrium constraints using the example of gas markets" within the Collaborative Research Center CRC/TRR 154 *Mathematical Modelling, Simulation, and Optimization Using the Example of Gas Networks*. The third phase of the project, if approved, would start in the summer of 2022.

Members of RG 8 actively participated and organized events in several international conferences. Michael Hintermüller co-organized the hybrid Oberwolfach workshop on "Challenges in Optimization with Complex PDE-Systems" in February 2021. Olivier Huber, Amal Alphonse, and Caroline Geiersbach were invited to give talks. Amal Alphonse and Guozhi Dong participated and gave talks at the 91th GAMM Annual Meeting in March 2021. Caroline Geiersbach presented at the SIAM Conference on Computational Science and Engineering in March 2021. Michael Hintermüller was an invited speaker at the online series "One World Optimization Seminar" in May 2021. Amal Alphonse participated in the Interfaces and Free Boundaries satellite virtual meeting in June 2021. At the SIAM Conference on Optimization in July 2021, Michael Hintermüller and Kostas Papafitsoros gave invited talks and Olivier Huber gave a talk. Caroline Geiersbach gave a talk at the International Conference on Spectral and High Order Methods in July 2021. Kostas Papafitsoros co-organized a minisymposium at the IFIP TC7 Conference in Quito, Ecuador, in September 2021. Michael Hintermüller was an invited speaker for the "Deep Learning and Inverse Problems" program of the Isaac Newton Institute for Mathematical Sciences in Cambridge, UK, in October 2021.

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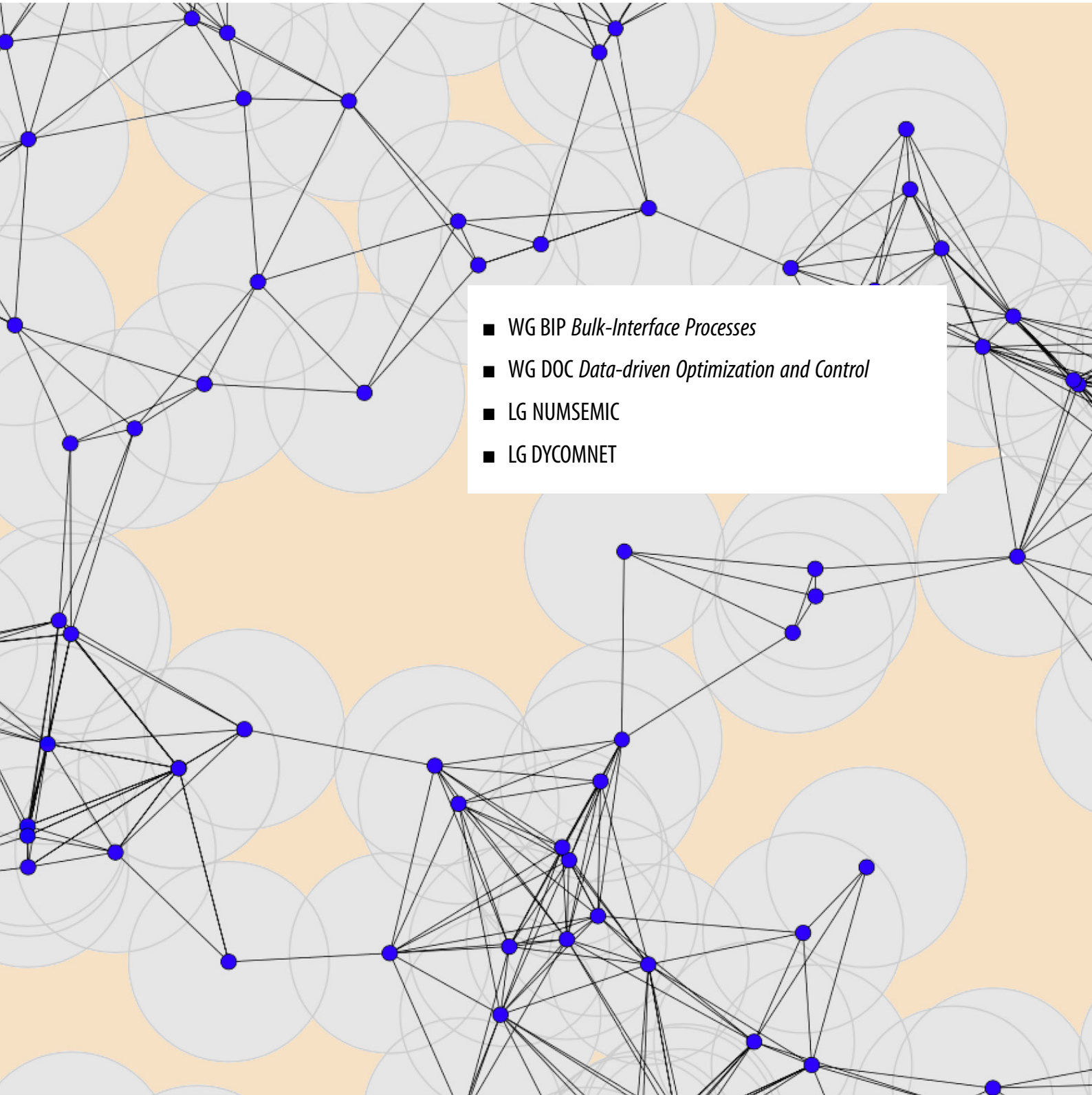
5 Flexible Research Platform



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

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

Head: Dr. Marita Thomas

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

Secretary: Andrea Eismann

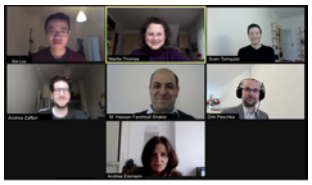


Fig. 1: *WG BIP, 2021, left–right: X. Liu, M. Thomas, S. Tornquist, A. Zafferi, M.H. Farshbaf-Shaker, D. Peschka, A. Eismann*

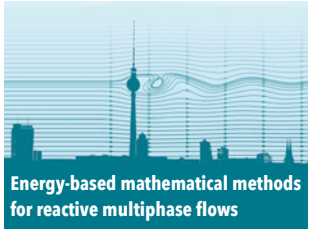
Weierstrass Group (WG) BIP was established as an element of the Flexible Research Platform at WIAS in April 2017, partially funded by WIAS budget resources. After a first successful period of three years, the group was positively evaluated in spring 2020, and a second three-year funding period was granted.

The 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 WIAS main application areas *Nano- and Opto-electronics*, *Materials Modeling*, and *Flow and Transport*. Since for the time being, the projects on mechanically strained optoelectronic devices are considered successfully closed, the group continues and intensifies its research on applications within the areas *Materials Modeling* and *Flow and Transport* in the second funding period that started in July 2020. In doing so, the focus is 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 was a co-organizer of the Thematic Einstein Semester (TES) on Energy-based Mathematical Methods for Reactive Multiphase Flows in winter term 2020/21. The TES was jointly organized by members of WG BIP, RG 1 *Partial Differential Equations*, and RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, together with Volker Mehrmann from Technische Universität Berlin. It combined a series of online workshops, conferences, and seminars with student courses and student projects and was closed with the three-day final conference "Structures in Evolution: Theory and Applications" in February 23–25, 2021.

The following summary reports on the results obtained in 2021 within the two topics (1) and (2):

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 "Reliability of efficient approximation schemes for material discontinuities described by functions of bounded variation" within the DFG-funded Priority Program 1748 *Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretisation Methods, Mechanical and Mathematical Analysis* finally expired in November 2021 after a second funding period of three years. It led to analytical results on the convergence of time- and space-discrete schemes for damage and fracture models with different types of coupled dynamics and to regularity results for the solutions; cf., e.g., [1]. Moreover, it also fostered the project "Nonlinear fracture dynamics: Modeling, analysis, approximation, and applications" of Marita Thomas in collaboration with Kerstin Weinberg (Universität Siegen) and Christian Wieners (Karlsruher Institut für Technologie) within the Priority Program SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*, where discretization methods as in [1] are also to be ultimately investigated in the nonlinear setting of dynamic fracture at finite strains. As a first step in this direction, an alternative discretization method for the dynamic phase-field fracture model from [1] using a coupled first-order system in combination with a discontinuous Galerkin approach is currently studied for convergence.

Moreover, within the student projects of the TES, structure-preserving discretization methods for phase-field models at finite strains for different applications were studied in the framework of gradient flows and GENERIC (General Equation for Non-Equilibrium Reversible Irreversible Coupling). In this context, [2] provides a discretization approach that preserves an appropriate gradient structure as much as possible for the application of phase separation and swelling of gels. This research is also part of the MATH+ project AA2-9 "Variational methods for viscoelastic flows and gelation," which saw its start in January 2021.

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 also aims at their extension to applications in geosciences, e.g., within project C09 "Dynamics of rock dehydration on multiple scales" in the DFG-funded CRC 1114 *Scaling Cascades in Complex Systems*.

In order to describe chemical reactions and reactive transport within rocks during subduction, in project C09, the work [3] studies and extends the GENERIC formalism. In this thermodynamical modeling framework, the thermodynamical and mechanical foundations for the treatment of reactive fluid flows are established. The paper [3] provides a clear relation and transformation rule between a Lagrangian and an Eulerian formulation of the thermodynamical system in the GENERIC formalism resulting in the corresponding systems of partial differential equations. Based on this result, further extensions to models of fluid-structure interaction are also obtained.

As a further geological application, [4] is concerned with the mathematical analysis of a model for sea ice dynamics. In collaboration with Edriss Titi (Texas A&M, Cambridge University, Weizmann Institute), well-posedness is established for the phenomenological sea ice model that was originally introduced by W.D. Hibler in 1979 and builds the core for many sea ice simulations in geoscientific literature. The techniques of [4] preserve the hyperbolic nature of the model and provide the well-posedness for strong solutions with sufficiently regular initial data when there is no open water.

As a part of the project “Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows” within the DFG-funded Priority Program 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates*, 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), cf. [2]. Additionally, higher-order schemes for free boundary problems were developed jointly with Luca Heltai (Scuola Internazionale Superiore di Studi Avanzati Trieste) in the WIAS Preprint 2887, 2021, and comparisons of hydrodynamic models with moving contact lines and molecular dynamics models were performed jointly with Marcello Sega et al. (Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien), see WIAS Preprint 2911, 2022. Based on these results, it is the future 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
Secretary: Patricia Rouland

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 Fall 2021, a Ph.D. student joined the group with a research focus on statistical learning theory and distributionally robust optimization. A postdoctoral scholar is envisioned to join the group in Spring 2022, as a part of the MATH+ project on distributionally robust optimization and control.

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

WG DOC also contributed to the Leibniz MMS Summer School 2021 that took place in the Dagstuhl Castle, Saarland. There, its leader Jia-Jie Zhu gave a mini-course on "Robust optimization and learning under distribution shift."

Robust machine-learning distribution shift and distributionally robust optimization. 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.

Our recent paper entitled "Adversarially robust kernel smoothing" [1], where Jia-Jie Zhu invented a new algorithm called the *adversarially robust kernel smoothing* (ARKS) for robust learning has been accepted as an oral presentation ($\leq$ 3% of the submitted paper) at the 25th International Conference on Artificial Intelligence and Statistics (AISTATS) 2022. This work builds upon our previous works in distributionally robust optimization and kernel methods using the maximum mean discrepancy (MMD), e.g., [2]. Here, we propose a novel *function majorant* in the sense of convex analysis and show that ARKS can be applied to large-scale robust machine learning tasks. For example, we demonstrate an application of ARKS in human face classification (whether sunglasses are present in this figure), where ARKS can robustly learn under the so-called *adversarial attacks* that produce artificial faces with sunglasses.

Fig. 1: *Training data samples from adversarially robust classification of presence of sunglasses. The bottom row shows the original training data, and the top row shows data perturbed by an adversarial attack algorithm. Figure taken from [1].*

In addition to empirical results, we further show a robustness certificate leveraging the theory of DRO, convex analysis, and empirical processes. We show that ARKS can robustify the learning algorithms in certified regions described by the Wasserstein distances in log-scale. This work was completed partially during Dr. Zhu's appointment at the Max Planck Institute for Intelligent Systems, Tübingen.

In addition, we have the following close-to-completion projects in addressing distributional robustness in learning and optimization:

- Conditional moment restriction and instrumental variable regression for robust causal inference. Collaboration with Bernhard Schölkopf's group at the Max Planck Institute for Intelligent Systems in Tübingen;
- Learning kernel sum-of-squares functions for distributionally robust optimization.

The members of WG DOC are also in active discussions with the WIAS research groups RG 1 *Partial Differential Equations* on dynamic optimal transport applications to machine learning, the Leibniz Group NUMSEMIC on approximation theory for machine learning, RG 4 *Nonlinear Optimization and Inverse Problems* on numerical optimization and chance-constrained stochastic programs, and RG 6 *Stochastic Algorithms and Nonparametric Statistics* on stochastic optimization and statistical machine learning.

Data-driven robust dynamical system modeling and distributionally robust control. Another focus of WG DOC is in data-driven dynamics modeling and distributionally robust control. This research directions draw from the foundational works in kernel discrepancy measures and data-driven modeling schemes principled in statistical learning theory. Currently, we have the following ongoing projects in addressing distributional robustness in learning and optimization:

- Scalable numerical methods for approximate learning-based model predictive control. Collaboration with Bernhard Schölkopf's group, MPI Tübingen, and Moritz Diehl's group, Universität Freiburg;
- Robust modeling of dynamic systems using Koopman operator and maximum mean discrepancy. Collaboration with Feliks Nüske, Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg;

- Distributionally robust optimization for model-based reinforcement learning. Collaboration with Jan Peters's group, Technische Universität Darmstadt.

We also envision further discussions with RG 6 on kernel regression for stochastic control, RG 4 on numerical optimal control and probilistic constraints, and RG 8 *Nonsmooth Variational Problems and Operator Equations* on partial differential equation-constrained optimization.

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

Head: Dr. Patricio Farrell
Team: Dr. Yiannis Hadjimichael
Dilara Abdel
Secretary: Marion Lawrenz

The Leibniz Group NUMSEMIC was established on WIAS' Flexible Research Platform 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 equations (PDE) models as well as physics-preserving numerical techniques for new semiconductor materials and technologies.

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

There were several highlights within the group in the report year: The head of the group was made an offer for an associate professorship at Heriot-Watt university and was invited to give a plenary talk at the "Asymptotic Behaviors of Systems of PDEs arising in Physics and Biology" conference. Dilara Abdel and Patricio Farrell visited INRIA Lille for a month to collaborate on the modeling and analysis of perovskite models. During a research visit to SISSA Trieste, the head of the research group collaborated on a comparison of hybridizable discontinous Galerkin and finite volume methods. Dilara Abdel received two SIAM student travel awards and a PROCOPE fellowship by the science department of the French embassy.

The following four specific research topics drive our research:

- Electro-mechanical models and simulations to understand transport in **bent nanowires**,
- The **lateral photovoltage scanning method** 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.

Bent nanowires. Together with Christian Merdon and Timo Streckenbach (both RG 3 *Numerical Mathematics and Scientific Computing*), 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 finite element methods.

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" that started in 2021. Apart from LG NUMSEMIC, this project involves Matthias Liero and Annegret Glitzky (both RG 1 *Partial Differential Equations*) as well as Barbara Zwicknagel from Humboldt-Universität zu Berlin.

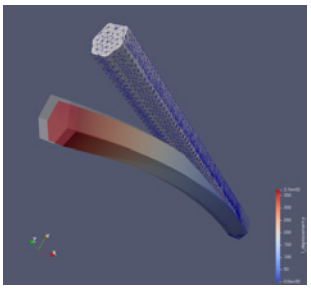

Fig. 2: *A bent nanowire*

The lateral photovoltage scanning method. In order to improve the crystal growth design, it is crucial to predict the temperature distribution in the furnace and especially in the growing crystal. Unfortunately, it is impossible to measure the temperature distribution during crystal growth without damaging the crystal structure and introducing impurities. Moreover, silicon, for example, melts at extremely high temperatures, around 1687 K.

However, during growth, microscopic variations in the crystal appear along the solid-liquid interface. These can be measured even in the cooled-down crystal and correspond to isothermal contour lines of the temperature field. The *lateral photovoltage scanning* method (LPS) helps to visualize these variations with a laser by creating a voltage difference at the sample edges that is proportional to the microscopic variations.

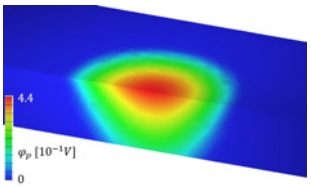

Fig. 3: *Simulation of a hole quasi-Fermi potential distribution generated by a laser during an LPS scan*

Our open-source code reduces the simulation time by two orders of magnitude. This is crucial since a future aim is to efficiently solve the corresponding inverse problem. Moreover, our method presented here also works well for very low doping concentrations that previously could not be simulated due to numerical instabilities. We also present a convergence study showing that the LPS voltage converges quadratically [2, 5].

Perovskites 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 29.15% has been demonstrated. Further efficiency gains are likely. However, the commercialization of PSCs is still in its early stages and several challenges need to be overcome: Commercially viable PSCs degrade significantly faster. Also some PSCs rely on environmentally unfriendly materials such as lead (Pb), yielding toxic chemical compounds (PbI2).

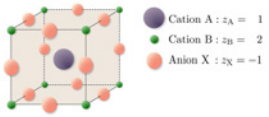

Fig. 4: *The perovskite unit cell*

Dilara Abdel and Patricio Farrell are working together with Petr Vágner and Jürgen Fuhrmann (both RG 3) on deriving models and simulations for PSCs. The idea is to derive from Maxwell–Stefan diffusion and general electrostatics a drift-diffusion model for charge transport in perovskite solar cells (PSCs) where any ion in the perovskite layer may flexibly be chosen to be mobile or immobile. Unlike other models in the literature, our model is based on quasi-Fermi potentials instead of densities. Our approach allows to easily include nonlinear diffusion (based on, for example, Fermi–Dirac, Gauss–Fermi, or Blakemore statistics) as well as limit the ion depletion (via the Fermi–Dirac integral of order -1). The latter is motivated by a grand-canonical formalism of ideal lattice gas. Furthermore, our model allows to use different statistics for different species [1].

Together with Nicola Courtier from the University of Oxford, the group organized a minisymposium at the "SIAM Conference on Mathematical Aspects of Materials Science MS21" with the title "Modelling and Simulation of Charge Transport in Perovskites." The minisymposium included talks by eight speakers from the UK, Israel, Argentina, Switzerland, and Germany. From WIAS Dilara Abdel gave a talk.

Coupling with atomistic effects. LG NUMSEMIC investigates together with researchers from Tyndall National Institute (Ireland) 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 the software `ddfermi` [6].

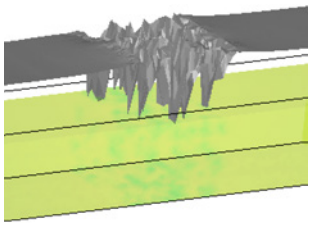

Fig. 5: *Random fluctuations in the band edge energy on atomic scale*

Other projects. Other projects in LG NUMSEMIC concern positivity-preserving time discretizations [3] as well as SIR (susceptible, infected, and recovered) models [4].

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

Head: Priv.-Doz. Dr. Benedikt Jahnel

Team: Anne Flöge (WIAS Female Master Students Program)
Alexander Hinsen
Dr. Sanjoy Kumar Jhawar
Anh Duc Vu

Secretary: Christina van de Sand

2021 was the first year within the five-year runtime of the Leibniz junior research group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks*, which is funded by the Leibniz Association through the *Leibniz Competition 2020*. Using methods from stochastic geometry and statistical physics, the group's general goal is to make cutting-edge contributions to the fundamental understanding of spatial communication system with a significant random component. Prototypically, and also in 2021, DYCOMNET investigates connectivity properties of so-called *device-to-device networks* in which randomly located mobile network components can communicate in a peer-to-peer fashion whenever they are sufficiently close to each other.

One of the key performance indicators of such networks is the emergence of large connected components, a phenomenon often called *percolation*, see Figure 1 for an illustration. The importance of percolation analysis for communication systems was, for example, highlighted in the title story of the April edition of the *Scientific American*, entitled *The Mathematics of How Connections Become Global: Percolation Theory Illuminates the Behavior of Many Kinds of Networks, From Cell-Phone Connections to Disease Transmission*, in which the head of the group was among the interviewed experts. More details on applications of percolation theory to communication systems are presented by the group in this year's Scientific Highlights article "Probabilistic Methods for Communication Systems" on page 10. Here, the LG DYCOMNET reports, for example, on their accomplishments regarding the analysis of connection times in large mobile infrastructure-augmented device-to-device networks, see also [2, 3]. Additionally, the Scientific Highlights article also features results on the limiting shape of the set of infected devices in pure device-to-device systems as well as scaling limits for the space-time dissipation of malware in such networks [1]. This work very much benefitted from the contributions of Alexander Hinsen who is funded by the *Berlin Mathematics Research Center MATH+* via the project "Influence of mobility on connectivity."

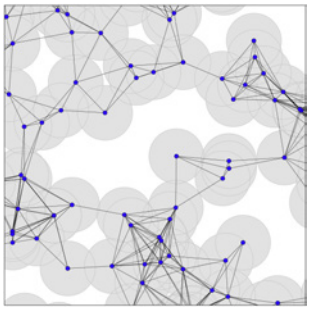


Fig. 1: *Realization of randomly placed devices (blue). Black edges are drawn whenever two devices have overlapping interaction zones (gray).*

But not only the scientific community is interested in percolation results and the like for communication systems. In 2021, the DYCOMNET group successfully completed another joint research project with their longterm partners from industry, Eli Cali and Jean-Philippe Wary at Orange SA in Paris, France. This project, under the title "Malware propagation in mobile device-to-device networks," investigated a model in which devices move independently along streets in a city topology sampled from a *Poisson–Voronoi tessellation*, and malware is transmitted between any pair of devices whenever they are sufficiently close for a sufficiently long time. The main results describe the multidimensional phase diagram for the presence, respectively absence, of percolation in the

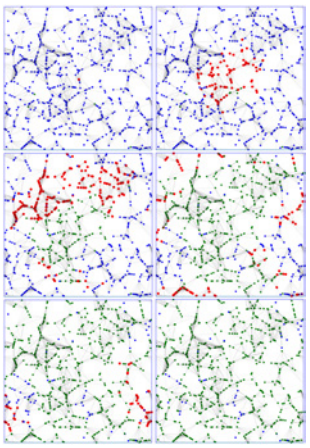


Fig. 2: *Snapshots of the mobile urban device-to-device network at six different times, based on a Python simulation. An infected device (red) is present at the center at initial time (up left), together with other susceptible devices (blue) and patch-holding devices (green). As time progresses, susceptible devices in the vicinity start to become infected. However, once patch-holding devices are attacked, they start to retaliate towards the infected devices.*

model and thus give insights into the parameter regimes in which malware can infect macroscopic portions of the system, respectively remains local. In the second part of the work, also the mitigating effects of a decentralized counter-measure were analyzed for a large set of system parameters, see Figure 2 for an illustration. Here, the main results feature parameter regimes in which the malware either survives or can be successfully eliminated from the system. Besides rigorous proofs, together with their collaborators, DYCOMNET also performed a variety of simulation studies of the space-time system.

In addition to the described projects, in 2021, the group also used its expertise on random graphs and stochastic geometry to make contributions in related fields of research. In [4], Sanjoy Jhawar contributed to the asymptotic analysis of dense connectivity models in which the probability of a point-to-point connection to be established depends on independent random weights associated to the points. In [5], a cross-disciplinary WIAS group around Anh Duc Vu investigated a class of nonlinear partial differential equations defined on a randomly perforated domain driven by Poisson point processes. Also here, percolation and ergodicity properties of point processes play a central role in the analysis. Finally, in [6] the loss, respectively the preservation, of locality properties of totally independent random fields under a local thinning transformation are investigated.

Another highlight of 2021 was the successful defense of the habilitation thesis “Stochastic Geometry and Communication Networks & Statistical Mechanics for Point Processes and Stochastic Dynamics” of the head of the group at the Technische Universität (TU) Berlin, reviewed by Wolfgang König (TU Berlin/WIAS), Sabine Jansen (München), Aernout van Enter (Groningen), and François Baccelli (Paris). The habilitation was followed by two offers for W2 professorships at the Technische Universität Braunschweig and the Philipps-Universität Marburg.

The year 2021 also brought multiple opportunities to present the work of the group, e.g., at the “Stochastic Geometry Days” in Dunkerque, France, the “Thematic Einstein Semester on Geometric and Topological Structure of Materials” at TU Berlin, the Workshop “Randomness Unleashed: Geometry, Topology, and Data” at the Rijksuniversiteit Groningen, Netherlands, the “DYOGENE Seminar” at INRIA Paris, France, the “Probability Seminar” at University of Bath, and the “MoDiRu Seminar” at Charité Berlin. As a newly appointed *EURANDOM Ambassador* at Eindhoven University of Technology, Netherlands, Benedikt Jahnel will have the opportunity to push forward the agenda of the group via two international conferences within the next four years.

References

[1] C. Coletti, L. de Lima, A. Hinsen, B. Jahnel, D. Valesin, *Limiting shape for first-passage percolation models on random geometric graphs*, arxiv Preprint no. 2109.07813, 2021.

[2] C. Hirsch, B. Jahnel, E. Cali, *Percolation and connection times in multi-scale dynamic networks*, arxiv Preprint no. 2103.03171, 2021.

[3] C. Hirsch, B. Jahnel, E. Cali, *Connection intervals in multi-scale dynamic networks*, arxiv Preprint no. 2111.13140, 2021.

[4] S.K. Jhawar, S.K. Iyer, *Poisson approximation and connectivity in a scale-free random connection model*, Electron. J. Probab., **26** (2021), pp. 1–23.

[5] M. Heida, B. Jahnel, A.D. Vu, *Homogenization on irregularly perforated domains*, arxiv Preprint no. 2110.03256 , 2021.

[6] B. Jahnel, C. Külske, *Gibbsianness and non-Gibbsianness for Bernoulli lattice fields under removal of isolated sites*, arxiv Preprint no. 2109.13997, 2021.

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. L. Andreis, Assistant Professorship, March 1, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Italy.
2. G. Dong, Associate Professorship, December 13, Central South University, School of Mathematics and Statistics, Changsa, Hunan Province, P.R. of China.
3. P. Farrell, Associate Professorship, June 16, Heriot-Watt University Edinburgh, School of Mathematical and Computer Sciences, UK.
4. B. Jahnel, W2 Professorship, August 11, Technische Universität Braunschweig, Carl-Friedrich-Gauß-Fakultät.
5. ———, W2 Professorship, November 25, Philipps-Universität Marburg, FB 12 – Mathematik und Informatik.
6. A. Kröner, W2 Professorship, September 6, Martin-Luther-Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II – Chemie, Physik und Mathematik.
7. G. Nika, Assistant Professorship, September 1, Karlstad University, Department of Mathematics and Computer Science, Sweden.

A.1.2 Awards and Distinctions

1. D. Abdel, *Scholarship "Procope Mobility 2021" of the French Embassy in Germany*, April 26.
2. ———, *SIAM CSE21 Student Travel Award*, February 9.
3. ———, *SIAM MS21 Student Travel Award*, May 5.
4. M. Ebeling-Rump, *Special prize of the Humboldt University Society for business and start-up ideas to combat climate changes and one of the two Audience awards from the Berliner Sparkasse for a concept of energy saving through mathematically optimized design of components*, June 22, 2021.
5. R. Henrion, *Member of Comité Scientifique International, Groupement de Recherche Mathématiques de l'Optimisation et Applications (GdR MOA), France.*
6. M. Hintermüller, *Co-chair and Member of the Council of the Berlin Mathematics Research Center MATH+.*
7. ———, *Member of the Integrative Research Institute for the Sciences IRIS Adlershof of the Humboldt-Universität zu Berlin.*
8. ———, *Member of the Scientific Advisory Board of the INM – Leibniz-Institut für Neue Materialien, Saarbrücken.*
9. ———, *Spokesperson of Forschungsverbund Berlin e.V.*
10. ———, *Spokesperson of Section 4, Technical Sciences and Engineering, of the initiative Berlin Research 50.*
11. D. Hömberg, *Chair of the European Consortium for Mathematics in Industry (ECMI)'s Research and Innovation Committee.*
12. ———, *Head of the Secretariat of the International Mathematical Union (IMU).*

13. ———, *Treasurer of IMU*.
14. ———, *Vice Chair of 7th Technical Committee (TC7) of the International Federation for Information Processing (IFIP) on System Modeling and Optimization*.
15. B. Jahnel, *EURANDOM Ambassador at Eindhoven University of Technology*, September 1.
16. M. Radziunas, *Honorary Associate Professor of Macquarie University 2021–2023, Sydney, Australia*, August 12.
17. A. Stephan, *SIAM Travel Award*, May 5, 2021.
18. V. Klika, M. Pavelka, P. Vágner, M. Grmela, *Entropy 2021 Best Paper Award*, May 26.

A.1.3 Habilitations

1. B. Jahnel, *Stochastic Geometry and Communication Networks & Statistical Mechanics for Point Processes and Stochastic Dynamics*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, May 10.

A.1.4 Defenses of Ph.D. Theses

1. J. Arenas Jaén, *Thermal cutting of steel plates – Modelling, simulation and optimal control of preheating strategies*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, February 26.
2. P. Hager, *Rough analysis with application in markets and related fields*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Prof. Dr. P. Friz, Dr. Ch. Bayer, September 15.
3. T. Keil, *Optimal control of a semi-discrete Cahn–Hilliard–Navier–Stokes system with variable fluid densities*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. M. Hintermüller, September 10.
4. R. Preiss, *Hopf algebras and non-associative algebras in the study of iterated-integral signatures and rough paths*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. P. Friz, October 5.
5. Y. Yuan, *Schramm–Loewner evolution and path regularity*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. P. Friz, October 26.
6. D. Dvinskikh, *Decentralized algorithms for Wasserstein barycenters*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, August 18.
7. F. Galarce Marín, *Inverse problems in hemodynamics. Fast estimation of blood flows from medical data*, INRIA Paris & LJLL. Faculté des Sciences, Sorbonne Université, supervisors: Prof. J.-F. Gerbeau, Prof. D. Lombardi, Prof. O. Mula, April 9.
8. A. Stephan, *Coarse graining for gradient systems and Markov processes*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, May 11.

A.1.5 Supervision of Undergraduate Theses

1. H. Aydin, *Fixierung für die aktivierte Irrfahrt und das stochastische Sandhaufenmodell* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. L. Taggi, January 19.

2. K. Brasch, *Geometric programming – Theory and application to smart grid households* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, May 4.
3. H. Busse, *Generalizations of the Lax–Milgram theorem* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. A. Mielke, April 29.
4. M. Domke, *Identifikation von Wärmeausdehnungskoeffizienten bei Faserverbundwerkstoffen* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, January 4.
5. A.K. El-Rahhal, *Approximation von Übertragungsfunktionen einer Werkzeugmaschine mittels mathematischer Modelle* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 5.
6. N.F. Engler, *Gibbsianness of locally thinned random fields* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Priv.-Doz. Dr. B. Jahnel, Prof. Dr. W. König, June 22.
7. M. Gaedke, *Verfahren für parabolische Differentialgleichungen am Beispiel der Wärmeleitungsgleichung* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 25.
8. Th.-M. Galanis, *Large deviations for high interferences* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, January 20.
9. E. Giesecke, *Deep learning meets optimal control: Network architectures based on neural ordinary differential equations and simulations of Runge–Kutta nets* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. A. Kröner, March 2.
10. T. Grahl, *Abweichungen des Durchsatzes bei zufälligen Mediumzugangsprotokollen* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, October 15.
11. D. Grinberg, *Analysis of codon usage bias based on optimal transport* (bachelor's thesis), Beuth Hochschule für Technik Berlin, supervisor: Dr. A. Suvorikova, April 21.
12. M. Haase, *Deep neural networks for topology optimisation under uncertainties* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. M. Eigel, June 28.
13. B. Hahn, *Optimierung verrauschter Funktionen mittels Implicit Filtering* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, May 4.
14. L. Henning, *Gradienten Verfahren zur Optimierung Neuronaler Netze* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 25.
15. P.J. Hossie, *Large interferences in spatial communication systems* (master's thesis), African Institute of Mathematical Science Ghana, supervisor: Prof. Dr. W. König, July 12.
16. T. Hu, *Bernstein polynomials and their application in the finite element method* (bachelor's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, September 23.
17. J. Kreich, *Multithreaded GMRES in the programming language Julia* (master's thesis), Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Dr. J. Fuhrmann, November 4.
18. A. Magraner Villalba, *Asymptotics of statistical experiments for extreme values* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, December 3.

19. M. Maibaum, *Lipschitz methods in global optimization* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, June 21.
20. S. Marschall, *Ein zufälliges Polymer mit vielen Attraktionspunkten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 13.
21. K. Mild, *Training separabler tiefer neuronaler Netzwerke mit Variable Projektion* (bachelor's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. A. Kröner, July 9.
22. A. Miwa, *Ein Prinzip großer Abweichungen für Clustergrößen in zufälligen Graphen mit fester Kantenzahl* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R. Patterson, November 30.
23. Z. Momo, *Particle size statistics in a coagulation model with constant kernel* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Dr. R. Patterson, November 30.
24. J. Pilarski, *Die Konvergenz des Random-Waypoint-Modells in die invariante Verteilung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, August 17.
25. S.L. Plato, *Analysis and numerics for a spatio-temporal predator-prey system* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, June 22.
26. M. Pudör, *Die Momente eines Verzweigungsprozesses in zufälligem Medium* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Prof. Dr. J. Blath, January 4.
27. F. Rehfeld, *Stokes–Darcy vs. Brinkman – Ein numerischer Vergleich* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, January 26.
28. M.E.V. Reiter, *Numerical approximation of dissipative solutions to the Ericksen–Leslie equations* (master's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. R. Lasarzik, October 20.
29. L. Scaglione, *Simulation of an elastic vascularized tissue via non-matching immersed methods* (bachelor's thesis), Politecnico di Milano, Dipartimento di Matematica, supervisors: Dr. A. Caiazzo, Dr. U. Wilbrandt, July 16.
30. Ch. Schmidt, *Konnektivität via empirische Maße und deren große Abweichungen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, June 7.
31. L.L.L. Schmollack, *Mathematische Herleitung und Analyse eines Fluid-Struktur-Interaktionsproblems* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. M. Thomas, June 30.
32. N. Siebken, *k-Hop-Perkolation* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, November 5.
33. F. Sun, *Die asymptotische Extremwertverteilung des Gaußprozesses* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 13.
34. K. Völkner, *Optimal control of a class of nonsmooth semilinear elliptic PDEs* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisors: Prof. Dr. M. Hintermüller, Dr. K. Papafitsoros, December 8.

35. A.D. Vu, *An application of stochastic two-scale convergence on a nonlinear Robin boundary problem* (master's thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Dr. M. Heida, February 10.

36. J. Yan, *Konvergenzgeschwindigkeit des Random-Waypoint-Modells gegen ihre invariante Verteilung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, October 21.

37. Y. Zhu, *Phasenübergang im freien Bose-Gas via große Abweichungen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisors: Prof. Dr. W. König, Priv.-Doz. Dr. B. Jahnel, October 8.

A.2 Grants[1]

European Union, Brussels

- **Seventh Framework Programme**

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

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

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

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

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

- **European Metrology Programme for Innovation and Research (EMPIR)**
  Invertible Neural Networks for applications in metrology (as 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 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

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

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

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

- **Förderprogramm IKT 2020 – Forschung für Innovationen** (Funding program 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).

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

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

In 2021, WIAS dedicated considerable financial and personal resources to the Center: Its director, Prof. M. Hintermüller (RG 8) was one of the three spokespersons and a member of the Executive Board of MATH+. He, Prof. A. Mielke (RG 1, as Chair of the MATH+ Council), Prof. W. König (RG 5), Prof. P. Friz (RG 6), Prof. V. Spokoiny (RG 6), and Dr. M. Thomas (WG BIP) 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:

AA1-12: "Mathematical modeling of cellular self-organization of stimuli responsive extra cellular matrix" (in 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)

AA2-15 "Random alloy fluctuations in semiconductors" (in RG 1 and RG 6)

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

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

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

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)

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

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

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

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

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

EF3-9 “Mathematical framework for MR poroelastography” (in RG 3 and RG 6)

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

EF4-10 “Trail formation in populations of auto-chemotactic agents” (from 2022 new name “Coherent movements in co-evolving agent-message systems”; in RG 5)

Approved projects, starting in 2022:

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

AA3-13 “Placing Steiner points in constrained tetrahedralizations” (in RG 3)

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)

EF1-15 “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)

EF3-11 “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)

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

- **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, will successfully be ended in June 2022. The center is facing a reorientation. An application for a third funding period until June 2026 has been submitted. The research center focuses on an efficient handling of gas transportation. The Weierstrass Institute participates in the subprojects “Chance constraints in models of gas markets” (in RG 4), “Multicriteria optimization subject to equilibrium constraints at the example of gas markets,” and “Galerkin methods for the simulation, calibration, and control of partial differential equations on networks” (both in RG 8).

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

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

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

  The center began its work on October 1, 2014 (second funding period until June 30, 2022). WIAS members participate in the subprojects: B01 “Fault networks and scaling properties of deformation accumulation” (in RG 1, with FU Berlin and GFZ Potsdam), C02 “Interface dynamics: Bridging stochastic and hydrodynamic descriptions” (in RG 1, with FU Berlin), C05 “Effective models for materials and interfaces with multiple

scales" (in RG 1), C08 "Stochastic spatial coagulation particle processes" (in RG 5), and C09 "Dynamics of rock dehydration on multiple scales" (in WG BIP with FU Berlin). CRC 1114 currently applies for its third funding period.

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

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

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

- **Priority Program SPP 1748: "Zuverlässige Simulationstechniken in der Festkörpermechanik – Entwicklung nichtkonventioneller Diskretisierungsverfahren, mechanische und mathematische Analyse" (Reliable Simulation Techniques in Solid Mechanics – Development of Non-standard Discretisation Methods, Mechanical and Mathematical Analysis)**, Universität Duisburg-Essen

  WG 1 participated in this priority program with the subproject "Finite-Elemente-Approximation von Funktionen beschränkter Variation mit Anwendungen in der Modellierung von Schädigung, Rissen und Plastizität" (Finite element approximation of functions of bounded variation and application to models of damage, fracture, and plasticity), which is a collaboration with Universität Freiburg (duration: Oct. 2014 – Sept. 2017) and then participated, also jointly with Universität Freiburg, from December 2017 to November 2021 in the subproject "Reliability of efficient approximation schemes for material discontinuities described by functions of bounded variation."

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

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

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

  The Director of WIAS, Prof. 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 until 2022 started in 2019.

  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 from 01.07.2019 and 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 projects: "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

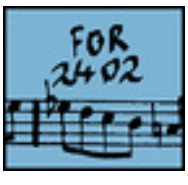
The head of RG 5, Prof. Wolfgang König, is the head of this priority programme, which aims at solving various problems that originate from a counterplay between randomness and space. There are many motivations from rich applications in the Sciences, but also intrinsic interest from researchers in probability.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

WIAS participates with the projects "Spatial coagulation and gelation" and "The statistical mechanics of the interlacement process" (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 (PDEs) 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 spokesmen 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.

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

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

- Approved Project:

  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) will examine 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 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.

- Approved Project:

  ANR-DFG Cooperation: Joint German-French Research Projects: "Hybrid chip-scale frequency combs combining III-V quantum-dash mode-locked lasers and high-Q silicon-nitride microresonator (HybridCombs)" (in RG 2)

- **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 planned for 2021 had to be cancelled, but a successful collaboration has been established on the basis of video conferencing and online communication.

- **Normalverfahren (Individual Grants)**

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

  "Numerische Multiskalen-Methoden zur inversen Schätzung der effektiven Eigenschaften poroelastischer Gewebe" (Computational multiscale methods for inverse estimation of effective properties of poroelastic tissues; in RG 3)

  Approved Project:

  "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)**

  "Numerische Methoden für innovative Halbleiter-Bauteile" (Numerical Methods for Innovative Semiconductor Devices; January 2020 – December 2024, in LG NUMSEMIC)

  "Probabilistische Methoden für dynamische Kommunikationsnetzwerke" (Probabilistic Methods for Dynamic Communication Networks; January 2021 – December 2025, in LG DYCOMNET)

  Approved Projects:

  "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).

Einstein Stiftung Berlin (Einstein Foundation Berlin)

- Thematic Einstein Semester "Energy-Based Mathematical Methods for Reactive Multiphase Flows" (October 2020 – March 2021, co-organized by RG 1, RG 7, and WG BIP)
- 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," started in July 2018, jointly with HU Berlin, in RG 5.
- **Program for Project-Related Personal Exchange (PPP) with India**, "Analysis and numerical methods for population balance equations" (in RG 3)

International projects

- Fondation Mathématique Jacques Hadamard (FMJH): Optimal control problems with probabilistic constraints (in RG 4)

Mission-oriented research (examples)

- Orange Labs Research, Paris, France:
  "Malware propagation in mobile device-to-device networks" (01.09.2020–31.12.2021; in LG DYCOMNET)
- Ferdinand Braun Institute, Berlin:
  "Simulation of external cavity and multi-section semiconductor lasers" (01.01.2021–31.07.2021; in RG 2)

  Approved Project:

  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, Managing 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. ———, Guest Editor, Frontiers in Physiology, Section Biophysics, Frontiers Media S.A., Lausanne, Switzerland.
8. P. Friz, Editor-in-Chief, Annals of Applied Probability, The Institute of Mathematical Statistics, Beachwood, OH, USA.
9. ———, Editorial Board, Electronic Communications in Probability, Institute of Mathematical Statistics, Bethesda, USA.
10. ———, Editorial Board, Electronic Journal of Probability, Institute of Mathematical Statistics, Bethesda, USA.
11. R. Henrion, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, Netherlands.
12. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, Netherlands.
13. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
14. ———, Editorial Board, Optimization — A Journal of Mathematical Programming and Operations Research, Taylor & Francis, Abingdon, UK.
15. M. Hintermüller, Associate Editor, ESAIM: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
16. ———, Associate Editor, Advances in Continuous and Discrete Models: Theory and Modern Applications, Springer Nature, New York, USA.
17. ———, Associate Editor, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, USA.
18. ———, Editorial Board, Interfaces and Free Boundaries, European Mathematical Society Publishing House, Zurich, Switzerland.
19. ———, Editorial Board, Annales Mathématiques Blaise Pascal, Laboratoire de Mathématiques CNRS-UMR 6620, Université Blaise Pascal, Clermont-Ferrand, France.
20. ———, Editorial Board, Journal of Nonsmooth Analysis and Optimization, Centre pour la Communication Scientifique Directe, Villeurbanne, France.
21. ———, Editorial Board, Optimization Methods and Software, Taylor & Francis, Oxford, UK.

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

22. ———, Editorial Board, Foundations of Data Science, American Institute of Mathematical Sciences, Springfield, USA.
23. ———, Series Editor, International Series of Numerical Mathematics, Springer-Verlag, Basel, Switzerland.
24. ———, Series Editor, Handbook of Numerical Analysis, Elsevier, Amsterdam, Netherlands.
25. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
26. ———, Editorial Board, Eurasian Journal of Mathematical and Computer Applications, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan.
27. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
28. ———, Editorial Board, Bernoulli Journal, International Statistical Institute/Bernoulli Society for Mathematical Statistics and Probability, The Hague, Netherlands.
29. ———, Series Editor, Pathways in Mathematics, Birkhäuser, Basel, Switzerland.
30. A. Mielke, Associate Editor, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
31. ———, Associate Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
32. ———, Editor-in-Chief, GAMM Lecture Notes in Applied Mathematics and Mechanics, Springer-Verlag, Heidelberg.
33. M. Radziunas, Editorial Board, Mathematical Modelling and Analysis, Vilnius, Lithuania.
34. J.G.M. Schoenmakers, Editorial Board, International Journal of Portfolio Analysis and Management, Interscience Enterprises Limited, Geneva, Switzerland.
35. ———, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
36. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
37. V. Spokoiny, Editor, Theory of Probability and its Applications, SIAM, Philadelphia, Pennsylvania, USA.
38. M. Thomas, Associate Editor, Discrete & Continuous Dynamical Systems – Series S, American Institute of Mathematical Sciences, Springfield, USA.
39. B. Wagner, Editorial Board, SIAM Journal on Applied Mathematics, Society for Industrial and Applied Mathematics, Philadelphia, USA.
40. ———, Guest Editor, European Journal of Applied Mathematics, Special Issue “The Mathematics in Renewable Energy”, Springer Nature, Heidelberg et al.

A.4 Conferences, Colloquia, and Workshops

Applied Probability Day 2021 (Online Event)
Berlin, January 8
Organized by: WIAS (RG 6), TU Berlin
Supported by: IMS, ERC Project GPSART 683164, WIAS

The purpose of this one-day meeting was to unite a number of leaders of modern applied probability theory, all presently serving on the board of the IMS Annals of Applied Probability, and allowing for an intimate change of ideas in a small setting of our immediate working groups. The resulting format was one with 40–50 online participants who followed a total of 10 senior speakers, 6 of them from outside Germany (3 from Paris, 1 from Luxembourg, 1 from Prague, 1 from Budapest).

The workshop was jointly organized by the WIAS group *Stochastic Algorithms and Nonparametric Statistics* (Peter Friz, ERC and DFG funded) and François Delarue (U Nice).

"Structures in Evolution: Theory and Applications" – Final Conference of the Thematic Einstein Semester on Energy-based Mathematical Methods for Reactive Multiphase Flows (Online Event)
Berlin, February 23–25
Organized by: WIAS (RG 1 (Matthias Liero, Alexander Mielke), RG 7 (Barbara Wagner), WG BIP (Marita Thomas, Dirk Peschka)), TU Berlin (Volker Mehrmann)
Supported by: Einstein Foundation Berlin

This three-day final conference of the Thematic Einstein Semester featured eight invited talks by internationally renowned scientists working in the field of variational methods for evolution equations. The range of topics included thermodynamic frameworks for multicomponent flows, structure-preserving discretization schemes, and the derivation of effective models for problems with multiple scales.

Due to the corona pandemic, this workshop was organized as an online event. On average, the workshop had about 40 online participants each day.

Finite volume methods for real-world applications (Online Event)
Berlin, April 29
Organized by: WIAS (RG 1 (Annegret Glitzky, Thomas Koprucki, Matthias Liero) and RG 3 (Alexander Linke))

This one-day online workshop on the occasion of Dr. Jürgen Fuhrmann's 60th birthday featured three invited talks by internationally renowned speakers in the field of finite-volume methods and mesh generation, as well as a "Hackathon" for the novel scientific programming language Julia. Robert Eymard (Université Gustave Eiffel, France) reported on finite-volume methods and monotony issues. The talk by Hang Si (WIAS) focused on numerical mesh generation, and Claire Chainais-Hillairet (Université de Lille, France) demonstrated an existence result for a corrosion model based on a computer-assisted proof.

Finally, the Hackathon allowed interested participants to actively learn and try the Julia language, which is tailored for applications in scientific computing and machine learning. Topics included first steps in Julia, meshes and visualization, automatic differentiation and machine learning and partial differential equations.

The event attracted about 80 participants from ten different countries.

SPDEs & friends (Online Event)
Berlin, May 31 – June 2
Organized by: WIAS (RG 6), TU Berlin
Supported by: DFG FOR 2402, MATH+, WIAS

The aim of the conference was to bring mathematicians from the Stochastic Partial Differential Equations, Liouville Quantum Gravity, Statistical Mechanics and Gaussian Free Field communities together in order to showcase recent result and open problems that may be attractive to researchers in these areas. In order to encourage

cross-discipline interactions, the conference was held in the "speaker-discussant" format, where talks by the invited speakers are followed by a summary and question session conducted by another researcher. Due to the ongoing pandemic, the meeting was held completely online via the Zoom platform. Moreover, coffee and lunch breaks were held on the Gather.Town platform.

The conference attracted more than 240 online participants and featured 36 invited speakers, divided into 18 main speakers and 18 discussants, including early career and senior researchers.

The conference was organized by the WIAS group *Stochastic Algorithms and Nonparametric Statistics* members Oleg Butkovsky (DFG funded), Peter Friz (ERC and DFG funded), and Nikolas Tapia (MATH+ funded).

Nonlinear Dynamics in Semiconductor Lasers (Online Event)

Berlin, June 16–18
Organized by: RG (2)
Supported by: MATH+, WIAS

The online Workshop "Nonlinear Dynamics in Semiconductor Lasers,", financially supported by WIAS and MATH+, brought together internationally renowned researchers working on theoretical, experimental, and applied aspects of the dynamics of semiconductor lasers and optoelectronic devices, as well as mathematical methods for modeling and analysis of these devices. The Workshop featured a good balance between theory, experiment, and numerics and provided the participants with the opportunity to present the latest developments and to exchange knowledge with their colleagues, including young scientists. The subjects of the Workshop included: dynamics of ring and edge-emitting multisection lasers, broad-area lasers and VCSELs, coupled laser systems, frequency-swept lasers, high-beta lasers, high-power tapered and broad-area lasers and amplifiers, lasers with delayed feedback, mode-locked lasers, narrow-linewidth lasers, and quantum-dot lasers. Special attention was drawn to the dynamics of single-photon sources and quantum light-emitting diodes, hybrid SOA-fiber lasers, generation of short optical pulses including spatial and temporal localized structures of light, as well as to analytical and numerical methods for modeling and simulations of optoelectronic devices. The program included 35 invited and 10 contributed online talks and 5 poster presentations on the Gather.Town platform. The Workshop was attended by 95 registered participants from 16 countries.

Minisymposium "Perspectives of Gradient-Robustness" (Online Event)

Berlin, July 8
Organized by: WIAS (RG 3: Jürgen Fuhrmann, Volker John, Christian Merdon)

This online mini-symposium gathered interested researchers to discuss recent developments and perspectives for gradient-robust discretizations in computational fluid dynamics and included three invited talks. Joachim Schöberl (Technische Universität Wien, Austria) presented software tools for robust finite element methods. Thomas Apel and Volker Kempf (both Universität der Bundeswehr München) talked about pressure-robust discretizations on anisotropic meshes. Michael Neilan (University of Pittsburgh, USA) focussed on novel quasi-optimal error estimates for pressure-robust schemes. A fourth talk by Christian Merdon (WIAS Berlin) focussed on the impact of gradient-robustness in convection stabilisation and compressible low Mach number flows.

The event attracted 75 participants from Germany, the Netherlands, Italy, Austria, France, the USA and Kuwait. The occasion was also used by the organizers and many present colleagues to thank Alexander Linke for his fundamental contributions in the field.

Leibniz MMS Summer School 2021 "Mathematical Methods for Machine Learning"

Schloss Dagstuhl, August 23–27
Organized by: WIAS: Martin Eigel (RG 4) and Christian Bayer (RG 6)
Supported by: MMS

In this school for more than 20 Ph.D. students from various Leibniz Institutes of the Mathematical Modeling and Simulation (MMS) network, fundamental and advanced aspects of Machine Learning methods were presented with the aim to enable the participants to apply such methods to their specific research problems. In particular,

the addressed topics included symbol image machine learning; fundamentals of statistical learning theory; introduction to machine learning with Python; signatures and learning of time-invariant features of time series; data-driven modeling of dynamical systems; distributed learning; robust methods for machine learning and data-driven decision-making; kernel methods.

AMaSiS2021: Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems (AMaSiS 2021, Online Event)
Berlin, September 6–9
Organized by: WIAS (RG 1 (Annegret Glitzky, Hans-Christoph Kaiser, Oliver Marquardt), RG 2 (Markus Kantner), RG 3 (Jürgen Fuhrmann), RG 7 (Manuel Landstorfer)) and Ansgar Jüngel (TU Vienna)
Supported by: DFG (funding not utilized), MATH+, WIAS

The interdisciplinary workshop was dedicated to the mathematical modeling of semiconductors and electrochemical systems. Due to inherent similarities between both disciplines, AMaSiS explored synergies in mathematical modeling, analysis, numerics, and simulation techniques. The conference brought together experts from applied mathematics, physics, engineering, chemistry, and material science and covered the topics electronic structure theory, non-equilibrium thermodynamics and transport theories, mathematical upscaling from quantum mechanics and particle systems to continuum scale, numerical methods, as well as special semiconductor devices, and electrochemical systems.

This online event hosted 12 invited presentations including two survey lectures for a broader scientific audience by Joachim Maier (Stuttgart) on “Ion conductors, electron conductors and mixed conductors in electrochemistry” and Eoin P. O’Reilly (Tyndall, Cork) on “Trends and challenges in semiconductor device and nanostructure modeling”. Furthermore, the program contained 14 contributed talks and a virtual poster session with 16 scientific posters. It attracted more than 100 participants from 17 countries.

15th International Conference on Free Boundary Problems: Theory and Applications 2021 (Online Event, FBP 2021)
Berlin, September 13–17
Organized by: WIAS (RG 8), FU Berlin, TU Berlin
Supported by: MATH+, WIAS

The FBP conference was a flagship event that brought together the free boundary and partial differential equation communities. This international conference has been organized every few years, the first of which took place in 1981.

More than 161 scientists from around the world participated in the online event, delivering a total of 159 scientific talks. FBP 2021 featured 17 minisymposia on topics related to free boundary problems, including surface PDEs, numerical methods, stochastic models, applications to life and physical sciences, and interface problems. The 12 plenary talks delivered by prominent mathematicians in the field, including a recent Fields medalist, were extremely well received by the community.

The organization was performed by the following members of WIAS Research Group RG 8: Michael Hintermüller, Amal Alphonse, Jo-Andrea Brüggemann, Caroline Geiersbach, Olivier Huber, and Axel Kröner. Other members of RG 8 provided technical support during the conference.

Junior Female Researchers in Probability (hybrid format)
Berlin, October 4–6
Organized by: IRTG 2544 Berlin-Oxford, WIAS (RG 5)
Supported by: MATH+, HU Berlin, TU Berlin

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 accomodation, and about 20–30 took this opportunity to present their Ph.D. work to a larger audience.

The workshop took place in a hybrid format, and about 45 participants (by far not only females) were present in person (65 participants online) at the wonderful location in the Harnack Haus in Berlin-Dahlem. 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 seven people, comprising one current (Alexandra Quitmann and one former member (Luisa Andreis) of the WIAS Research Group RG 5 *Interacting Random Systems*.

Kick-off Workshop of the MATH+ Thematic Einstein Semester on "Mathematics of Imaging in Real-World Challenges" (hybrid format)
Berlin, October 6–8
Organized by: WIAS (RG 8, ZIB, TU Berlin, PTB)
Supported by: Einstein Foundation, MATH+, HU Berlin, TU Berlin, PTB, ZIB, WIAS

This workshop served as a kick-off event for the MATH+ Thematic Einstein Semester on "Mathematic of Imaging in Real-world Challenges" October 2021 – March 2022. The event brought together practitioners, biomedical engineers, computer vision and machine learning experts as well as applied mathematicians in order to exchange on the current applications and theory of imaging science. The meeting was successfully organized in a hybrid fashion with the first day taking place entirely online and the following two days taking place in Physikalisch-Technische Bundesanstalt (PTB) in a hybrid manner with most speakers and attendants being physically present. The workshop consisted of 16 invited talks, a poster session for young researchers (9 posters), dedicated sessions on "Software and Practice," "Real-world Applications" as well as a lively panel discussion on "Public Software and Rewarding in Science" and "Career Pathways." The conference was attended by more than 80 participants, mainly from Germany, as well as from Austria, UK, USA, and Hong Kong.

A.4.1 Oberwolfach Workshops co-organized by WIAS

Challenges in Optimization with Complex PDE-Systems (hybrid format)
Mathematisches Forschungsinstitut Oberwolfach, February 14–20
Organized by: Michael Hintermüller (RG 8), Karl Kunisch (Graz), Günter Leugering (Erlangen), Elisabetta Rocca (Pavia)

The workshop concentrated on various aspects of optimization problems with systems of nonlinear partial differential equations (PDEs) or variational inequalities (VIs) as constraints. In particular, discussions around several keynote presentations in the areas of optimal control of nonlinear or non-smooth systems, optimization problems with functional and discrete or switching variables leading to mixed integer nonlinear PDE-constrained optimization, shape and topology optimization, feedback control and stabilization, multi-criteria problems and multiple optimization problems with equilibrium constraints as well as versions of these problems under uncertainty or stochastic influences, and the respectively associated numerical analysis as well as design and analysis of solution algorithms were promoted. Moreover, aspects of optimal control of data-driven PDE constraints (e.g., related to machine learning) were addressed.

The workshop consisted of 13 keynote presentations, which were complemented by 17 short communications.

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

1. U. Bandelow, member of the Program Committee, *21st International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD, Online Conference)*, Torino, Italy, September 13–17.
2. Ch. Bayer, organizer of the Minisymposium "UQ for Rough Volatility and Predictive Models in Finance", *SIAM Conference on Financial Mathematics and Engineering (FM21, Online Event)*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, USA, June 1–4.
3. P. Farrell, co-organizer of the Minisymposium MS63 "Modelling and Simulation of Charge Transport in Perovskites", *SIAM Conference on Mathematical Aspects of Materials Science MS21 (Online Event)*, Basque Center for Applied Mathematics, Bilbao, Spain, May 17–28.
4. P. Friz, co-organizer, *14th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis (Online Event)*, University of Oxford, Mathematical Institute, UK, February 10–12.
5. ———, co-organizer, *Higher Structures Emerging from Renormalisation*, Universität Wien, Erwin-Schrödinger-Institut für Mathematische Physik (ESI), Austria, November 8–19.
6. P. Friz, N. Tapia, co-organizers, *Cumulants in Stochastic Analysis (Online Event)*, Technische Universität Berlin, Institut für Mathematik, February 25–26.
7. K. Papafitsoros, co-organizer of the Minisymposium "Bilevel Optimization Approaches for Image and Data Analysis", *IFIP TC7 Conference on Modelling and Optimization (Online Conference)*, Quito, Ecuador, August 30 – September 3.
8. D. Peschka, M. Thomas, co-organizers of the Section S11 "Interfacial Flows", *91st Annual Meeting of the International Association of Applied Mathematics and Mechanics (Online Event)*, Universität Kassel, March 15–19.
9. L. Schmeller, co-organizer, *Workshop on Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates (SPP2171) (Online Event)*, Universität Münster, June 28 – July 1.
10. V. Spokoiny, co-organizer, *Conference Optimization without Borders*, Sirius University of Science and Technology, Sochi, Russian Federation, July 12–18.
11. ———, co-organizer, *Machine Learning and Nonparametric Statistics*, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, December 12–17.
12. K. Tabelow, Th. Koprucki, co-organizers of Minisymposium MS12 "Ready for MaRDI, am I a Digital Mathematician?", *DMV-ÖMG Annual Meeting 2021 (Online Event)*, Universität Passau, September 27 – October 1.
13. N. Tapia, co-organizer, *Young Researchers between Geometry and Stochastic Analysis 2021 (Online Event)*, University of Agder, Institute of Mathematics, Kristiansand, Norway, June 16–18.
14. ———, co-organizer, *Noncommutative Algebra, Probability and Analysis in Action (Hybrid Event)*, Universität Greifswald, Alfried Krupp Wissenschaftskolleg, September 20–25.
15. M. Thomas, co-organizer of the Minisymposium MSDI4 "Modeling and Analysis of Geological Fluid Flows", *CRC 1114 Conference 2021 (Online Event)*, Freie Universität Berlin, March 1–3.
16. A.G. Vladimirov, member of the Scientific and Organizing Committee, *Solvay Workshop on Dissipative Solitons and Optical Frequency Comb Generation*, International Solvay Institutes, Brussels, Belgium, September 15–16.
17. B. Wagner, principal investigator and co-organizer, *748th WE-Heraeus-Seminar on "Nanoscale Physics of Electrochemical and Biological Media" (Online Event)*, May 10–12.

A.6 Publications

A.6.1 Editorship of Proceedings and Collected Editions

[1] H. Abels, K. Disser, H.-Chr. Kaiser, A. Mielke, M. Thomas, eds., *Issue on Partial Differential Equations in Fluids and Solids*, vol. 14 of Discrete and Continuous Dynamical Systems – Series S, no. 11, American Institute of Mathematical Sciences, Springfield, 2021, 292 pages.

[2] M. Liero, S. Reichelt, G. Schneider, F. Theil, M. Thomas, eds., *Analysis of Evolutionary and Complex Systems: Issue on the Occasion of Alexander Mielke's 60th Birthday*, vol. 14 of Discrete and Continuous Dynamical Systems – Series S, no. 1, American Institute of Mathematical Sciences, Springfield, 2021, 453 pages.

[3] A. Mielke, M. Peletier, D. Slepcev, eds., *Variational Methods for Evolution*, vol. 17 of Oberwolfach Reports, no. 2/3, European Mathematical Society Publishing House, Zurich, 2021, 76 pages. DOI: 10.4171/OWR/2020/29.

[4] V.A. Garanzha, L. Kamenski, H. Si, eds., *Numerical Geometry, Grid Generation and Scientific Computing. Proceedings of the 10th International Conference, NUMGRID 2020 / Delaunay 130, Celebrating the 130th Anniversary of Boris Delaunay, Moscow, Russia, November 2020*, vol. 143 of Lecture Notes in Computational Science and Engineering, Springer Nature Switzerland AG, Cham, 2021, 417 pages. DOI: 10.1007/978-3-030-76798-3.

A.6.2 Outstanding Contributions to Monographs

[1] M. Hintermüller, T. Keil, *Chapter 3: Optimal Control of Geometric Partial Differential Equations, in: Geometric Partial Differential Equations: Part 2*, A. Bonito, R.H. Nochetto, eds., vol. 22 of Handbook of Numerical Analysis, Elsevier, 2021, pp. 213–270. DOI: 10.1016/bs.hna.2020.10.003.

[2] H. Si, *On decomposition of embedded prismatoids in R^3 without additional points*, V.A. Garanzha, L. Kamenski, H. Si, eds., vol. 143 of Lecture Notes in Computational Science and Engineering, Springer Nature Switzerland AG, Cham, 2021, pp. 95–112. DOI: 10.1007/978-3-030-76798-3.

[3] Z. Erkoç, A. Aman, U. Güdükbay, H. Si, *Out-of-core constrained Delaunay tetrahedralizations for large scenes*, V.A. Garanzha, L. Kamenski, H. Si, eds., vol. 143 of Lecture Notes in Computational Science and Engineering, Springer Nature Switzerland AG, Cham, 2021, pp. 113–124. DOI: 10.1007/978-3-030-76798-3.

[4] L. Starke, K. Tabelow, Th. Niendorf, A. Pohlmann, *Chapter 34: Denoising for Improved Parametric MRI of the Kidney: Protocol for Nonlocal Means Filtering, in: Preclinical MRI of the Kidney: Methods and Protocols*, A. Pohlmann, Th. Niendorf, eds., vol. 2216 of Methods in Molecular Biology, Springer Nature Switzerland AG, Cham, 2021, pp. 565–576. DOI: 10.1007/978-1-0716-0978-1_34.

Contributions to Monographs (to appear)

[1] A. Hinsen, B. Jahnel, *Agent-based modeling and simulation for malware spreading in D2D networks*, International Conference on Autonomous Agents and Multiagent Systems 2022, The University of Auckland, 2022.

A.6.3 Articles in Refereed Journals[3]

[1] P. Colli, G. Gilardi, J. Sprekels, *An asymptotic analysis for a generalized Cahn–Hilliard system with fractional operators*, J. Evol. Equ., 21 (2021), pp. 2749–2778. DOI: 10.1007/s00028-021-00706-1.

[2] ———, *Deep quench approximation and optimal control of general Cahn–Hilliard systems with fractional operators and double obstacle potentials*, Discrete Contin. Dyn. Syst. Ser. S, 14 (2021), pp. 243–271. DOI: 10.3934/dcdss.2020213.

[3] P. Colli, A. Signori, J. Sprekels, *Second-order analysis of an optimal control problem in a phase field tumor growth model with singular potentials and chemotaxis*, ESAIM Control Optim. Calc. Var., 27 (2021), pp. 73/1–73/46. DOI: 10.1051/cocv/2021072.

[4] J. Sprekels, F. Tröltzsch, *Sparse optimal control of a phase field system with singular potentials arising in the modeling of tumor growth*, ESAIM Control Optim. Calc. Var., 27 (2021), pp. S26/1–S26/27. DOI: 10.1051/cocv/2020088.

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[6] D. Abdel, P. Vágner, J. Fuhrmann, P. Farrell, *Modelling charge transport in perovskite solar cells: Potential-based and limiting ion depletion*, Electrochim. Acta, 390 (2021), pp. 138696/1–138696/12. DOI: 10.1016/j.electacta.2021.138696.

[7] A. Alphonse, C.N. Rautenberg, J.F. Rodrigues, *Analysis of a quasi-variational contact problem arising in thermoelasticity*, Nonlinear Anal., 217 (2022), pp. 112728/1–112728/40 (published online on 13.12.2021). DOI: 10.1016/j.na.2021.112728.

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[11] Ch. Bayer, F. Harang, P. Pigato, *Log-modulated rough stochastic volatility models*, SIAM J. Financial Math., 12 (2021), pp. 1257–1284. DOI: 10.1137/20M135902X.

[12] M. Redmann, Ch. Bayer, P. Goyal, *Low-dimensional approximations of high-dimensional asset price models*, SIAM J. Financial Math., 12 (2021), pp. 1–28. DOI: 10.1137/20M1325666.

[13] Ch. Bayer, D. Belomestny, P. Hager, P. Pigato, J.G.M. Schoenmakers, *Randomized optimal stopping algorithms and their convergence analysis*, SIAM J. Financial Math., 12 (2021), pp. 1201–1225. DOI: 10.1137/20M1373876.

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[15] M. Bongarti, I. Lasiecka, R. Triggiani, *The SMGT equation from the boundary: Regularity and stabilization*, Appl. Anal., published online on 30.11.2021. DOI: 10.1080/00036811.2021.1999420.

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[6] A. Grin, K.R. Schneider, *Global algebraic Poincaré–Bendixson annulus for van der Pol systems*, Preprint no. 2864, WIAS, Berlin, 2021.

[7] P. Krejčí, E. Rocca, J. Sprekels, *Analysis of a tumor model as a multicomponent deformable porous medium*, Preprint no. 2842, WIAS, Berlin, 2021.

[8] A. Agazzi, L. Andreis, R.I.A. Patterson, D.R.M. Renger, *Large deviations for Markov jump processes with uniformly diminishing rates*, Preprint no. 2816, WIAS, Berlin, 2021.

[9] Ch. Bayer, S. Breneis, *Markovian approximations of stochastic Volterra equations with the fractional kernel*, Preprint no. 2868, WIAS, Berlin, 2021.

[10] Ch. Bayer, M. Eigel, L. Sallandt, P. Trunschke, *Pricing high-dimensional Bermudan options with hierarchical tensor formats*, Preprint no. 2821, WIAS, Berlin, 2021.

[11] L. Heltai, A. Caiazzo, L.O. Müller, *Multiscale coupling of one-dimensional vascular models and elastic tissues*, Preprint no. 2830, WIAS, Berlin, 2021.

[12] D. Bothe, W. Dreyer, P.-É. Druet, *Multicomponent incompressible fluids – An asymptotic study*, Preprint no. 2825, WIAS, Berlin, 2021.

[13] P.-É. Druet, *Maximal mixed parabolic-hyperbolic regularity for the full equations of multicomponent fluid dynamics*, Preprint no. 2869, WIAS, Berlin, 2021.

[14] A. Sadiev, A. Beznosikov, P. Dvurechensky, A. Gasnikov, *Zeroth-order algorithms for smooth saddle-point problems*, Preprint no. 2827, WIAS, Berlin, 2021.

[15] A. Agafonov, D. Kamzolov, P. Dvurechensky, A. Gasnikov, *Inexact tensor methods and their application to stochastic convex optimization*, Preprint no. 2818, WIAS, Berlin, 2021.

[16] P. Ostroukhov, R. Kamalov, P. Dvurechensky, A. Gasnikov, *Tensor methods for strongly convex strongly concave saddle point problems and strongly monotone variational inequalities*, Preprint no. 2820, WIAS, Berlin, 2021.

[17] M. Ebeling-Rump, D. Hömberg, R. Lasarzik, *Two-scale topology optimization with heterogeneous mesostructures based on a local volume constraint*, Preprint no. 2908, WIAS, Berlin, 2021.

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

[18] M. Eigel, N. Farchmin, S. Heidenreich, P. Trunschke, *Adaptive non-intrusive reconstruction of solutions to high-dimensional parametric PDEs*, Preprint no. 2897, WIAS, Berlin, 2021.

[19] ———, *Efficient approximation of high-dimensional exponentials by tensor networks*, Preprint no. 2844, WIAS, Berlin, 2021.

[20] M. Eigel, R. Gruhlke, D. Moser, *Numerical upscaling of parametric microstructures in a possibilistic uncertainty framework with tensor trains*, Preprint no. 2907, WIAS, Berlin, 2021.

[21] M. Eigel, R. Schneider, D. Sommer, *Dynamical low-rank approximations of solutions to the Hamilton–Jacobi–Bellman equation*, Preprint no. 2896, WIAS, Berlin, 2021.

[22] Th. Eiter, *On the Oseen-type resolvent problem associated with time-periodic flow past a rotating body*, Preprint no. 2888, WIAS, Berlin, 2021.

[23] ———, *On the Stokes-type resolvent problem associated with time-periodic flow around a rotating obstacle*, Preprint no. 2876, WIAS, Berlin, 2021.

[24] Th. Eiter, K. Hopf, R. Lasarzik, *Weak-strong uniqueness and energy-variational solutions for a class of viscoelastoplastic fluid models*, Preprint no. 2904, WIAS, Berlin, 2021.

[25] Th. Eiter, K. Hopf, A. Mielke, *Leray–Hopf solutions to a viscoelastic fluid model with nonsmooth stress-strain relation*, Preprint no. 2829, WIAS, Berlin, 2021.

[26] A.H. Erhardt, S. Solem, *Analysis and simulation of a modified cardiac cell model gives accurate predictions of the dynamics of the original one*, Preprint no. 2848, WIAS, Berlin, 2021.

[27] G. Arumgam, A.K. Dond, A.H. Erhardt, *Global existence of solutions to Keller–Segel chemotaxis system with heterogeneous logistic source and nonlinear secretion*, Preprint no. 2847, WIAS, Berlin, 2021.

[28] P. Friz, P. Hager, N. Tapia, *Unified signature cumulants and generalized Magnus expansions*, Preprint no. 2814, WIAS, Berlin, 2021.

[29] B. Gaudeul, J. Fuhrmann, *Entropy and convergence analysis for two finite volume schemes for a Nernst–Planck–Poisson system with ion volume constraints*, Preprint no. 2811, WIAS, Berlin, 2021.

[30] F. Galarce Marín, D. Lombardi, O. Mula, *State estimation with model reduction and shape variability: Application to biomedical problems*, Preprint no. 2850, WIAS, Berlin, 2021.

[31] V. Matyukhin, S. Kabanikhin, M. Shishlenin, N. Novikov, A. Vasin, A. Gasnikov, *Convex optimization with inexact gradients in Hilbert space and applications to elliptic inverse problems*, Preprint no. 2815, WIAS, Berlin, 2021.

[32] A. Vasin, A. Gasnikov, V. Spokoiny, *Stopping rules for accelerated gradient methods with additive noise in gradient*, Preprint no. 2812, WIAS, Berlin, 2021.

[33] N. Yudin, A. Gasnikov, *Flexible modification of Gauss–Newton method and its stochastic extension*, Preprint no. 2813, WIAS, Berlin, 2021.

[34] C. Geiersbach, M. Hintermüller, *Optimality conditions and Moreau–Yosida regularization for almost sure state constraints*, Preprint no. 2862, WIAS, Berlin, 2021.

[35] A. Glitzky, M. Liero, G. Nika, *A coarse-grained electrothermal model for organic semiconductor devices*, Preprint no. 2822, WIAS, Berlin, 2021.

[36] Y. Hadjimichael, D.I. Ketcheson, L. Lóczi, *Positivity preservation of implicit discretizations of the advection equation*, Preprint no. 2846, WIAS, Berlin, 2021.

[37] B. Takács, Y. Hadjimichael, *High order discretization methods for spatial-dependent epidemic models*, Preprint no. 2805, WIAS, Berlin, 2021.

[38] M. Heida, *Precompact probability spaces in applied stochastic homogenization*, Preprint no. 2852, WIAS, Berlin, 2021.

[39] ———, *Stochastic homogenization on perforated domains I: Extension operators*, Preprint no. 2849, WIAS, Berlin, 2021.

[40] ———, *Stochastic homogenization on perforated domains II – Application to nonlinear elasticity models*, Preprint no. 2865, WIAS, Berlin, 2021.

[41] M. Heida, St. Neukamm, M. Varga, *Stochastic two-scale convergence and Young measures*, Preprint no. 2885, WIAS, Berlin, 2021.

[42] M. Heida, B. Jahnel, A.D. Vu, *Stochastic homogenization on irregularly perforated domains*, Preprint no. 2880, WIAS, Berlin, 2021.

[43] M. Heida, M. Landstorfer, M. Liero, *Homogenization of a porous intercalation electrode with phase separation*, Preprint no. 2905, WIAS, Berlin, 2021.

[44] M. Heida, M. Thomas, *GENERIC for dissipative solids with bulk-interface interaction*, Preprint no. 2872, WIAS, Berlin, 2021.

[45] H. Berthold, H. Heitsch, R. Henrion, J. Schwientek, *On the algorithmic solution of optimization problems subject to probabilistic/robust (probust) constraints*, Preprint no. 2835, WIAS, Berlin, 2021.

[46] H. Heitsch, R. Henrion, Th. Kleinert, M. Schmidt, *On convex lower-level black-box constraints in bilevel optimization with an application to gas market models with chance constraints*, Preprint no. 2828, WIAS, Berlin, 2021.

[47] M. Branda, R. Henrion, M. Pištěk, *Value at risk approach to producer's best response in electricity market with uncertain demand*, Preprint no. 2831, WIAS, Berlin, 2021.

[48] R. Henrion, A. Jourani, B.S. Mordukhovich, *Controlled polyhedral sweeping processes: Existence, stability, and optimality conditions*, Preprint no. 2892, WIAS, Berlin, 2021.

[49] C.F. Coletti, L.R. de Lima, A. Hinsen, B. Jahnel, D.R. Valesin, *Limiting shape for first-passage percolation models on random geometric graphs*, Preprint no. 2877, WIAS, Berlin, 2021.

[50] M. Gugat, J. Habermann, M. Hintermüller, O. Huber, *Constrained exact boundary controllability of a semilinear model for pipeline gas flow*, Preprint no. 2899, WIAS, Berlin, 2021.

[51] M. Hintermüller, A. Kröner, *Differentiability properties for boundary control of fluid-structure interactions of linear elasticity with Navier–Stokes equations with mixed-boundary conditions in a channel*, Preprint no. 2871, WIAS, Berlin, 2021.

[52] M. Hintermüller, St.-M. Stengl, *A generalized Γ-convergence concept for a type of equilibrium problems*, Preprint no. 2879, WIAS, Berlin, 2021.

[53] K. Hopf, *Singularities in L^1-supercritical Fokker–Planck equations: A qualitative analysis*, Preprint no. 2860, WIAS, Berlin, 2021.

[54] ———, *Weak-strong uniqueness for energy-reaction-diffusion systems*, Preprint no. 2808, WIAS, Berlin, 2021.

[55] K. Hopf, M. Burger, *On multi-species diffusion with size exclusion*, Preprint no. 2883, WIAS, Berlin, 2021.

[56] J. Fischer, K. Hopf, M. Kniely, A. Mielke, *Global existence analysis of energy-reaction-diffusion systems*, Preprint no. 2807, WIAS, Berlin, 2021.

[57] Ch. Hirsch, B. Jahnel, E. Cali, *Connection intervals in multi-scale dynamic networks*, Preprint no. 2895, WIAS, Berlin, 2021.

[58] B. Jahnel, Ch. Hirsch, E. Cali, *Percolation and connection times in multi-scale dynamic networks*, Preprint no. 2823, WIAS, Berlin, 2021.

[59] B. Jahnel, Ch. Külske, *Gibbsianness and non-Gibbsianness for Bernoulli lattice fields under removal of isolated sites*, Preprint no. 2878, WIAS, Berlin, 2021.

[60] V. John, B. Moreau, J. Novo, *Error analysis of a SUPG-stabilized POD-ROM method for convection-diffusion-reaction equations*, Preprint no. 2874, WIAS, Berlin, 2021.

[61] H. Wenzel, M. Kantner, M. Radziunas, U. Bandelow, *Semiconductor laser linewidth theory revisited*, Preprint no. 2838, WIAS, Berlin, 2021.

[62] L. Andreis, W. König, H. Langhammer, R.I.A. Patterson, *A large-deviations principle for all the components in a sparse inhomogeneous random graph*, Preprint no. 2898, WIAS, Berlin, 2021.

[63] A. Kröner, C.N. Rautenberg, S. Rodrigues, *Existence, uniqueness, and stabilization results for parabolic variational inequalities*, Preprint no. 2870, WIAS, Berlin, 2021.

[64] M. Landstorfer, M. Ohlberger, St. Rave, M. Tacke, *A modeling framework for efficient reduced order simulations of parametrized lithium-ion battery cells*, Preprint no. 2882, WIAS, Berlin, 2021.

[65] M. Landstorfer, R. Müller, *Thermodynamic models for a concentration and electric field dependent susceptibility in liquid electrolytes*, Preprint no. 2906, WIAS, Berlin, 2021.

[66] R. Lasarzik, *On the existence of weak solutions in the context of multidimensional incompressible fluid dynamics*, Preprint no. 2834, WIAS, Berlin, 2021.

[67] X. Liu, M. Thomas, E. Titi, *Well-posedness of Hibler's dynamical sea-ice model*, Preprint no. 2833, WIAS, Berlin, 2021.

[68] L. Mertensk̈otter, K. Busch, R. de J. León-Montiel, *Entangled two-photon absorption spectroscopy with varying pump wavelength*, Preprint no. 2837, WIAS, Berlin, 2021.

[69] A. Mielke, S. Reichelt, *Traveling fronts in a reaction-diffusion equation with a memory term*, Preprint no. 2836, WIAS, Berlin, 2021.

[70] A. Mielke, R. Rossi, *Balanced-Viscosity solutions to infinite-dimensional multi-rate systems*, Preprint no. 2902, WIAS, Berlin, 2021.

[71] G. Nika, *Derivation of effective models from heterogenous Cosserat media via periodic unfolding*, Preprint no. 2817, WIAS, Berlin, 2021.

[72] ———, *An existence result for a class of nonlinear magnetorheological composites*, Preprint no. 2804, WIAS, Berlin, 2021.

[73] F. Agnelli, G. Nika, A. Constantinescu, *Design of thin micro-architectured panels with extension-bending coupling effects using topology optimization*, Preprint no. 2873, WIAS, Berlin, 2021.

[74] T. Orenshtein, *Rough invariance principle for delayed regenerative processes*, Preprint no. 2809, WIAS, Berlin, 2021.

[75] A. Jha, O. Pártl, N. Ahmed, D. Kuzmin, *An assessment of solvers for algebraically stabilized discretizations of convection-diffusion-reaction equations*, Preprint no. 2889, WIAS, Berlin, 2021.

[76] Z. Mokhtari, R.I.A. Patterson, F. Höfling, *Spontaneous trail formation in populations of autochemotactic walkers*, Preprint no. 2900, WIAS, Berlin, 2021.

[77] R.I.A. Patterson, D.R.M. Renger, U. Sharma, *Variational structures beyond gradient flows: A macroscopic fluctuation-theory perspective*, Preprint no. 2826, WIAS, Berlin, 2021.

[78] M. Horák, M. Kružík, P. Pelech, A. Schlömerkemper, *Gradient polyconvexity and modeling of shape memory alloys*, Preprint no. 2851, WIAS, Berlin, 2021.

[79] P. Pelech, K. Tůma, M. Pavelka, M. Šípka, M. Sýkora, *On compatibility of the natural configuration framework with general equation for non-equilibrium reversible-irreversible coupling (GENERIC): Derivation of anisotropic rate-type models*, Preprint no. 2856, WIAS, Berlin, 2021.

[80] D. Peschka, L. Heltai, *Model hierarchies and higher-order discretisation of time-dependent thin-film free boundary problems with dynamic contact angle*, Preprint no. 2887, WIAS, Berlin, 2021.

[81] D. Peschka, A. Zafferi, L. Heltai, M. Thomas, *Variational approach to fluid-structure interaction via GENERIC*, Preprint no. 2903, WIAS, Berlin, 2021.

[82] S. Slepneva, A. Pimenov, *Nonlinear dynamical properties of frequency swept fiber-based semiconductor lasers*, Preprint no. 2839, WIAS, Berlin, 2021.

[83] A. Zeghuzi, J.-P. Koester, M. Radziunas, H. Christopher, H. Wenzel, A. Knigge, *Spatially modulated broad-area lasers for narrow lateral far-field divergence*, Preprint no. 2857, WIAS, Berlin, 2021.

[84] X. Yu, G. Hu, W. Lu, A. Rathsfeld, *PML and high-accuracy boundary integral equation solver for wave scattering by a locally defected periodic surface*, Preprint no. 2866, WIAS, Berlin, 2021.

[85] D.R.M. Renger, *Anisothermal chemical reactions: Onsager–Machlup and macroscopic fluctuation theory*, Preprint no. 2893, WIAS, Berlin, 2021.

[86] N. Nüsken, D.R.M. Renger, *Stein variational gradient descent: Many-particle and long-time asymptotics*, Preprint no. 2819, WIAS, Berlin, 2021.

[87] D.R.M. Renger, St. Schindler, *Gradient flows for bounded linear evolution equations*, Preprint no. 2881, WIAS, Berlin, 2021.

[88] R. Shiri, L. Schmeller, R. Seemann, D. Peschka, B. Wagner, *On the spinodal dewetting of thin liquid bilayers*, Preprint no. 2861, WIAS, Berlin, 2021.

[89] D. Belomestny, J.G.M. Schoenmakers, *From optimal martingales to randomized dual optimal stopping*, Preprint no. 2810, WIAS, Berlin, 2021.

[90] D. Belomestny, Ch. Bender, J.G.M. Schoenmakers, *Solving optimal stopping problems via randomization and empirical dual optimization*, Preprint no. 2884, WIAS, Berlin, 2021.

[91] A. Stephan, *Coarse-graining and reconstruction for Markov matrices*, Preprint no. 2891, WIAS, Berlin, 2021.

[92] A. Stephan, H. Stephan, *Positivity and polynomial decay of energies for square-field operators*, Preprint no. 2901, WIAS, Berlin, 2021.

[93] A. Neumann, N. Peitek, A. Brechmann, K. Tabelow, Th. Dickhaus, *Utilizing anatomical information for signal detection in functional magnetic resonance imaging*, Preprint no. 2806, WIAS, Berlin, 2021.

[94] A.G. Vladimirov, *Non-local and local temporal cavity soliton interaction in delay models of mode-locked lasers*, Preprint no. 2894, WIAS, Berlin, 2021.

[95] A.G. Vladimirov, S. Suchkov, G. Huyet, S.K. Turitsyn, *A delay differential equation NOLM–NALM mode-locked laser model*, Preprint no. 2858, WIAS, Berlin, 2021.

[96] A.G. Vladimirov, M. Tlidi, M. Taki, *Dissipative soliton interaction in Kerr resonators with high-order dispersion*, Preprint no. 2843, WIAS, Berlin, 2021.

[97] M. Nizette, A.G. Vladimirov, *A generalized Haus master equation model for mode-locked class-B lasers*, Preprint no. 2840, WIAS, Berlin, 2021.

[98] A.K. Barua, R. Chew, L. Shuwang, J. Lowengrub, A. Münch, B. Wagner, *Sharp-interface problem of the Ohta–Kawasaki model for symmetric diblock copolymers*, Preprint no. 2855, WIAS, Berlin, 2021.

[99] E. Meca, A.W. Fritsch, J. Iglesias-Artola, S. Reber, B. Wagner, *Predicting disordered regions driving phase separation of proteins under variable salt concentration*, Preprint no. 2875, WIAS, Berlin, 2021.

[100] A. Hajizadeh, A. Matysiak, M. Wolfrum, P.J.C. May, R. König, *Auditory cortex modelled as a dynamical network of oscillators: Understanding event-related fields and their adaptation*, Preprint no. 2854, WIAS, Berlin, 2021.

[101] M. Wolfrum, S. Yanchuk, O. D'Huys, *Multiple self-locking in the Kuramoto–Sakaguchi system with delay*, Preprint no. 2890, WIAS, Berlin, 2021.

[102] S. Yanchuk, M. Wolfrum, T. Pereira, D. Turaev, *Absolute stability and absolute hyperbolicity in systems with discrete time-delays*, Preprint no. 2824, WIAS, Berlin, 2021.

[103] I. Franović, O.E. Omel'chenko, M. Wolfrum, *Bumps, chimera states, and Turing patterns in systems of coupled active rotators*, Preprint no. 2886, WIAS, Berlin, 2021.

[104] V.V. Klinshov, S.Y. Kirillov, V.I. Nekorkin, M. Wolfrum, *Noise-induced dynamical regimes in a system of globally coupled excitable units*, Preprint no. 2853, WIAS, Berlin, 2021.

[105] A. Zafferi, D. Peschka, M. Thomas, *GENERIC framework for reactive fluid flows*, Preprint no. 2841, WIAS, Berlin, 2021.

[106] A. Zass, *Gibbs point processes on path space: Existence, cluster expansion and uniqueness*, Preprint no. 2859, WIAS, Berlin, 2021.

A.7.2 Preprints/Reports in other Institutions

[1] O. Butkovsky, K. Dareiotis, M. Gerencsér, *Optimal rate of convergence for approximations of SPDEs with non-regular drift*, arXiv:2110.06148, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[2] O. Butkovsky, V. Margarint, Y. Yuan, *Law of the SLE tip*, arXiv:2110.11247, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[3] M. Coghi, W. Dreyer, P. Gajewski, C. Guhlke, P. Friz, M. Maurelli, *A McKean–Vlasov SDE and particle system with interaction from reflecting boundaries*, Preprint no. 2102.12315v1, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[4] A. Rogozin, A. Beznosikov, D. Dvinskikh, D. Kovalev, P. Dvurechensky, A. Gasnikov, *Decentralized distributed optimization for saddle point problems*, arXiv:2102.07758, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[5] A. Agafonov, P. Dvurechensky, G. Scutari, A. Gasnikov, D. Kamzolov, A. Lukashevich, A. Daneshmand, *An accelerated second-order method for distributed stochastic optimization*, arXiv:2103.14392, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[6] A. Beznosikov, P. Dvurechensky, A. Koloskova, V. Samokhin, S.U. Stich, A. Gasnikov, *Decentralized local stochastic extra-gradient for variational inequalities*, arXiv:2106.08315, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[7] E. Gladin, A. Sadiev, A. Gasnikov, P. Dvurechensky, A. Beznosikov, M. Alkousa, *Solving smooth min-min and min-max problems by mixed oracle algorithms*, arXiv:2103.00434, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[8] E. Gorbunov, M. Danilova, I. Shibaev, P. Dvurechensky, A. Gasnikov, *Near-optimal high probability complexity bounds for non-smooth stochastic optimization with heavy-tailed noise*, arXiv:2106.05958, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[9] P. Dvurechensky, D. Kamzolov, A. Lukashevich, S. Lee, E. Ordentlich, C.A. Uribe, A. Gasnikov, *Hyperfast second-order local solvers for efficient statistically preconditioned distributed optimization*, arXiv:2102.08246, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[10] D. Pasechnyuk, P. Dvurechensky, S. Omelchenko, A. Gasnikov, *Stochastic optimization for dynamic pricing*, arXiv:2106.14090, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[11] A. Rogozin, M. Bochko, P. Dvurechensky, A. Gasnikov, V. Lukoshkin, *An accelerated method for decentralized distributed stochastic optimization over time-varying graphs*, arXiv:2103.15598, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[12] P. Dvurechensky, M. Staudigl, *Hessian barrier algorithms for non-convex conic optimization*, arXiv:2111.00100, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[13] P. Dvurechensky, M. Staudigl, S. Shtern, *First-order methods for convex optimization*, arXiv:2101.00935, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[14] A. Daneshmand, G. Scutari, P. Dvurechensky, A. Gasnikov, *Newton method over networks is fast up to the statistical precision*, arXiv:2102.06780, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[15] V. Tominin, Y. Tominin, E. Borodich, D. Kovalev, A. Gasnikov, P. Dvurechensky, *On accelerated methods for saddle-point problems with composite structure*, arXiv:2103.09344, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[16] M. O'Donovan, P. Farrell, T. Streckenbach, Th. Koprucki, St. Schulz, *Multiscale simulations of unipolar hole transport in (In,Ga)N quantum well systems*, arXiv:2111.01644, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[17] V. Novitskii, A. Gasnikov, *Improved exploiting higher order smoothness in derivative-free optimization and continuous bandit*, arXiv:2101.03821, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[18] V. Grimm, M. Hintermüller, O. Huber, L. Schewe, M. Schmidt, G. Zöttl, *A PDE-constrained generalized Nash equilibrium approach for modeling gas markets with transport*, Preprint no. 458, Dokumentserver des Sonderforschungsbereichs Transregio 154, https://opus4.kobv.de/opus4-trr154/home, 2021.

[19] N. Fountoulakis, T. Iyes, *Condensation phenomena in preferential attachment trees with neighbourhood influence*, arXiv:2101.027, Cornell University Library, arXiv.org, Ithaka, USA, 2021.

[20] V. John, P. Knobloch, *On algebraically stabilized schemes for convection-diffusion-reaction problems*, Preprint no. 2111.08697, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[21] A. Bianchi, F. Collet, E. Magnanini, *The GHS and other inequalities for the two-star model*, arXiv:2107.08889, Cornell University Library, arXiv.org, Ithaka, USA, 2021.

[22] ———, *Limit theorems for exponential random graphs*, arXiv:2105.06312, Cornell University Library, arXiv.org, Ithaka, USA, 2021.

[23] V. Pagliari, K. Papafitsoros, B. Ralță, A. Vikelis, *Bilevel training schemes in imaging for total-variation-type functionals with convex integrands*, arXiv:2112.10682, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[24] A. Kroshnin, V. Spokoiny, A. Suvorikova, *Multiplier bootstrap for Bures–Wasserstein barycenters*, arXiv:2111.12612, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[25] H. Abdulsamad, T. Dorau, B. Belousov, J.-J. Zhu, J. Peters, *Distributionally robust trajectory optimization under uncertain dynamics via relative-entropy trust regions*, arXiv:2103.15388, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[26] J.-J. Zhu, Ch. Kouridi, Y. Nemmour, B. Schölkopf, *Adversarially robust kernel smoothing*, arXiv:2102.08474, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[27] D. Agudelo-España, Y. Nemmour, B. Schölkopf, J.-J. Zhu, *Shallow representation is deep: Learning uncertainty-aware and worst-case random feature dynamics*, arXiv:2106.13066, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

[28] Y. Nemmour, B. Schölkopf, J.-J. Zhu, *Distributional robustness regularized scenario optimization with application to model predictive control*, arXiv:2110.13588, Cornell University Library, arXiv.org, Ithaca, USA, 2021.

A.8 Talks and Posters

A.8.1 Main and Plenary Talks

1. P. Dvurechensky, *Accelerated gradient methods and their applications to Wasserstein barycenter problem (online talk)*, The XIII International Scientific Conference and Young Scientist School "Theory and Numerics of Inverse and Ill-posed Problems" (Online Event), April 12–22, Mathematical Center in Akademgorodok, Novosibirsk, Russian Federation, April 14.
2. ———, *A short introduction to optimization (online talk)*, ITaS Interdisciplinary Conference 2021 (Online Event), November 15–17, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russian Federation, November 15.
3. P. Farrell, *Numerical methods for innovative semiconductor devices*, Conference "Asymptotic Behaviors of Systems of PDE arising in Physics and Biology: Theoretical and Numerical Points of View", November 16–19, Université de Lille, Laboratoire Paul Painlevé, France, November 17.
4. P. Friz, *Rough stochastic differential equations (online talk)*, Pathwise Stochastic Analysis and Applications (Online Event), March 8–12, Centre International de Rencontres Mathématiques, France, March 8.
5. ———, *Unified cumulants and Magnus expansions*, Noncommutative Algebra, Probability and Analysis in Action (Hybrid Event), September 20–25, Universität Greifswald, Alfried Krupp Wissenschaftskolleg, September 21.
6. R. Henrion, *Dealing with probust constraints in stochastic optimization*, Workshop "Applications of Semi-Infinite Optimization" (Online Event), May 20–21, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Kaiserslautern, May 21.
7. ———, *Contraintes en probabilité au-delà de la recherche opérationnelle (online talk)*, 13e Journée Normandie-Mathématique (Hybrid Event), Rouen, France, June 24.
8. M. Hintermüller, *Optimization with learning-informed differential equation constraints and its applications*, Online Conference "Industrial and Applied Mathematics", January 11–15, The Hong Kong University of Science and Technology, Institute for Advanced Study, January 13.
9. ———, *Mathematics of quantitative MRI (online talk)*, The 5th International Symposium on Image Computing and Digital Medicine (ISICDM 2021), December 17–20, Guilin, China, December 18.
10. D. Hömberg, *Industry 4.0 – Mathematical concepts and new challenges (online talk)*, International Conference on Direct Digital Manufacturing and Polymers (ICDDMAP 2021) (Online Event), May 20–22, Polytechnic of Leiria, Portugal, May 21.
11. A. Linke, *On the role of the Helmholtz–Leray projector for a novel pressure-robust discretization theory for the incompressible Navier–Stokes equations*, Ecole de Recherche CIMPA & Workshop, May 31 – June 7, Nador, Morocco, June 2.

A.8.2 Scientific Talks (Invited)

1. A. Alphonse, *Directional differentiability and optimal control for elliptic quasi-variational inequalities (online talk)*, Workshop "Challenges in Optimization with Complex PDE-Systems" (Hybrid Workshop), February 14–20, Mathematisches Forschungsinstitut Oberwolfach, February 17.
2. ———, *Some aspects of sensitivity analysis and optimal control for elliptic QVIs (online talk)*, Annual Meeting of the DFG SPP 1962 (Virtual Conference), March 24–25, WIAS Berlin, March 25.

3. L. Andreis, *Introduction to large deviations and random graphs (online minicourse)*, 4 talks, cycle of doctoral seminars (8-hour course) for the Ph.D. program of Turin University, Università degli Studi di Torino, Dipartimento di Matematica, Italy, January 14–25.
4. U. Bandelow, *Modeling and simulation of the dynamics in semiconductor lasers (online talk)*, 91st Annual Meeting of the International Association of Applied Mathematics and Mechanics, MS1: "Computational Photonics"' (Online Event), March 15–19, Universität Kassel, March 16.
5. ———, *Ultrashort solitons in the regime of event horizons in nonlinear dispersive optical media*, Solvay Workshop on Dissipative Solitons and Optical Frequency Comb Generation, September 15–16, International Solvay Institutes, Brussels, Belgium, September 16.
6. Ch. Bayer, *A pricing BSPDE for rough volatility (online talk)*, MATH4UQ Seminar (Online Event), Rheinisch-Westfälische Technische Hochschule Aachen, Mathematics for Uncertainty Quantification, April 6.
7. ———, *Log-modulated rough stochastic volatility models (online talk)*, SIAM Conference on Financial Mathematics and Engineering (FM21, Online Event), Minisymposium MS46: "UQ for Rough Volatility and Predictive Models in Finance", June 1–4, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, USA, June 4.
8. ———, *Pricing of American options using high-dimensional non-linear networks*, Next Generation Models of Financial Data, September 20–22, Technischen Universität München, Fakultät für Mathematik, Burghausen, September 21.
9. S. Breneis, *On variation functions and their moduli of continuity (online talk)*, Methods of Nonlinear Analysis in Differential and Integral Equations (Online Event), May 15–16, Rzeszów University of Technology, Department of Nonlinear Analysis, Poland, May 16.
10. ———, *Markovian approximations of stochastic Volterra equations with the fractional kernel*, 2021 Summer School of Berlin-Oxford IRTG Stochastic Analysis in Interaction (Hybrid Event), September 20–24, Technische Universität Berlin, Institut für Mathematik, September 24.
11. O. Butkovsky, *Skew fractional Brownian motion: Going beyond the Catellier–Gubinelli setting (online talk)*, 14th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis (Online Event), February 10–12, University of Oxford, Mathematical Institute, UK, February 11.
12. ———, *New coupling techniques for exponential ergodicity of SPDEs in the hypoelliptic and effectively elliptic settings (online talk)*, Applied and Computational Mathematics Research Seminar, Tulane University, School of Science and Engineering, New Orleans, USA, April 30.
13. ———, *Regularization by noise for SPDEs and SDEs: A stochastic sewing approach (online talk)*, Bernoulli-IMS 10th World Congress in Probability and Statistics (Online Event), July 19–23, Seoul National University, Korea (Republic of), July 22.
14. ———, *Skew fractional Brownian motion (online talk)*, LSA Autumn Meeting 2021 (Online Event), September 20–24, National Research University – Higher School of Economics (HSE), Laboratory of Stochastic Analysis and its Applications, Moscow, Russian Federation, September 22.
15. ———, *Regularization by noise via stochastic sewing with random controls*, German Probability and Statistics Days (GPSD) 2021, September 27 – October 1, DMV-Fachgruppe Stochastik e.V., Mannheim, September 27.
16. G. Dong, M. Hintermüller, K. Papafitsoros, *Learning-informed model meets integrated physics-based method in quantitative MRI (online talk)*, 91st Annual Meeting of the International Association of Applied Mathematics and Mechanics, S21: "Mathematical Signal and Image Processing" (Online Event), March 15–19, Universität Kassel, March 18.
17. P.-É. Druet, *The free energy of incompressible fluid mixtures: An asymptotic study (online talk)*, TES-Seminar on Energy-based Mathematical Methods and Thermodynamics, Thematic Einstein Semester on

Energy-based Mathematical Methods for Reactive Multiphase Flows, Technische Universität Berlin, WIAS Berlin, January 21.

18. P.-E. Druet, *Well-posedness results for mixed-type systems modelling pressure-driven multicomponent fluid flows (online talk)*, 8th European Congress of Mathematics (8ECM), Minisymposium ID 42 "Multicomponent Diffusion in Porous Media" (Online Event), June 20–26, Portorož, Slovenia, June 22.

19. ———, *Modeling and analysis for multicomponent incompressible fluids (online talk)*, 8th European Congress of Mathematics (8ECM), Minisymposium ID 51 "Partial Differential Equations describing Far-from-Equilibrium Open Systems" (Online Event), June 20–26, Portorož, Slovenia, June 23.

20. D. Dvinskikh, *Decentralized algorithms for Wasserstein barycenters (online talk)*, Moscow Conference on Combinatorics and Applications (Online Event), May 31 – June 4, Moscow Institute of Physics and Technology, School of Applied Mathematics and Computer Science, Moscow, Russian Federation, June 2.

21. ———, *A clever mean: Wasserstein barycenters*, Education Program: Modern Methods of Information Theory, Optimization and Management, July 19 – August 8, Sirius University of Science and Technology, Sochi, Russian Federation, July 19.

22. P. Dvurechensky, *Wasserstein barycenters from the computational perspective (online talk)*, Moscow Conference on Combinatorics and Applications (Online Event), May 31 – June 4, Moscow Institute of Physics and Technology, School of Applied Mathematics and Computer Science, Moscow, Russian Federation, June 2.

23. ———, *Decentralize and randomize: Faster algorithm for Wasserstein barycenters (online talk)*, EUROPT 2021, 18th International Workshop on Continuous Optimization (Online Event), July 7–9, Toulouse, France, July 7.

24. ———, *Primal-dual accelerated gradient methods with alternating minimization (online talk)*, Conference Optimization without Borders, July 12–18, Sirius University of Science and Technology, Sochi, Russian Federation, July 15.

25. ———, *Newton method over networks is fast up to the statistical precision (online talk)*, Thirty-eighth International Conference on Machine Learning (Online Event), July 18–24, Carnegie Mellon University, Pittsburgh, USA, July 20.

26. ———, *On a combination of alternating minimization and Nesterov's momentum (online talk)*, Thirty-eighth International Conference on Machine Learning (Online Event), July 18–24, Carnegie Mellon University, Pittsburgh, USA, July 20.

27. ———, *Distributed optimization algorithms for Wasserstein barycenters (online talk)*, 2021 INFORMS Annual Meeting, October 24–27, Institute for Operations Research and the Management Sciences (Hybrid Event), Anaheim, California, USA, October 24.

28. M. Ebeling-Rump, *Topology optimization subject to a local volume constraint (online talk)*, European Conference on Mathematics for Industry (ECMI2021), MS07: "Maths for the Digital Factory" (Online Event), April 13–15, Bergische Universität Wuppertal, April 15.

29. M. Eigel, *An adaptive tensor reconstruction for Bayesian inversion (online talk)*, School for Simulation and Data Science (SSD) Seminar, RWTH Aachen, IRTG Modern Inverse Problems, July 5.

30. A. Erhardt, *Modelling and analysis of cardiac dynamics (online talk)*, Applied Analysis Group Seminar (Online Event), Universität Bremen, June 1.

31. P. Farrell, *Modelling and simulation of the lateral photovoltage scanning method (online talk)*, European Conference on Mathematics for Industry (ECMI2021), MSOEE: "Mathematical Modeling of Charge Transport in Graphene and Low dimensional Structures" (Online Event), April 13–15, Bergische Universität Wuppertal, April 13.

32. P. Farrell, *Finite volume and meshfree strategies to solve PDEs numerically (online talk)*, Heriot-Watt University, Maxwell Institute for Mathematical Sciences, Edinburgh, Scotland, UK, June 2.

33. ———, *Numerical methods for innovative semiconductor devices*, SISSA – International School for Advanced Studies, Research Group "Mathematical Analysis, Modelling, and Applications", mathLab Seminar, Trieste, Italy, December 9.

34. P. Friz, *New perspectives on rough paths, signatures and signature cumulants (online talk)*, DataSig Seminar Series (Online Event), University of Oxford, Mathematical Institute, UK, May 6.

35. ———, *Rough stochastic differential equations*, Probability Seminar, Maxwell Institute for Mathematical Science, Edinburgh, UK, October 7.

36. ———, *On rough SDEs (online talk)*, International Seminar on SDEs and Related Topics (Online Event), hosted by University of Jyväskylä, Department of Mathematics and Statistics, October 29.

37. ———, *Liouville Brownian rough paths (online talk)*, Probability Seminar, Universität Wien, Fakultät für Mathematik, Austria, November 14.

38. ———, *Local volatility under rough volatility*, QuantMinds International 2021, December 6–9, Barcelona, Spain, December 7.

39. ———, *What can mathematics do for artificial intelligence? (online talk)*, Berlin Research 50 Workshop on Artificial Intelligence in Research (Online Event), December 13, Berlin Research 50, December 13.

40. C. Geiersbach, *Optimality conditions and regularization for convex stochastic optimization with almost sure state constraints (online talk)*, Workshop "Challenges in Optimization with Complex PDE-Systems" (Hybrid Workshop), February 14–20, Mathematisches Forschungsinstitut Oberwolfach, February 16.

41. ———, *Almost sure state constraints with an application to stochastic Nash equilibrium problems (online talk)*, SIAM Conference on Computational Science and Engineering – CSE21 (Virtual Conference), Minisymposium MS 114 "Risk-Averse PDE-Constrained Optimization", March 1–5, Virtual Conference Host: National Security Agency (NSA), March 2.

42. ———, *Optimality conditions and regularization for stochastic optimization with almost sure state constraints (online talk)*, Oberseminar Numerical Optimization (Online Event), Universität Konstanz, June 29.

43. ———, *Stochastic approximation for optimization in shape spaces (online talk)*, International Conference on Spectral and High Order Methods (ICOSAHOM), Session: "Shape and Topology Optimization" (Online Event), Technische Universität Wien / Universität Wien, Austria, July 13.

44. ———, *Stochastic approximation for optimization in shape spaces*, 15th International Conference on Free Boundary Problems: Theory and Applications 2021 (FBP 2021, Online Event), Minisymposium "UQ in Free Boundary Problems", September 13–17, WIAS, Berlin, September 14.

45. ———, *Optimal conditions & regularization for stochastic optimization with almost sure state constraints*, Vienna Colloquium on Decision Making under Uncertainty, October 1, Vienna, Austria, October 1.

46. ———, *Optimality conditions and regularization for stochastic optimization with almost sure state constraints*, Forschungsseminar Algorithmische Optimierung, Humboldt-Universität zu Berlin, November 18.

47. M. Heida, *Stochastic homogenization on randomly perforated domains (online talk)*, SIAM Conference on Mathematical Aspects of Materials Science (MS21, Online Event), Minisymposium "Stochastic Homogenization and Related Topics", May 17–28, Basque Center for Applied Mathematics, Bilbao, Spain, May 24.

48. ———, *Stochastic homogenization on random geometries (online talk)*, Applied Analysis Seminar, Universität Heidelberg, June 17.

49. H. Heitsch, *An algorithmic approach for solving optimization problems with probabilistic/robust (probust) constraints*, Workshop "Applications of Semi-Infinite Optimization" (Online Event), May 20–21, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Kaiserslautern, May 21.

50. R. Henrion, *Adaptive grid refinement for optimization problems with probabilistic/robust (probust) constraints*, PGMO DAYS 2021, Session 12E "Stochastic Optimization I", November 30 – December 1, Gaspard Monge Program for Optimization, Operations Research and their Interaction with Data Science, EDF Lab Paris-Saclay, Palaiseau, France, December 1.

51. M. Hintermüller, *Non smooth and complementarity-based distributed parameter systems: Simulation and hierarchical optimization (online talk)*, 91th Annual Meeting of the International Association of Applied Mathematics and Mechanics (Online Event), Session DFG-PP 1962 Non-smooth and Complementarity-based Distributed Parameter Systems, March 15–19, Universität Kassel, March 16.

52. ———, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, Seminar CMAI, George Mason University, Center for Mathematics and Artificial Intelligence, Fairfax, USA, March 19.

53. ———, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, One World Optimization Seminar, Universität Wien, Fakultät für Mathematik, Austria, May 10.

54. ———, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, INdAM Workshop 2021: "Analysis and Numerics of Design, Control and Inverse Problems" (Online Event), July 1–7, Istituto Nazionale di Alta Matematica, Rome, Italy, July 5.

55. ———, *Semi-smooth Newton methods: Theory, numerical algorithms and applications I (online talk)*, International Forum on Frontiers of Intelligent Medical Image Analysis and Computing 2021 (Online Forum), Xidian University, Southeastern University, and Hong Kong Baptist University, China, July 19.

56. ———, *Optimal control of quasi-variational inequalities (online talk)*, SIAM Conference on Optimization (OP21) (Online Event), Minisymposium MS93 "Nonsmooth Problems and Methods in Large-scale Optimization", July 20–23, July 23.

57. ———, *Semi-smooth Newton methods: Theory, numerical algorithms and applications II (online talk)*, International Forum on Frontiers of Intelligent Medical Image Analysis and Computing 2021 (Online Forum), Xidian University, Southeastern University, and Hong Kong Baptist University, China, July 26.

58. ———, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, Deep Learning and Inverse Problems (MDLW02), September 27 – October 1, Isaac Newton Institute for Mathematical Sciences (Hybrid Event), Oxford, UK, October 1.

59. ———, *Quantitative imaging: Physics integrated and machine learning based models in MRI (online talk)*, MATH-IMS Joint Applied Mathematics Colloquium Series, The Chinese University of Hong Kong, Center for Mathematical Artificial Intelligence, China, December 3.

60. ———, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, Oberseminar Numerical Optimization, Universität Konstanz, Fachbereich Mathematik und Statistik, December 14.

61. D. Hömberg, *Mathematics for steel production and manufacturing (online talk)*, Cardiff University, School of Mathematics, UK, March 2.

62. ———, *Modelling and simulation of high-frequency induction welding (online talk)*, European Conference on Mathematics for Industry (ECMI2021), MS08: "Modelling, Simulation and Optimization in Electrical Engineering" (Online Event), April 13–15, Bergische Universität Wuppertal, April 13.

63. T. Iyer, *Degrees of fixed vertices and power law degree distributions in preferential attachment trees with neighbourhood influence*, Probability Seminar, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Florence, Italy, November 17.

64. B. Jahnel, *Phase transitions for the Boolean model for Cox point processes (online talk)*, DYOGENE Seminar (Online Event), INRIA Paris, France, January 11.

65. ———, *Gibbsian representation for point processes via hyperedge potentials (online talk)*, Thematic Einstein Semester on Geometric and Topological Structure of Materials, Summer Semester 2021, Technische Universität Berlin, May 20.

66. ———, *Stochastic geometry for epidemiology (online talk)*, Monday Biostatistics Roundtable, Institute of Biometry and Clinical Epidemiology (Online Event), Campus Charité, June 14.

67. ———, *Connectivity improvements in mobile device-to-device networks (online talk)*, Telecom Orange Paris, France, July 6.

68. ———, *Phase transitions for the Boolean model for Cox point processes*, Workshop on Randomness Unleashed Geometry, Topology, and Data, September 22–24, University of Groningen, Faculty of Science and Engineering, Groningen, Netherlands, September 23.

69. ———, *Phase transitions for the Boolean model for Cox point processes (online talk)*, Probability Seminar Bath (Online Event), University of Bath, Department of Mathematical Sciences, UK, October 18.

70. ———, *First-passage percolation and chase-escape dynamics on random geometric graphs*, Stochastic Geometry Days, November 15–19, Dunkerque, France, November 17.

71. V. John, *On the convergence order of the finite element error in the kinetic energy for high Reynolds number incompressible flows (online talk)*, International Symposium on Recent Trends in Differential Equations: Theory, Computation & Application, Symposium on Recent Trends in Numerical Method for PDEs and Applications (Online Event), March 19–22, Indian Institute of Technology Kanpur, India, March 19.

72. ———, *Techniques for improving finite element solutions of steady-state convection-diffusion equations (online talk)*, BIRS-CMO Workshop "Bound-Preserving Space and Time Discretizations for Convection-Dominated Problems" (Online Event), August 22–27, Banff International Research Station for Mathematical Innovation and Discovery, Casa Matemática Oaxaca (CMO), Mexico, August 25.

73. ———, *Modeling and discretization techniques for partial differential equations*, 4 talks, Graduiertenkollegs 2433 DAEDALUS, Weierstrass Institute Berlin, November 23–25.

74. M. Kantner, *Mathematical modeling and optimal control of the COVID-19 pandemic (online talk)*, Mathematisches Kolloquium, Bergische Universität Wuppertal, April 27.

75. S. Katz, *Modeling and discretization techniques for partial differential equations*, 4 talks, Graduiertenkollegs 2433 DAEDALUS, Weierstrass Institute Berlin, November 23–25.

76. W. König, *A grid version of the interacting Bose gas (online talk)*, Probability Seminar (Online Event), University of Bath, Department of Mathematical Sciences, UK, February 15.

77. ———, *Cluster size distributions in a classical many-body system (online talk)*, Thematic Einstein Semester on Geometric and Topological Structure of Materials, Summer Semester 2021, Technische Universität Berlin, May 20.

78. ———, *A box version of the interacting Bose gas*, Workshop on Randomness Unleashed Geometry, Topology, and Data, September 22–24, University of Groningen, Faculty of Science and Engineering, Groningen, Netherlands, September 23.

79. ———, *A large-deviations principle for all the components in a sparse inhomogeneous Erdős–Rényi graph (online talk)*, UC San Diego Probability Seminar (Online Event), University of California, Department of Mathematics, San Diego, USA, October 14.

80. ———, *Das interagierende Bosegas im Lichte der Wahrscheinlichkeitstheorie*, Sommerfeld Seminar, Arnold–Sommerfeld–Gesellschaft e.V., Leipzig, October 21.

81. ———, *A box version of the interacting Bose gas*, Stochastic Geometry Days, November 15–19, Dunkerque, France, November 18.

82. A. Kröner, *Optimal control and deep learning*, Research Seminar: Mathematical Modelling and Simulation, Humboldt-Universität zu Berlin, July 15.

83. M. Landstorfer, *Modeling of concentration and electric field dependent susceptibilities in electrolytes (online talk)*, AA2 – Materials, Light, Devices, Freie Universität Berlin, Humboldt-Universität zu Berlin, WIAS Berlin, February 26.

84. ———, *Modeling electrochemical systems with continuum thermodynamics – From fundamental electrochemistry to porous intercalation electrodes (online talk)*, Stochastic & Multiscale Modeling and Computation Seminar (Online Event), Illinois Institute of Technology, Chicago, USA, October 28.

85. R. Lasarzik, *Energy-variational solutions for incompressible fluid dynamics*, Oberseminar Angewandte Analysis, Universität Ulm, Institut für Angewandte Analysis, October 25.

86. ———, *Energy-variational solutions for incompressible fluid dynamics*, Technische Universität Berlin, Institut für Mathematik, November 8.

87. J. Leake, *Lorentzian polynomials on cones and the Heron–Rota–Welsh conjecture*, Monday Colloquium of Graduiertenkolleg "Facets of Complexity" (GRK 2434), Technische Universität Berlin, November 22.

88. ———, *Continuous maximum entropy distributions (online talk)*, Optimization Under Symmetry, November 29 – December 3, University of California at Berkeley, Simons Institute for the Theory of Computing, USA, November 30.

89. ———, *Sampling matrices from HCIZ densities (online talk)*, Frontiers of Statistical Mechanics and Theoretical Computer Science 2021 (Hybrid Event), December 13–15, University of Illinois at Chicago, USA / Durham University, UK, December 14.

90. M. Liero, *Heat and carrier flow in organic semiconductor devices – Modeling, analysis, and simulation (online talk)*, AMaSiS 2021: Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems (Online Event), September 6–9, WIAS Berlin, September 6.

91. ———, *Mathematical research data in Applied Analysis (online talk)*, MaRDI Kickoff Workshop, November 2–4, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 2.

92. X. Liu, *Justification of the primitive equations (online talk)*, Global Scientist Interdisciplinary Online Forum 2021, Southern University of Science and Technology, Shenzhen, China, January 9.

93. E. Magnanini, *Limit theorems for the edge density in exponential random graphs*, Probability Seminar, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Italy, November 17.

94. O. Marquardt, *Modelling the electronic properties of semiconductor nanowire heterostructures (online talk)*, PDI-Seminar, Paul-Drude-Institut für Festkörperelektronik, August 23.

95. A. Mielke, *Gradient structures and EDP convergence for reaction and diffusion (online talk)*, Recent Advances in Gradient Flows, Kinetic Theory, and Reaction-Diffusion Equations (Online Event), July 13–16, Universität Wien, July 15.

96. ———, *On a rigorous derivation of a wave equation with fractional damping from a system with fluid-structure interaction (online talk)*, Tbilisi Analysis and PDE Seminar (Online Event), The University of Georgia, School of Science and Technology, December 20.

97. R. Müller, *Modeling of ion transport by a Maxwell–Stefan approach and numerical results (online talk)*, 8th European Congress of Mathematics (8ECM), Minisymposium "Multicomponent Diffusion in Porous Media", June 20–26, Portorož, Slovenia, June 22.

98. R. Müller, *Modeling of complex polycristalline electrodes and numerical study (online talk)*, DMV–ÖMG Annual Meeting 2021 (Online Event), Minisymposium 8: "PDE Models Describing Interfaces and Complex Structures", September 27 – October 1, Universität Passau, September 30.

99. T. Orenshtein, *Rough walks in random environment (online talk)*, Argentina–Brasil–Portugal Joint Probability Seminar (Online Event), Instituto Nacional de Matemática Pura e Aplicada (IMPA), Brazil, May 19.

100. ———, *A discussant for a talk by Jeremy QUASTEL (UBC) titled "The KPZ fixed point" (online talk)*, SPDEs & friends (Online Event), May 31 – June 2, Technische Universität Berlin, May 31.

101. ———, *Rough walks in random environment (online talk)*, Bernoulli-IMS 10th World Congress in Probability and Statistics (Online Event), July 19–23, Seoul National University, Korea (Republic of), July 22.

102. ———, *Rough walks in random environments (online talk)*, Chilean Probability Seminar (Online Event), Pontificia Universidad Católica de Chile, Facultad de Matemáticas, Santiago de Chile, Chile, December 1.

103. K. Papafitsoros, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, University of Graz, Institute of Mathematics and Scientific Computing, Austria, January 21.

104. ———, *Optimization with learning-informed differential equation constraints and its applications (online talk)*, Seminar Modern Methods in Applied Stochastics and Nonparametric Statistics, WIAS Berlin, March 16.

105. ———, *Automatic distributed regularization parameter selection in total generalized variation based image reconstruction via bilevel optimization (online talk)*, SIAM Conference on Optimization (Online Event), Minisymposium "Bilevel Optimization: Theory, Applications and Algorithms", July 20–23, July 21.

106. ———, *Total variation methods in image reconstruction*, Departmental Seminar, National Technical University of Athens, Department of Mathematics, Greece, December 21.

107. K. Papafitsoros, A. Kofler, *Classical vs. data driven regularization methods in imaging (online tutorial)*, MATH+ Thematic Einstein Semester on Mathematics of Imaging in Real-Word Challenges, Berlin, October 29.

108. R. Patterson, *Decomposing large deviations rate functions into reversible and irreversible parts (online talk)*, The British Mathematical Colloquium (BMC) and the British Applied Mathematics Colloquium (BAMC) : BMC-BAMC GLASGOW 2021, April 6–9, University of Glasgow (Online Event), UK, April 7.

109. P. Pelech, *Separately global solutions to rate-independent systems – Applications to large-strain deformations of damageable solids (online talk)*, SIAM Conference on Mathematical Aspects of Materials Science (MS21), Minisymposium 33 "Asymptotic Analysis of Variational Models in Solid Mechanics" (Online Event), May 17–28, Basque Center for Applied Mathematics, Bilbao, Spain, May 24.

110. D. Peschka, *Energy-based variational approach to moving interfaces and contact lines (online talk)*, SIAM Conference on Mathematical Aspects of Materials Science (MS21), Minisymposium 46 "Multi-phase Flow and Dynamics of Interfaces: Analysis and Numerics" (Online Event), May 17–28, Basque Center for Applied Mathematics, Bilbao, Spain, May 19.

111. ———, *Thin-film problems with dynamic contact angle (online talk)*, 8th European Congress of Mathematics (8ECM), Minisymposium ID 43 "Higher-order Evolution Equations" (Online Event), June 20–26, Portoroč, Slovenia, June 23.

112. M. Radziunas, *Modeling, simulation, and analysis of dynamics in semiconductor lasers (online talk)*, Research seminar of the Institute of Computer Science (Online Event), Vilnius University, Lithuania, September 29.

113. D. Sommer, *Robust nonlinear model predictive control using tensor networks (online talk)*, European Conference on Mathematics for Industry (ECMI2021), MS23: "Data-Driven Optimization" (Online Event), April 13–15, Bergische Universität Wuppertal, April 14.

114. V. Spokoiny, *Bayesian inference in Bernoulli model with application to ranking from pairwise comparison (online talk)*, Data Seminar, Université Grenoble Alpes, Laboratoire Jean Kuntzmann, France, January 21.

115. ———, *Random gradient free optimization: Bayesian view*, Conference Optimization without Borders, July 12–18, Sirius University of Science and Technology, Sochi, Russian Federation, July 12.

116. ———, *Adaptive manifold recovery*, Conference Optimization without Borders, July 12–18, Sirius University of Science and Technology, Sochi, Russian Federation, July 15.

117. ———, *Inference for nonlinear inverse problems (online talk)*, Bernoulli-IMS 10th World Congress in Probability and Statistics (Online Event), July 19–23, Seoul National University, Korea (Republic of), July 20.

118. ———, *Adaptive graph clustering*, Statistics, Artificial Intelligence, Machine Learning, Probability, Learning Theory Event – SAMPLE, October 26–30, National Research University Higher School of Economics, International Laboratory of Stochastic Algorithms and High-Dimensional Inference, Gelendzhik, Russian Federation, October 27.

119. A. Stephan, *Gradient systems and mulit-scale reaction networks (online talk)*, Limits and Control of Stochastic Reaction Networks (Online Event), July 26–30, American Institute of Mathematics, San Jose, USA, July 29.

120. A. Suvorikova, *Optimal transport in machine learning (onlne talk)*, Seminar of the International Laboratory of Stochastic Algorithms and High-dimensional Inference (HDI Lab), National Research University – Higher School of Economics (HSE), Faculty of Computer Science (Online Event), Moscow, Russian Federation, April 29.

121. ———, *Statistics for non-statisticians (online talk)*, ITaS Interdisciplinary Conference 2021 (Online Event), November 15–17, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russian Federation, November 16.

122. ———, *Survey of methods of k-means clustering with optimal transport (online talk)*, Third HSE-Yandex Autumn School on Generative Models (Hybrid Event), November 23–26, National Research University – Higher School of Economics (HSE), Yandex SDA Campus, Moscow, Russian Federation, November 26.

123. K. Tabelow, *MaRDI – The mathematical research data Initiative within the NFDI (online talk)*, SFB 1294 Colloquium (Online Event), Universität Potsdam, Institut für Mathematik, April 16.

124. N. Tapia, *Approximation of controlled rough paths (online talk)*, 14th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis (Online Event), February 10–12, University of Oxford, Mathematical Institute, UK, February 10.

125. ———, *Transport and continuity equations with (very) rough noise (online talk)*, Seminario de Probabilidad Hispanohablante (Online Event), Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Argentina, March 1.

126. ———, *Unified signature cumulants and generalized Magnus expansions*, Pathwise Stochastic Analysis and Applications (Online Event), March 8–12, Centre International de Rencontres Mathématiques, France, March 11.

127. ———, *Numerical schemes for rough partial differential equations (online talk)*, DNA Seminar (Online Event), Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, March 12.

128. ———, *Series iteradas para clasificación de series de tiempo (online talk)*, Seminario Chileno de Probabilidades (Online Event), Universidad de Chile, Centro de Modelamiento Matemático, Santiago de Chile, Chile, March 31.

129. ———, *Transport and continuity equations with (very) rough noise (online talk)*, Bernoulli-IMS 10th World Congress in Probability and Statistics (Online Event), July 19–23, Seoul National University, Korea (Republic of), July 20.

130. ———, *Iterated sums for time series classification*, Leibniz MMS Summer School "Mathematical Methods for Machine Learning", August 22–27, Schloss Dagstuhl, Leibniz-Zentrum für Informatik, Wadern, August 23.

131. ———, *Robustness of ResNets*, Forschungsseminar, Universität des Saarlandes, Fakultät für Mathematik und Informatik, Saarbrücken, October 29.

132. M. Thomas, *Convergence analysis for fully discretized damage and phase-field fracture models (online talk)*, 15th International Conference on Free Boundary Problems: Theory and Applications 2021 (FBP 2021, Online Event), Minisymposium "Phase Field Models", September 13–17, WIAS, Berlin, September 14.

133. W. van Zuijlen, *Large time behaviour of the parabolic Anderson model (online talk)*, Probability Meeting (Online Event), University of Oxford, Department of Statistics, UK, February 10.

134. ———, *Large time behaviour of the parabolic Anderson model (online talk)*, Probability and Statistical Physics Seminar (Online Event), The University of Chicago, Department of Mathematics, Statistics, and Computer Science, USA, February 12.

135. ———, *Quantitative heat kernel estimates for diffusions with distributional drift (online talk)*, 14th Oxford-Berlin Young Researchers Meeting on Applied Stochastic Analysis (Online Event), February 10–12, University of Oxford, Mathematical Institute, UK, February 12.

136. ———, *Total mass asymptotics of the parabolic Anderson model (online talk)*, SPASS – Probability, Stochastic Analysis and Statistics Seminar (Online Event), Pisa, Italy, June 8.

137. A.G. Vladimirov, *Short pulse solutions of time-delay laser models (online talk)*, Dynamics Days Europe 2021 (Online Event), Minisymposium MS34 "Time Delayed Systems: Theory and Experiments", August 23–27, Université Côte d'Azur, Nice, France, August 27.

138. B. Wagner, R. Seemann, *Liquid dewetting from liquid and soft substrates (online talk)*, SPP2171 Kolloquium, May 27.

139. M. Wolfrum, *Temporal dissipative solitons in systems of delay-differential equations (online talk)*, SIAM Conference on Applications of Dynamical Systems (Online Event), Minisymposium 184 "Traveling Pulses in Delay and Lattice Differential Equations", May 23–27, Portland, Oregon, USA, May 27.

140. ———, *Stability properties of temporal dissipative solitons in DDE systems (online talk)*, Dynamics Days Europe 2021 (Online Event), Minisymposium MS34: "Time Delayed Systems: Theory and Experiment", August 23–27, Université Côte d'Azur, Nice, France, August 27.

141. ———, *Bumps, chimera states, and Turing patterns in systems of coupled active rotators*, Control of Self-Organizing Nonlinear Systems, August 29 – September 2, Potsdam, September 2.

142. ———, *Mode-locking and coherence echoes in systems of globally coupled phase oscillators (online talk)*, Nonlinear Dynamics of Oscillatory Systems (Online Event), September 19–22, Nizhny Novgorod, Russian Federation, September 21.

143. A. Zafferi, *Coupling of thermoviscoelastic solids and reactive flows via GENERIC (online talk)*, CRC 1114 Conference 2021 (Online Event), MSDI4: "Modeling and Analysis of Geological Fluid Flows", March 1–3, Freie Universität Berlin, March 2.

144. A. Zass, *A marked Gibbs point process on path space: Existence and uniqueness*, Oberseminar Stochastik, Universität zu Köln, Department Mathematik/Informatik, Abteilung Mathematik, November 4.

145. ———, *Gibbs point processes on path space: Existence, cluster expansion and uniqueness*, AG Stochastische Geometrie, Karlsruher Institut für Technologie, Fakultät für Mathematik, December 10.

146. J.-J. Zhu, *Robust optimization and learning under distribution shift*, 4 talks, Leibniz MMS Summer School "Mathematical Methods for Machine Learning", August 22–27, Schloss Dagstuhl, Leibniz-Zentrum für Informatik, Wadern, August 26–27.

A.8.3 Talks for a More General Public

1. P. Friz, *Mathematik: Wie wahrscheinlich ist es? Von Risiko, zufälliger Mathematik und absolutem Chaos*, Aktionstag "Einstein macht Schule", Technische Universität Berlin, June 18.

2. C. Geiersbach, *Energie (MATH+)*, MitWissenschaft, Humboldt Forum, Berlin, October 28.
3. W. König, *Murphys Gesetz, tippende Affen und Unendlichkeit in der Wahrscheinlichkeitsrechnung*, 2 talks, Tag der Wissenschaften 2021, Weinberg-Gymnasium Kleinmachnow, November 12.
4. M. Liero, *Lügen mit Statistik? Jein! (online talk)*, Aktionstag "Einstein macht Schule" (Online Event), Technische Universität Berlin, June 18.

A.8.4 Posters

1. D. Abdel, P. Vágner, J. Fuhrmann, P. Farrell, *Modelling charge transport in perovskite solar cells: Potential-based and limiting ion depletion*, SIAM Conference on Computational Science and Engineering – CSE21 (Online Event), Texas, USA, March 1–5.
2. ———, *Modeling and simulation of charge transport in perovskite solar cells*, AMaSiS 2021: Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems (Online Event), September 6–9.
3. ———, *Modeling and simulation of charge transport in perovskite solar cells*, Conference "Asymptotic Behaviors of Systems of PDEs arising in Physics and Biology: Theoretical and Numerical Points of View", Lille, Laboratoire Paul Painlevé, France, November 16–19.
4. A. Caiazzo, F. Galarce Marín, J. Polzehl, I. Sack, K. Tabelow, *Physics based assimilation of displacements data from magnetic resonance elastography*, Kick-off Workshop of the MATH+ Thematic Einstein Semester on Mathematics of Imaging in Real-World Challenges (Hybrid Event), Berlin, October 6–8.
5. D. Dvinskikh, D. Tiapkin, *Improved complexity bounds in Wasserstein barycenter problem (online presentation)*, The 24th International Conference on Artificial Intelligence and Statistics (Online Event), April 13–15.
6. M. Eigel, *A neural multilevel method for high-dimensional parametric PDEs*, Thirty-fifth Conference on Neural Information Processing Systems (NeurIPS 2021) (Online Event), December 6–14.
7. A.H. Erhardt, S. Checa, A. Petersen, B. Wagner, *AA1-12: Mathematical modelling of cellular self-organization on stimuli responsive extracellular matrix (online poster)*, MATH+ Day 2021 (Online Event), Technische Universität Berlin, November 5.
8. P. Farrell, St. Kayser, N. Rotundo, *Modeling and simulation of the lateral photovoltage scanning method*, SIAM Conference on Computational Science and Engineering – CSE21 (Online Event), Texas, USA, March 1–5.
9. P. Farrell, Y. Hadjimichael, Ch. Merdon, T. Streckenbach, *Toward charge transport in bent nanowires*, AMaSiS 2021: Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems (Online Event), September 6–9.
10. M.H. Farshbaf Shaker, D. Peschka, M. Thomas, B. Wagner, *Variational methods for viscoelastic flows and gelation*, MATH+ Day 2021 (Online Event), Technische Universität Berlin, November 5.
11. B. Gaudeul, J. Fuhrmann, *Two entropic finite volume schemes for a Nernst–Planck–Poisson system with ion volume constraints*, AMaSiS 2021: Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems (Online Event), September 6–9.
12. A. Gerdes, *Synchronization patterns in globally coupled Stuart–Landau oscillators*, Control of Self-Organizing Nonlinear Systems, Potsdam, August 29 – September 2.
13. S. Katz, *C^1 finite elements with interpolated boundary conditions and applications to the Willmore flow of graphs*, DAEDALUS Research Training Group "Interdisciplinary Welcome Week", October 20.
14. M. Landstorfer, M. Eigel, M. Heida, A. Selahi, *Recovery of battery ageing dynamics with multiple timescales (online poster)*, MATH+ Day 2021 (Online Event), Technische Universität Berlin, November 5.

15. X. Liu, *Second law of thermodynamics and bounded entropy solutions in the compressible Navier–Stokes system*, Summer School 2021 "Wave Phenomena: Analysis and Numerics" (Hybrid Event), September 27–30.

16. A. Maltsi, *Quantum dots and TEM images from a mathematician's perspective*, Women in Mathematics Webinar (Online Event), UK, February 11–12.

17. ———, *Model-based geometry reconstruction of TEM images*, MATH+ Day 2021 (Online Event), Technische Universität Berlin, November 5.

18. L. Mertenskötter, M. Kantner, H. Wenzel, U. Bandelow, *Modeling and optimization of semiconductor lasers for quantum metrology applications*, MATH+ Day 2021 (Online Event), Technische Universität Berlin, November 5.

19. A. Mielke, A. Stephan, *Effective models for materials and interfaces with multiple scales*, CRC 1114 Conference 2021 (Online Event), March 1–3.

20. G. Nika, *Derivation of an effective bulk-surface thermistor model for OLEDs*, AMaSiS 2021: Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems (Online Event), September 6–9.

21. D. Peschka, *Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows*, Conference "Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates" of the SPP 2171, Freiburg, November 8–10.

22. L. Plato, R. Lasarzik, D. Hömberg, E. Emmrich, *Nonlinear electrokinetics in anisotropic microfluids — Analysis, simulation, and optimal control*, MATH+ Day 2021 (Online Event), Technische Universität Berlin, November 5.

23. L. Schmeller, B. Wagner, *Dynamic wetting and dewetting of viscous liquid droplets films on viscoelastic substrates*, Conference "Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates" of the SPP 2171, Freiburg, November 8–10.

24. A. Selahi, M. Landstorfer, *The double layer capacity of non-ideal electrolyte solutions – A numerical study (online poster)*, 240th ECS meeting (Online Event), October 10–14.

25. M. Stöhr, *Bifurcations and instabilities of temporal dissipative solitons in DDE systems with large delay*, Control of Self-Organizing Nonlinear Systems, Potsdam, August 29 – September 2.

26. A. Zafferi, *Dynamics of rock dehydration on multiple scales*, CRC 1114 Conference 2021 (Online Event), March 1–3.

A.9 Visits to other Institutions[5]

1. D. Abdel, Université de Lille, Laboratoire Paul Painlevé, France, October 18 – November 19.
2. O. Butkovsky, Technische Universität Wien, Fakultät für Mathematik und Geoinformation, Austria, November 13–20.
3. P. Farrell, Université de Lille, Laboratoire Paul Painlevé, France, October 18 – November 19.
4. ———, SISSA – International School for Advanced Studies, Trieste, Italy, December 6–17.
5. D. Hömberg, Adjunct Professorship, Norwegian University of Science and Technology, Department of Mathematical Sciences, Trondheim, Norway, November 1–12.
6. T. Iyer, University of Birmingham, School of Mathematics, Birmingham, UK, September 3–13.
7. ———, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Italy, November 12–28.
8. V. John, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, August 30 – September 3.
9. W. König, Universität zu Köln, Department Mathematik/Informatik, Abteilung Mathematik, November 1–5.
10. Z. Lakdawala, Technische Universität Kaiserslautern, Department of Computer Science, October 4–15.
11. X. Liu, Université Savoie Mont Blanc, Laboratoire de Mathématiques, Chambéry, France, November 30 – December 10.
12. E. Magnanini, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Italy, November 12–28.
13. T. Orenshtein, Technion — Israel Institute of Technology, Faculty of Industrial Engineering and Management, Haifa, Israel, November 5–19.
14. A. Quitmann, Università di Roma la Sapienza, Dipartimento di Matematica, Italy, June 20 – July 10.
15. ———, Università di Roma la Sapienza, Dipartimento di Matematica (DAAD Fellowship), Italy, November 6 – December 11.
16. M. Radziunas, Vilnius University, Institute of Computer Science, Lithuania, September 8–11.
17. V. Spokoiny, Higher School of Economics, International Laboratory of Stochastic Algorithms and High-Dimensional Inference, Moscow, Russian Federation, July 6–10.
18. ———, July 23–27.
19. A. Suvorikova, Higher School of Economics, Faculty of Computer Science, Moscow, Russian Federation, June 15 – September 15.
20. P. Vágner, University of Chemistry and Technology, Department of Petroleum Technology and Alternative Fuels, Prague, Czech Republic, August 2–13.
21. W. van Zuijlen, Radboud University Nijmegen, Department of Mathematics, Nijmegen, Netherlands, June 30 – July 5.
22. ———, August 25–31.
23. ———, October 20–25.
24. A. Zass, Universität zu Köln, Department Mathematik/Informatik, Abteilung Mathematik, November 1–5.

[5] Only stays of more than three days are listed.

A.10 Academic Teaching[6]

Winter Semester 2020/2021

1. U. Bandelow, *Online: Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. P.-É. Druet, *Online: Nonlinear Partial Differential Equations* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
3. ———, *Online: Nonlinear Partial Differential Equations* (practice), Humboldt-Universität zu Berlin, 2 SWS.
4. P. Dvurechensky, *Online: Theory of Optimization Algorithms for Large-scale Problems Motivated by Machine Learning Applications* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
5. ———, *Online: Theory of Optimization Algorithms for Large-scale Problems Motivated by Machine Learning Applications* (practice), Humboldt-Universität zu Berlin, 1 SWS.
6. M.H. Farshbaf Shaker, *Online: Mathematik für Ingenieure C1* (lecture), Friedrich-Alexander-Universität Erlangen-Nürnberg, 4 SWS.
7. ———, *Online: Übungen zur Mathematik für Ingenieure C1* (practice), Friedrich-Alexander-Universität Erlangen-Nürnberg, 4 SWS.
8. P. Friz, *Online: Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
9. J. Fuhrmann, *Online: Wissenschaftliches Rechnen (Scientific Computing)* (lecture), Technische Universität Berlin, 4 SWS.
10. A. Glitzky, A. Mielke, B. Zwicknagl, *Online: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
11. D. Hömberg, *Online: Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
12. V. John, *Online: Numerical Mathematics 2* (lecture), Freie Universität Berlin, 4 SWS.
13. O. Klein, *Online: Spezielle Themen der Mathematik (M39): Einführung in die Quantifizierung von Unsicherheiten, Uncertainty Quantification* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
14. ———, *Online: Spezielle Themen der Mathematik (M39): Einführung in die Quantifizierung von Unsicherheiten, Uncertainty Quantification* (practice), Humboldt-Universität zu Berlin, 1 SWS.
15. W. König, *Online: Probability Theory II* (lecture), Technische Universität Berlin, 4 SWS.
16. M. Landstorfer, *Online: Numerische Mathematik II für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
17. A. Linke, *Online: Mathematik für Geowissenschaftler I* (lecture), Freie Universität Berlin, 2 SWS.
18. V. Spokoiny, *Online: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
19. V. Spokoiny, W. Härdle, M. Reiss, S. Greven, *Online: Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/Universität Potsdam/WIAS Berlin, 2 SWS.
20. V. Spokoiny, P. Dvurechensky, M. Hintermüller, *Online: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
21. K. Tabelow, *Online: Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.

[6] SWS = semester periods per week

22. M. Wolfrum, B. Fiedler, I. Schneider, E. Schöll, *Online: Nonlinear Dynamics* (senior seminar), Freie Universität Berlin/WIAS Berlin/Technische Universität Berlin, 2 SWS.

Summer Semester 2021

1. U. Bandelow, *Online: Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
2. U. Bandelow, S. Amiranashvili, *Online: Nichtlineare Dynamik in der Photonik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
3. Ch. Bayer, *Online: Computational Finance* (lecture), Technische Universität Berlin, 2 SWS.
4. P. Friz, *Online: Wahrscheinlichkeitstheorie III* (lecture), Technische Universität Berlin, 2 SWS.
5. ———, *Online: Oberseminar Rough Paths, Stochastic Partial Differential Equations and Related Topics* (senior seminar), Technische Universität Berlin, 2 SWS.
6. A. Glitzky, A. Mielke, B. Zwicknagl, *Online: Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
7. M. Hintermüller, *Online: Ausgewählte Themen der Optimierung (M23): Mathematische Bildbearbeitung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
8. ———, *Online: Joint Research Seminar on Nonsmooth Variational Problems and Operator Equations / Mathematical Optimization* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
9. D. Hömberg, *Online: Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
10. V. John, *Online: Numerik III* (lecture), Freie Universität Berlin, 4 SWS.
11. R. Lasarzik, *Online: Differentialgleichungen III* (lecture), Technische Universität Berlin, 4 SWS.
12. A. Linke, *Online: Mathematik für Geowissenschaftler II* (lecture), Freie Universität Berlin, 2 SWS.
13. A. Mielke, M. Liero, *Online: Partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
14. V. Spokoiny, *Online: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
15. V. Spokoiny, W. Härdle, M. Reiss, S. Greven, *Online: Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin/Universität Potsdam/WIAS Berlin, 2 SWS.
16. V. Spokoiny, P. Dvurechensky, M. Hintermüller, *Online: Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), WIAS Berlin, 2 SWS.
17. K. Tabelow, *Online: Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
18. W. van Zuijlen, *Online: Integraltransformationen und partielle Differentialgleichungen für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
19. 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 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 (29)* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
15. ———, *Nonparametric Statistics (29)* (practice), Humboldt-Universität zu Berlin, 2 SWS.
16. V. Spokoiny, M. Reiss, S. Greven, W. Härdle, A. Carpentier, *Hybrid: Mathematical Statistics (M28)* (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, *Online: Mathematik* (seminar), Steinbeis-Hochschule Berlin, 2 SWS.
19. W. van Zuijlen, *Hybrid: Theory of Function Spaces and Applications* (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.

A.11 Visiting Scientists[7]

A.11.1 Guests

1. L. Andreis, Università degli Studi di Firenze, Dipartimento di Matematica e Informatica "Ulisse Dini", Firenze, Italy, June 21–30.
2. ———, July 19–28.
3. ———, September 26 – October 8.
4. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, November 2–6.
5. M. Brokate, Technische Universität München, Zentrum Mathematik, Garching, January 1 – December 31.
6. Ch. Giraudo, Università degli Studi di Trento, Dipartimento di Matematica, Italy, September 1 – November 30.
7. E. Gladin, Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin Mathematical School (BMS), September 20, 2021 – September 19, 2022.
8. O. Huber, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – December 31.
9. R. Kravchenko, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1 – December 31.
10. M. Meinlschmidt, Friedrich-Alexander Universität Erlangen-Nürnberg, Department of Data Science (DDS), Erlangen, October 4–7.
11. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, November 8 – December 8.
12. L. Scaglione, École Polytechnique, Centre de Mathématiques Appliquées, Palaiseau, France, April 19 – July 16.
13. E. Stepanov, Russian Academy of Sciences, Steklov Institute, St. Petersburg, Russian Federation, October 4–8.
14. ———, November 1–4.
15. L. Taggi, Sapienza Università di Roma, Dipartimento di Matematica, Italy, August 2–5.
16. ———, October 21–25.
17. ———, December 17–21.
18. D. Ueltschi, University of Warwick, Department of Mathematics, Coventry, UK, December 16–22.
19. K. Wiśniewski, Warsaw University of Technology, Faculty of Physics, Warsaw, Poland, September 1–30.

A.11.2 Scholarship Holders

1. Ch. Kwofie, University of Energy and Natural Resources, Sunyani, Ghana, DAAD Fellowship, February 1, 2018 – June 30, 2021.
2. Ch. Kwofie, University of Energy and Natural Resources, Sunyani, Ghana, DAAD Fellowship, October 1 – December 31.

[7] Only stays of more than three days are listed.

A.11.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. E. Gladin, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. V. Spokoiny, Berlin Mathematical School, doctoral candidate, September 20 – December 31.
2. P. Hager, Technische Universität Berlin, Institut für Mathematik, supervisors: Prof. Dr. P. Friz, Dr. Ch. Bayer, MATH+, doctoral candidate, January 1 – September 15.
3. R. Kravchenko, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. V. Spokoiny, MATH+, doctoral candidate, January 1 – December 31.
4. Ch. Kwofie, The African Institute for Mathematical Sciences (AIMS), supervisor: Prof. Dr. W. König, DAAD, doctoral candidate, July 1 – December 31.
5. Th. Lucke, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. W. König, doctoral candidate, January 1 – December 31.
6. Y. Sun, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, Berlin Mathematical School, doctoral candidate, January 1 – December 31.

A.12 Guest Talks

1. E. Bänsch, Friedrich-Alexander Universität Erlangen-Nürnberg, Department Mathematik, *The Buongiorno model for nanofluids (online talk)*, February 4.
2. C. Bartsch, genua GmbH, *Career opportunities for WIAS alumni in IT security? A personal case study (online talk)*, November 8.
3. M. Brokate, Technische Universität München, Zentrum Mathematik, Garching, *A variational inequality for the derivative of the play operator (online talk)*, June 23.
4. S. Budday, Friedrich-Alexander Universität Erlangen-Nürnberg, Department Maschinenbau (MB), *Brain mechanics across scales (online talk)*, November 23.
5. C. Conradi, Hochschule für Technik und Wirtschaft, Bioprozessführung und -simulation, Berlin, *Monomial parameterizations in the analysis of biochemical reaction networks (online talk)*, July 6.
6. A. Dickenstein, Universidad de Buenos Aires, Department of Mathematics, Argentina, *Algebra and geometry in the study of enzymatic networks? (online talk)*, May 11.
7. M. Efendiyev, Helmholtz Zentrum, Institute of Computational Biology, München, *Mathematical modeling of biofilms and their long-time dynamics (online talk)*, July 13.
8. A. Eikmeier, Technische Universität Berlin, Institut für Mathematik, *Existence of weak solutions to a general multivalued differential equation (online talk)*, December 7.
9. M. Engel, Freie Universität Berlin, Department of Mathematics and Computer Science, *Lyapunov exponents in random dynamical systems and how to find and use them (online talk)*, May 4.
10. P.E. Farrell, University of Oxford, Mathematical Institute, UK, *Computing disconnected bifurcation diagrams of partial differential equations (online talk)*, July 5.
11. J. Fischer, Institute of Science and Technology Austria (IST Austria), Fischer Group – Theorie der partiellen Differentialgleichungen, Angewandte und Numerische Analysis, Klosterneuburg, *Uniqueness and stability properties of multiphase mean curvature flow: An approach based on the variational (gradient flow) structure of the problem (online talk)*, June 9.
12. F. Galarce, Centre de Recherche INRIA de Paris & Laboratoire Jacques-Louis Lions, Faculté des Sciences de Sorbonne Université, France, *Inverse problems in haemodynamics – Fast estimation of blood flows from medical data (online talk)*, January 21.
13. G.P. Galdi, University of Pittsburgh, Mechanical Engineering & Materials Science, USA, *On the self-propelled motion of a rigid body in a viscous liquid by time-periodic boundary data (online talk)*, February 17.
14. B. Gaudeul, Université de Lille, Laboratoire Paul Painlevé, France, *Two entropic finite volume schemes for a Nernst–Planck–Poisson system with ion volume constraints (online talk)*, March 25.
15. S. Giere, felmo GmbH, *A conversation about transition from science to data science*, November 22.
16. I. Gijbels, Catholic University of Leuven, Statistics and Risk, Netherlands, *Extremiles and extremile regression (online talk)*, June 16.
17. Ch. Giraud, Université Paris-Saclay, Institut de Mathématiques d'Orsay, France, *A geometric approach to fair online learning (hybrid talk)*, November 17.
18. E. Gladin, Moscow Institute of Physics and Technology, Department of Control and Applied Mathematics, Russian Federation, *Solving convex min-min problems with smoothness and strong convexity in one variable group and small dimension of the other (online talk)*, February 2.

19. S. Gratton, École Nationale Supérieure d'Électrotechnique, d'Électronique, d'Informatique, d'Hydraulique et des Télécommunications (ENSEEIHT), Toulouse, France, *On a multilevel Levenberg–Marquardt method for the training of artificial neural networks and its application to the solution of partial differential equations (online talk)*, March 29.
20. P. Hagemann, Technische Universität Berlin, Institut für Mathematik, *Stochastic normalizing flows and inverse problems (online talk)*, November 30.
21. P. Hager, Technische Universität Berlin, Institut für Mathematik, *Optimal stopping with signatures (online talk)*, May 11.
22. J. Hauffen, Technische Universität Berlin, Institut für Mathematik, *Deep unfolding: Learned block regularization with application in photothermal superresolution (online talk)*, October 19.
23. L. Henze, Humboldt-Universität zu Berlin, Institut für Mathematik, *Classification of quantum dot images using machine learning (online talk)*, June 15.
24. D. Heydecker, University of Cambridge, Faculty of Mathematics, UK, *Large deviations of Kac's elastic particle system (online talk)*, March 17.
25. T. Hothorn, Universität Zürich, Institut für Epidemiologie, Biostatistik und Prävention, Switzerland, *Understanding and applying transformation models (online talk)*, February 24.
26. Y. Huang, Ludwig-Maximilians-Universität München, Tierärztliche Fakultät, *Advanced data analysis for traction force microscopy and data-driven discovery of physical equations (online talk)*, March 2.
27. M. Hütter, Eindhoven University of Technology, Materials Technology, Netherlands, *Finite-size effects in complex fluids: Phenomenology of fluctuations, stochastics, and statistical mechanics (online talk)*, January 28.
28. F. Iurlano, Sorbonne Université Paris, Laboratoire Jacques-Louis Lions (LJLL), France, *Shape optimization of light structures (online talk)*, April 14.
29. S. Jansen, Universität München, Mathematisches Institut, *Virial inversion and density functionals (online talk)*, January 13.
30. B. Jurgelucks, Humboldt-Universität zu Berlin, Institut für Mathematik, *Material parameter identification and sensitivity optimization for piezoelectric ceramics (online talk)*, February 12.
31. G. Keilbar, Humboldt-Universität zu Berlin, School of Business and Economics, *Finite sample bounds for quantiles using SGD (online talk)*, February 17.
32. M.-A. Keip, Universität Stuttgart, Institut für Mechanik (Bauwesen), *Multiscale analysis of instability-induced pattern transformations of composite active solids (online talk)*, July 15.
33. V. Kempf, Universität der Bundeswehr München, Institute for Mathematics and Computer-Based Simulation, *Anisotropic and pressure-robust finite element discretizations for the Stokes equations (online talk)*, February 2.
34. H. Leeb, University of Vienna, Department of Statistics and Operations Research, Austria, *A (tight) upper bound for the length of confidence intervals with conditional coverage (online talk)*, May 19.
35. P. Lorenz-Spreen, Max-Planck-Institut für Bildungsforschung, Forschungsbereich Adaptive Rationalität, Berlin, *Modeling radicalization dynamics and polarization in temporal networks (online talk)*, June 15.
36. Th. Lucke, Technische Universität Berlin, Institut für Mathematik, *Influence of mobility on telecommunication networks — Some thoughts (online talk)*, February 17.
37. C. Mailler, The University of Bath, Department of Mathematical Sciences, UK, *The ants walk: Finding geodesics in graphs using reinforcement learning (online talk)*, March 3.

38. D. Matignon, Université Fédérale Toulouse Midi-Pyrénées, Institut Supérieur de l'Aéronautique et de l'Espace (ISAE), France, *The partitioned finite element method for port-Hamiltonian systems: Structure-preserving numerics for physics-based PDEs with boundary control (online talk)*, January 14.
39. G. Medvedev, Drexel University, Department of Mathematics, Philadelphia, USA, *Unfolding chimeras: Where Turing meets Penrose (online talk)*, June 1.
40. V. Miloš, University of Chemistry and Technology, Department of Inorganic Technology, Prague, Czech Republic, *Modelling of YSZ LSM O_2 electrode with experimental validation (online talk)*, February 25.
41. H.-G. Müller, University of California at Davis, Department of Statistics, USA, *Functional models for time-varying random objects (online talk)*, May 26.
42. Th. Nagel, Technische Universität Berlin, Institut für Mathematik, *Surface detection of clouds by using simple artificial neural networks (online talk)*, February 23.
43. A. Naumov, Higher School of Economics, Faculty of Computer Science, Moscow, Russian Federation, *Finite time analysis of linear two-timescale stochastic approximation with Markovian noise (online talk)*, January 6.
44. E. Nijholt, University of Illinois at Urbana-Champaign, Department of Mathematics, Champaign, USA, *Exotic symmetry in networks (online talk)*, April 27.
45. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Madrid, Spain, *Error analysis of proper orthogonal decomposition stabilized methods for incompressible flows (online talk)*, April 15.
46. N. Nüsken, Universität Potsdam, Institut für Mathematik, *The Stein geometry in machine learning: Gradient flows, large deviations and convergence properties (online talk)*, April 21.
47. D.M. Ostrovskii, University of Southern California, Department of Industrial and Systems Engineering, Los Angeles, USA, *Near-optimal model discrimination with non-disclosure (online talk)*, January 19.
48. D. Paindaveine, Université Libre de Bruxelles, European Center for Advanced Research in Economics and Statistics (ECARES), Belgium, *Hypothesis testing on high-dimensional spheres: The Le Cam approach (online talk)*, December 8.
49. V. Panaretos, École Polytechnique Fédérale de Lausanne, Institute of Mathematics, Lausanne, Switzerland, *Testing for the rank of a covariance operator (online talk)*, July 7.
50. A. Pannier, Imperial College London, Stochastic Analysis and Mathematical Finance, UK, *Large and moderate deviations for stochastic Volterra systems (online talk)*, February 16.
51. S. Perotto, Politecnico di Milano, Dipartimento di Matematica, Italy, *Adaptive topology optimization in the design of structures and metamaterials (online talk)*, March 30.
52. K.H. Poelstra, Technische Universität Dortmund, Fakultät für Mathematik, *Dimension reduction for elasto-plastic rods and homogenization of elastoplastic lattices*, July 7.
53. A. Prevost, University of Cambridge, Faculty of Mathematics, Cambridge, UK, *Cluster capacity functionals and isomorphism theorems for Gaussian free fields (online talk)*, April 14.
54. N. Puchkin, Higher School of Economics Moscow, Faculty of Computer Science, Russian Federation, *Rates of convergence for density estimation with GANs (online talk)*, December 1.
55. E. Pulvirenti, Delft University of Technology, Applied Probability, Delft, Netherlands, *The Widom–Rowlinson model: Metastability, mesoscopic and microscopic fluctuations for the critical droplet (online talk)*, February 3.
56. L. Rebholz, Clemson University, Department of Mathematical Sciences, USA, *Anderson acceleration and how it speeds up convergence in fixed point iterations (online talk)*, March 18.
57. M. Reimherr, Pennsylvania State University, Department of Statistics, State College, USA, *Pure differential privacy in functional data analysis (online talk)*, November 24.

58. M. Reiter, Technische Universität Berlin, Institut für Mathematik, *Numerical approximation of the Ericksen–Leslie equations (online talk)*, June 15.

59. A. Rendall, Johannes Gutenberg-Universität Mainz, Institut für Mathematik, *Bogdanov–Takens bifurcations and the regulation of enzymatic activity by autophosphorylation (online talk)*, April 20.

60. Th. Richter, Universität Magdeburg, Institut für Analysis und Numerik, *Deep neural networks for accelerating fluid-dynamics simulations (online talk)*, May 20.

61. R. Rossi, Università degli Studi di Brescia, Ingegneria Meccanica e Industriale (DIMI), Italy, *Jump processes as generalized gradient systems (online talk)*, May 26.

62. T. Roubíček, Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czech Republic, *Viscoplastic elastodynamics at large deformations by Eulerian approaches (online talk)*, November 24.

63. L. Ruthotto, Emery College, Mathematics and Computer Sciences, Atlanta, USA, *A machine learning framework for mean field games and optimal control*, May 3.

64. U. Sauerland, A. Benz, Leibniz-Zentrum Allgemeine Sprachwissenschaft, Forschungsbereich Semantik & Pragmatik, *Numerical challenges in linguistic pragmatics (online talk)*, December 14.

65. T. Schäffter, Physikalisch-Technische Bundesanstalt, Abteilung 8, Medizinphysik und metrologische Informationstechnik, *Quantitative MR imaging – Added value (online talk)*, November 12.

66. A. Schlichting, Westfälische Wilhelms-Universität Münster, Angewandte Mathematik: Institut für Analysis und Numerik, *Dynamic behavior of growth processes: Phase separation, self-similarity, and oscillations (online talk)*, November 17.

67. B. Schmitzer, G. Steidl, Universität Göttingen, Institut für Informatik / Technische Universität Berlin, Institut für Mathematik, *Christmas talk: Santa Claus needs optimal transport (online talk)*, December 10.

68. E. Solea, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Data Science at the Service of Neurosciences, Rennes, France, *Nonparametric and high-dimensional functional graphical models (online talk)*, February 10.

69. E. Stepanov, Russian Academy of Sciences, Steklov Institute, St. Petersburg, *The story of a fish in a turbulent ocean: How to survive and how to return home (online talk)*, November 3.

70. W. Sun, Technische Universität Berlin, Berlin Mathematical School, *Pathwise large deviation for the pure jump k-nary interacting particle systems (online talk)*, June 9.

71. Y. Sun, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *Graph-spanning ratio test with application to change-point detection problem (online talk)*, April 13.

72. L. Taggi, University of Rome "La Sapienza", Mathematics Department, Italy, *Exponential decay of correlations for O(N) spin systems (online talk)*, January 20.

73. B. Thakur, Jacobs University, Physics & Earth Sciences, Bremen, *Data driven identification of nonlinear dynamics using sparse regression with applications in plasma physics (online talk)*, June 22.

74. S. Throm, Westfälische Wilhelms-Universität Münster, Institut für Analysis und Numerik, *Universal long-time asymptotics for coagulation equations (online talk)*, January 27.

75. A. Tóbiás, Technische Universität Berlin, Institut für Mathematik, *Absence of percolation in graphs based on stationary point processes with degrees bounded by two (online talk)*, May 26.

76. ———, *Virus dynamics in the presence of contact-mediated host dormancy (online talk)*, October 27.

77. L. Trussardi, Universität Konstanz, Fachbereich Mathematik und Statistik, *Two structure-preserving time discretizations for gradient flow. An application to GENERIC systems (online talk)*, December 15.

78. D. Ueltschi, University of Warwick, Department of Mathematics, Coventry, UK, *Loop models and the universal distribution of the loop lengths*, December 17.

79. D. Wang, Leiden University, Netherlands, *The parabolic Anderson model on a Galton–Watson tree with unbounded degrees (online talk)*, July 7.

80. S. Wang, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, *On polynomial-time computation of high-dimensional posterior measures by Langevin-type algorithms (online talk)*, January 20.

81. L. Wessels, Technische Universität Berlin, Institut für Mathematik, *Pontryagin's maximum principle for SPDEs and its relation to dynamic programming (online talk)*, December 1.

82. S. Wieczorek, University College Cork, Mathematical Sciences, Ireland, *Rate-induced tipping points (online talk)*, June 29.

83. Ch. Zheng, Max Planck Institute for Physics of Complex Systems, Division of Biological Physics, Dresden, *Transition to synchrony in the three-dimensional noisy Kuramoto model (online talk)*, June 8.

84. N. Zhivotovskiy, Eidgenössische Technische Hochschule Zürich, Departement Mathematik, Switzerland, *Distribution-free robust linear regression (online talk)*, November 10.

A.13 Software

AWC – Adaptive Weights Clustering (contact: V. Spokoiny, phone: +49 30/20372-575, e-mail: vladimir.spokoiny@wias-berlin.de)

`AWC` is an open source Python package containing implementation of the novel non-parametric clustering algorithm **A**daptive **W**eights **C**lustering. The method is fully automatic and does not require to specify the number of clusters or their structure. The procedure is numerically feasible and applicable for high-dimensional datasets.

More information: https://www.wias-berlin.de/software/awc/

AWS – Adaptive Weights Smoothing (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

`AWS` is a contributed package within the R-Project for Statistical Computing containing a reference implementation of the **A**daptive **W**eights **S**moothing algorithms for local constant likelihood and local polynomial regression models. Binaries for several operating systems are available from the Comprehensive R Archive Network (http://cran.r-project.org).

More information: https://www.wias-berlin.de/software/aws/

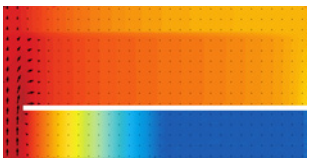
BALaser (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.radziunas@wias-berlin.de)

`BALaser` is the software tool used for simulations of the nonlinear dynamics in high-power edge-emitting **B**road-**A**rea semiconductor **Laser**s. It integrates numerically the laterally extended dynamic traveling wave model (one- and two-dimensional partial differential equations), executes different data post-processing routines, and visualizes the obtained data. When required, the traveling-wave-model-based solver is self-consistently coupled to the quasi-three-dimensional inhomogeneous current-spreading and heat-flow solvers, both developed using the WIAS `pdelib` toolkit.

More information: https://www.wias-berlin.de/software/balaser/

ddfermi (contact: Th. Koprucki, phone: +49 30/20372-508, e-mail: thomas.koprucki@wias-berlin.de, J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, P. Farrell, phone: +49 30/20372-401, e-mail: patricio.farrell@wias-berlin.de)

`ddfermi` is an open-source software prototype that simulates the carrier transport in classical or organic semiconductor devices based on drift-diffusion models.



Current density for single photon system

The key features are

- finite volume discretization of the semiconductor equations (van Roosbroeck system),
- thermodynamically consistent Scharfetter–Gummel flux discretizations beyond Boltzmann,
- general statistics: Fermi–Dirac, Gauss–Fermi, Blakemore, and Boltzmann,
- generic carrier species concept,
- one-, two- and three-dimensional devices,
- C++ code based on `pdelib` and interfaced via Python,
- in-situ visualization.

Please find further information under https://www.wias-berlin.de/software/ddfermi/.

DiPoG (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@wias-berlin.de)

The program package DiPoG (**D**irect and **i**nverse **P**roblems for **o**ptical **G**ratings) provides simulation and optimization tools for periodic diffractive structures with multilayer stacks.

The direct solver computes the field distributions and efficiencies of given gratings for TE and TM polarization as well as, under conical mounting, for arbitrary polygonal surface profiles. The inverse solver deals with the optimal design of gratings, realizing given optical functions, for example, far-field patterns, efficiency, or phase profiles. The algorithms are based on coupled generalized finite/boundary elements and gradient-type optimization methods.

For detailed information please see https://www.wias-berlin.de/software/DIPOG/.

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.radziunas@wias-berlin.de)

LDSL-tool (**L**ongitudinal **D**ynamics in **S**emiconductor **L**asers) is a **tool** for the simulation and analysis of the nonlinear longitudinal dynamics in multisection semiconductor lasers and different coupled laser devices. This software is used to investigate and design laser devices that exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, mutual synchronization, and frequency entrainment by an external modulated optical or electrical signal.

LDSL-tool combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.

Detailed information: https://www.wias-berlin.de/software/ldsl

WIAS-MeFreSim (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@wias-berlin.de)

WIAS-MeFreSim allows for the three-dimensional simulation of induction heat treatment for workpieces made of steel using single- and multi-frequency currents. It is the aim of the heat treatment to produce workpieces with hard, wear-resistant surface and soft, ductile core. The boundary layer of the workpiece is heated up by induced eddy currents and rapidly cooled down by the subsequent quenching process. The resulting solid-solid phase transitions lead to a hardening of the surface of the workpiece.

WIAS-MeFreSim is based on the WIAS software pdelib. It solves coupled systems of PDEs consisting of Maxwell's equations, the heat equation, and the equations of linear elasticity.

Fore more information see https://www.wias-berlin.de/software/MeFreSim/.

ParMoon (contact: U. Wilbrandt, phone: +49 30/20372-571, e-mail: ulrich.wilbrandt@wias-berlin.de)

ParMooN is a flexible finite element package for the solution of steady-state and time-dependent convection-diffusion-reaction equations, incompressible Navier–Stokes equations, and coupled systems consisting of these types of equations, like systems coupling free flows and flows in porous media.

Please find more information under http://cmg.cds.iisc.ac.in/parmoon/.

Important features of ParMooN are

- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, non-conforming, discontinuous, higher-order, vector-valued, isoparametric, with bubbles),
- the use of implicit time-stepping schemes (θ-schemes, DIRK schemes, Rosenbrock–Wanner schemes),
- the application of a multiple-discretization multi-level (MDML) preconditioner in Krylov subspace methods,
- tools for using reduced-order models based on proper orthogonal decomposition (POD) are available,
- hybrid parallelization with MPI and OpenMP.

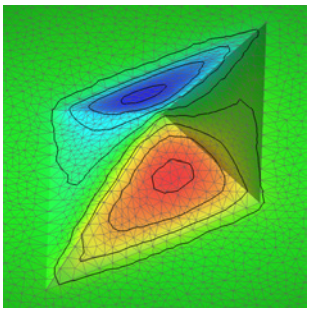
ParMooN is a joint development with the group of Prof. S. Ganesan (IISc Bangalore) and the group of Prof. G. Matthies (TU Dresden).

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, T. Streckenbach, phone: +49 30/20372-476, e-mail: timo.streckenbach@wias-berlin.de)

pdelib is a collection of software components that are useful to create simulators and visualization tools for partial differential equations. The main idea of the package is modularity, based on a bottom-up design realized in the C++ programming language. Among others, it provides

- iterative solvers for linear and nonlinear systems of equations,
- sparse matrix structures with preconditioners and direct solver interfaces,
- dimension-independent simplex grid handling in one, two, and three space dimensions,
- finite-volume-based solution of coupled parabolic reaction-diffusion-convection systems and pressure-robust discretizations for Navier–Stokes,
- finite-element-based solution of variational equations (especially thermoelasticity) with goal-oriented error estimators,
- optimization tool box,
- parallelization on SMP architectures,
- graphical output during computation using OpenGL,
- scripting interface based on the languages Python and Lua,
- graphical user interface based on the FLTK toolkit,
- modular build system and package manager for the installation of third-party software used in the code.

Please see also https://www.wias-berlin.de/software/pdelib/.



Displacement (y-component) from FEM simulation of elastic relaxation of a pyramidal InAs quantum dot with a rhomboidal base in GaAs matrix. Used as input for TEM image simulation.

PDELib.jl (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de, T. Streckenbach, phone: +49 30/20372-476, e-mail: timo.streckenbach@wias-berlin.de, Ch. Merdon, phone: +49 30/20372-452, e-mail: christian.merdon@wias-berlin.de)

PDELib.jl is being developed as the successor of pdelib in the Julia programming language. It is a collection of open source Julia packages dedicated to the handling of sparse matrices, mesh generation, and visualization. It wraps the Julia package VoronoiFVM.jl that implements the Voronoi box-based finite volume method for nonlinear systems of partial differential equations and the Julia package GradientRobustMultiPhysics.jl implementing gradient robust finite element methods in Julia.

Please see also https://github.com/WIAS-BERLIN/PDELib.jl.

SPHInX (contact: O. Marquardt, phone: +49 30/20372-474, e-mail: oliver.marquardt@wias-berlin.de)

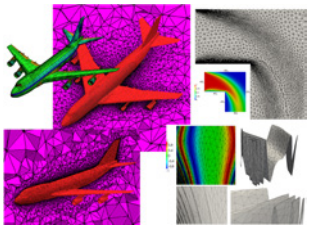
SPHInX is an open-source C++ library for materials simulation hosted by the Max-Planck-Institut für Eisenforschung GmbH in Düsseldorf. The multiband $\mathbf{k} \cdot \mathbf{p}$ and continuum elasticity modules of SPHInX for the calculation of elastic and optoelectronic properties of semiconductor heterostructures are maintained at WIAS Berlin.

Please see https://sxrepo.mpie.de/.

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/.



Adapted tetrahedral meshes and anisotropic meshes for numerical methods and scientific computation

WIAS-TeSCA (contact: H. Stephan, phone: +49 30/20372-442, e-mail: holger.stephan@wias-berlin.de)

`WIAS-TeSCA` is a **T**wo-dimensional **S**emi-**C**onductor **A**nalysis package. It serves to simulate numerically the charge carrier transport in semiconductor devices based upon the drift-diffusion model. This van Roosbroeck system is augmented by a vast variety of additional physical phenomena playing a role in the operation of specialized semiconductor devices as, e.g., the influence of magnetic fields, optical radiation, temperature, or the kinetics of deep (trapped) impurities.

The strategy of `WIAS-TeSCA` for solving the resulting highly nonlinear system of partial differential equations is oriented towards the Lyapunov structure of the system describing the currents of electrons and holes within the device. Thus, efficient numerical procedures for both the stationary and the transient simulation 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, 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).