Abstract Booklet

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Wednesday 27th September

15:30 - 17:30

Parallel sessions

Shapes, Geometry, Number Theory and Algebra I
Room 2.058
Chair: Andreas Ott

A tropical approach to consensus tree methods

Andrei Comăneci

In phylogenetics, one studies the evolutionary history of different species which is represented as a labeled tree. Due to very different available data and methods, one rarely can reconstruct a unique tree, so there is a need of a summary containing the most frequent characteristics. The summary is called a "consensus tree".

A large variety of consensus methods exist today, but most of them involve unweighted trees. For the weighted case, a geometric method was proposed by Billera, Holmes, and Vogtmann (2001), where they see a consensus method as a location estimator. Since Ardila and Klivans (2006) noticed a relationship of the aforementioned model to tropical geometry, much interest was put into exploiting alternative geometric structures.

We present recent work on the consensus method that exploits tropical convexity. We show that this is possible studying a Fermat–Weber problem under a specific asymmetric distance. This leads to a method that is fast to compute and has some desirable properties.

The performance on different data sets will be also presented. We will emphasize the phylogenetic meaning of the good properties provided by tropical convexity, but we will also point out some drawbacks of the current model. We will conclude with a few remarks about possible future improvements.

This is based on joint work with Michael Joswig (TU Berlin).

Algebraic Path Problems for Graph Metrics

Enrique Fita Sanmartin

Finding paths with optimal properties is a foundational problem in computer science. The notions of shortest paths (minimal sum of edge costs), minimax paths (minimal maximum edge weight), reliability of a path and many others all arise as special cases of the "algebraic path problem" (APP). Indeed, the APP formalizes the relation between different semirings such as min-plus, minmax and the distances they induce. We here clarify the relation between the potential distance and the log-semiring. We also present a new unifying family of algebraic structures that include all above-mentioned path problems as well as the commute cost and others as special or limiting cases. The family comprises not only semirings but also strong bimonoids (that is, semirings without distributivity). We call this new and very general distance the "log-norm distance". Finally, we also comment on some sufficient conditions which ensure that the APP associated with a semiring defines a metric over an arbitrary graph.

Topologically Autoencoding Cognitive Maps

Maxim Beketov

Cognitive maps is a term used to describe the inner mental representation of various spaces, including the physical space – perceived by the animal present in it (or imagined, for species capable of so). These maps are encoded in the neural activity of so-called place cells (in particular – other similar neurons have also been found) – neurons found in a certain region of the hippocampus, the discovery of which has been acknowledged by a Nobel Prize in Physiology and Medicine 2014, awarded to John O'Keefe, May-Britt Moser and Edvard I. Moser. In this work, we apply AutoEncoders (AEs, a family of ANNs) to the place cells' neural activity data recorded (with the optical technique of calcium imaging) from mice placed into arenas of different topologies – ones with 0, 1, 2, 3 holes (impenetrable obstacles) in it. The goal is, having the true coordinates of mice locations (synced with their neural activity) – to reconstruct this "true map" from the high-dimensional neural activity time series, preserving the topology of the arena. Applying vanilla AEs to this problem in a supervised manner (additionally penalising for metric dissimilarity of the inner, latent, representation of the time-series from the true map), we find that mices' cognitive maps are well reconstructed by quite shallow (3-4 layers) AEs – which provides some empirical implications for neuroscience. We also try a novel technique of Topological AutoEncoders (TopoAE) to solve this

problem in an unsupervised manner – the TopoAE is not being shown the true coordinates – rather being penalised for a difference in topological properties (persistent homologies) of the input point cloud and its latent representation. We slightly modify this approach to have different regularisation strengths for homologies of different order – in our problem, 1-homologies (cycles) are more important than others – and overall demonstrate the success of applying such nonlinear topologically-regularised dimension reduction techniques to such neural data.

Fluid Dynamics

Room: 2.066

Chair: Björn de Rijk

Unsteady flow and mass transfer induced by Rayleigh-Bénard-Marangoni Convection

Herlina Herlina

Evaporative cooling at the water surface is often modelled by imposing a constant heat flux at the surface. This boundary condition allows for variations in the water surface temperature T, inducing variations in surface tension. The resulting Marangoni forces tend to move surface water from low surface tension (high T) to high surface tension (low T) regions and generate small recirculation areas immediately underneath the surface. Buoyant convection, on the other hand, is characterised by thermal plumes that typically penetrate quite deep into the bulk of the water.

Fully resolved numerical simulations were performed to study the development of the Rayleigh-Bénard-Marangoni instability and its effect on interfacial mass transfer for various Rayleigh (Ra) and Marangoni (Ma) numbers. The domain was periodic in the horizontal directions. A flat surface was assumed with a fixed temperature flux and a fully saturated scalar concentration. The Marangoni effect on the horizontal velocities was modelled by

$du/dx = -M\ a\ dt/dX|_S$ and

$dv/dz = -M\ a\ d\ T/dY|_S$,

where S denotes the surface. At the bottom, zero flux conditions were employed for all scalars in combination with a free-slip condition for the velocity. The incompressible Navier-Stokes equations were discretised using fourth-order central methods for convection and diffusion, while the scalar convection-diffusion equations were solved using a fifth-order WENO scheme for the convection and a fourth-order central discretisation for the diffusion.

The results presented will focus on the development of convection cells from initially random disturbances added to the temperature field, thereby highlighting the differences between the Marangoni-force- and Buoyancy-induced convection as well as a comparison of the effectiveness of these two instability sources in promo+ng the mixing of cold, saturated surface water with warm, unsaturated water from the upper bulk.

On simple invariant solutions in rectangular duct flows

Markus Scherer

During the past decades, concepts borrowed from dynamical systems theory have significantly contributed to further the understanding of coherent dynamics both in transitional and fully-developed turbulent flows. Of particular relevance was in this context the identification of fully nonlinear ‘invariant solutions’ to the Navier-Stokes equations with a simple dynamics (typically stationary or time-periodic) that reveal a striking similarity to the coherent structures embedded in the chaotic turbulent attractor.

Most of the solutions known today have been detected in canonical wall-bounded flows including plane Couette, plane channel and circular pipe flow. On the other hand, less is known about such ‘exact coherent structures’ for more complex flow geometries such as the flow in a duct with rectangular cross-section, which inherently features a mean secondary flow pattern. While a handful of travelling-wave solutions (equilibria in an appropriate co-moving frame of reference) have been identified in the past, no time-dependent solution in rectangular duct flow is known to date.

In this talk, we will revisit the properties of the known solutions and present preliminary results of our search for invariant solutions in rectangular duct flow that reveal a certain time dependence. In this context, we will mainly focus on invariant states which live on the edge between the laminar and turbulent basins of attraction and which are therefore of direct relevance for transitional flows. We will conclude with a brief outlook on how the identified invariant solutions can be used as low-dimensional models of fully chaotic turbulent states, for instance when studying multiphase systems such as the dynamics of finite size-particles in a turbulent environment.

Integrated Engineering of fiber reinforced polymers

Room: 2.066

Chair: Loredana Kehrer & Tobias Karl

Mathematical methods for fiber orientation tensor interpolation and microstructure generation based on X-ray images of carbon fiber reinforced polymers

Juliane Blarr

The complex microstructure of fiber-reinforced polymers is difficult to characterize. Typically, CT images and subsequent image analysis methods help to determine quantitative parameters such as fiber orientation tensors. However, especially in the case of carbon fiber reinforced plastics, the contrast between fiber and matrix is low and due to the small diameter of the fibers, a high resolution is required. Both of these challenges introduce a lot of noise into the images and push previous algorithms and approaches to their limits. Both conventional mathematical methods and image processing methods as well as AI-based approaches offer new possibilities. In particular, the comparison of these methods is of interest. Two work insights will be given in the talk. First, it will be shown how a decomposition method based on the eigenvalue problem allows the interpolation of fiber orientation tensors and thus addresses one of the biggest problems in the field of microstructure characterization, i.e. up- and down-scaling, or scale bridging in general. In the process, a separate interpolation of the shape and orientation of the tensors has been implemented. On the other hand, the generation of microstructures offers a good opportunity for a better understanding of the same. Conventionally, this is done by sphere-packing algorithms, which however reach their limits at high fiber volume contents or fiber curvature. The novel capabilities offered by generative adversarial networks (GAN) were tested and a CT image generator was developed. This resulted in generated images that are difficult to distinguish from the training data by the untrained eye. It revealed a lot of potential for development: Apart from image information, quantities such as fiber volume content, fiber length distributions, and fiber orientation distributions could be included in the input data in the future to generate physically informed microstructures.

Implicit fiber orientation tensor closures

Tobias Karl

In the framework of lightweight composites, considering microstructural information is essential for industrial applications in view of predicting anisotropic material properties on the macroscale. For the special case of short-fiber reinforced composites, orientation tensors of the first kind are widely used as an efficient way of describing strongly heterogeneous and anisotropic microstructures. Typically, only the second-order fiber orientation tensor is known as a result of mold-filling simulations. In order to perform these mold-filling simulations, the fourth-order orientation tensor is needed for solving the corresponding evolution equation for the second-order orientation tensor. In addition, the approximation of the effective behavior requires the fourth-order orientation tensor when combining mean-field homogenization and orientation averaging. In this context, closure methods for fiber orientation tensors are used to approximate the fourth-order orientation tensor as a function of the second-order orientation tensor.

A novel closure approximation for fiber orientation tensors is proposed namely the fully symmetric implicit closure. Both the quadratic and hybrid versions of the novel closure are compared against classical approximations in terms of orientation evolution in a simple shear flow. Furthermore, the capability of predicting the effective viscous and elastic behavior of fiber suspensions and solid composites is investigated for a given fiber orientation state. The results show that both proposed implicit closures can be used to approximate the maximum entropy closure. Thereby, both the quadratic and the hybrid approach alleviate the high computational burden of the maximum entropy closure, as their formulation may be reduced to a one-dimensional problem. In addition, the predicted effective behavior based on the implicit closures shows an overall good agreement with predictions based on measured orientation data. In case of orientation evolution, the proposed implicit closures show oscillatory behavior, closely following the maximum entropy closure.

Viscoelastic modeling of PA6 under hydrothermal influences

Loredana Kehrer

Polymer-based composites are increasingly applied as resource-efficient semi-structural materials in many different engineering applications. In this context, polyamide 6 (PA6) serves as matrix material with advantageous properties such as high specific strength and great design freedom. In industrial applications, the material is exposed to environmental influences such as moisture, which can significantly affect its behavior and technical performance. Due to the hydrophobic nature of PA6, not only the temperature- but also the humidity-dependent behavior of PA6 is investigated in this work. To capture these effects, a generalized Maxwell model for the linear viscoelastic material properties under hydrothermal influences is presented and results for PA6 are discussed. In addition, the nonlinear viscoelastic material behavior is modeled based on the Schapery

integral model with internal variables. In this context, a one-dimensional formulation with strain-dependent nonlinear functions for a sinusoidal load case is presented. In addition to the viscoelastic storage and loss modulus, the higher order harmonic oscillations in the stress response are compared to experimental data from Fourier transform rheology of PA6 and results are discussed.

FFT-based homogenization and modeling of the viscosity of fiber suspensions

Benedikt Sterr

The viscosity of fiber suspensions plays an important role in manufacturing fiber reinforced composite components, for example in injection and compression molding. Therefore, an accurate understanding of the viscous properties of fiber suspensions is important for appropriate industrial application. Taking microstructural parameters into account, Fast Fourier Transform (FFT) based simulations enable high fidelity homogenization of viscous properties of fiber suspensions, thus laying the foundation for computational two-scale strategies. Previous work on FFT-based two-scale strategies has been limited to the assumption of a Newtonian polymer melt. However, polymer melts typically show non-Newtonian behavior. Here we investigate scale transition in the viscosity of fiber suspensions using the Cross-WLF material model and an extended computational method. We study the influence of loading direction and magnitude, as well as microstructural parameters on the effective viscosity of fiber suspensions with a non-Newtonian matrix. We compare our results to effective viscosities of fiber suspensions with a Newtonian matrix.

Mathematical modelling and control

Room: 2.067

Chair: Niklas Baumgarten

Numerical modelling of lava dome evolution

Natalya Zeinalova

Lava domes form during non-explosive volcanic eruptions due to an extrusion of highly viscous magmas from volcanic vents. We develop a numerical model of the lava dome growth at Volcán de Colima, Mexico during 2007-2009. The mathematical model treats the lava dome extrusion dynamics as a thermomechanical problem. The equations of motion (the Navier-Stokes equations), continuity, and heat transfer are solved with the relevant boundary and initial conditions in the assumption that magma viscosity depends on the volume fraction of crystals and temperature. Numerical experiments have been performed to analyse the internal structure of the lava dome (i.e., the distributions of the temperature, crystal content, viscosity, and velocity) depending on various heat sources and thermal boundary conditions. We show that cooling plays a significant role during long (up to several years) dome-building episodes. A carapace (a highviscous layer) develops as a response to a convective cooling at the lava dome interface with the air, and it becomes thicker if the radiative heat loss at the interface is also considered. The thick carapace influences the lava dome dynamics preventing its lateral advancement. The latent heat of crystallization leads to higher temperatures inside the lava dome and to a relative flattening of the dome. Meanwhile, the heat source due to viscous dissipation is negligible, and it does not influence the lava dome growth. The developed thermomechanical model can be used elsewhere to analyze non-explosive eruptions, dome carapace evolution, and its failure potentially leading to pyroclastic flow hazards.

Robust capture pursuit based on differential games

Vladimir Turetsky

For a planar engagement of two vehicles with time-dependent velocities, the problem of robust pursuit of uncertain evader is considered. If the pursuer's feedback control guarantees the capture (zero miss distance) at the prescribed time moment, against any admissible evader's behavior from some set of the initial positions (the capture zone), it is called the robust capture control. In this presentation, several types of robust capture controls are designed, and their capture zones are constructed. In the first approach, the problem is formulated as a differential zero-sum game with bounded controls. The original game is scalarized and then solved by the game space decomposition into regular and singular domains. A novel recursive procedure of the singular domain construction is proposed. The optimal minimizer's feedback strategy is a robust capture control. Its capture zone is a closed set in the plane (time, scalar state variable). The interior of this capture zone represents the maximal part of the game's singular region which closure is a simply connected set, and this set contains the point (final game time instant, zero). The aforementioned robust capture control has a bang-bang structure which leads to sliding modes and produces an undesirable chattering phenomenon. In the second approach, this drawback is circumvented by a preliminary design of a pursuer's feedback control with required properties like continuity/smoothness/linearity with respect to the state variable. In this presentation, two robust capture controls are designed in the form of saturated linear strategy. The first one is based on the

simplest strategy tracking the boundary of the maximal capture zone. The second strategy is saturated optimal minimizer's strategy in the auxiliary linear-quadratic differential game. Under proper conditions, the capture zones of these strategies coincide with the maximal one. Illustrative examples of the pursuit-evasion engagement between two flying vehicles are presented.

Simulation techniques and software packages

Room: 2.067
Chair: Mehdi Elasmi

MESHFREE Simulations for Industrial Applications

Fabian Castelli

Numerical simulations have become an indispensable tool for industrial research and development processes. Despite recent advances in numerical methods, software and hardware, the simulation of industrial applications is computationally challenging. Classical discretization methods, such as the finite element or finite volume method, are meshbased and face crucial challenges for example in case of complex model geometries, large deformations, or free surfaces. Meshfree approaches overcome the expensive meshing step for classical methods. At Fraunhofer ITWM and Fraunhofer SCAI, we develop and implement the MESHFREE software (www.meshfree.eu) providing a simulation tool for industrial applications. The discretization is based on a Generalized Finite Difference Method (GFDM). The method is purely meshfree and suited for fluid as well as continuum mechanical processes. Due to its discretization based on a scattered set of numerical points, MESHFREE is flexible and particularly efficient for applications with moving geometric parts, free surfaces, phase boundaries, or fluid-structure interaction. Examples include water management of vehicles or metal cutting processes. The talk presents the MESHFREE software and introduces the mathematical formulation as well as theory behind the GFDM. The capabilities of MESHFREE are demonstrated with an overview of successfully simulated industrial applications.

Machine Learning-Optimized Approach for Parameter Selection in MESHFREE Simulations: Enhancing Accuracy and Efficiency

Paulami Banerjee

Meshfree simulation methods have emerged as a valuable alternative to traditional mesh-based approaches in fields like computational fluid dynamics (CFD) and continuum mechanics. These methods offer the ability to handle complex flow domains, moving geometries and free surfaces. In our research, we focus on Fraunhofer's software MESHFREE (https://www.meshfree.eu/) which utilizes a numerical point cloud based on a generalized finite difference method. This approach enables users to control the local refinement of the point cloud and other quality-based parameters that influence the simulation results. Thus, the optimal balance between computation time and accuracy can potentially be exploited for the respective application.

However, the process of determining the optimal parameter combination in the MESHFREE software is currently manual and poses challenges, particularly for inexperienced users. To address this issue, this ongoing research aims to develop a machine learning (ML)-optimized approach that determines the best parameter combination based on specified requirements.

Unlike traditional Big Data-driven ML techniques, our methodology relies on simulation data obtained from flow simulations around a cylinder using the MESHFREE software. Initial focus is placed on determining optimal hyperparameters governing point-cloud resolution, neighborhood update strategies, and simulation quality. We apply a Latin Hypercube-based design of experiments for data generation, with active learning strategies effectively identifying regions within the hypercube that yield favorable outcomes while minimizing outliers. Subsequently, by employing data visualization techniques, and a combination of tree-based regression algorithms as well as gradient boosting techniques, we aim to gain a comprehensive understanding of the relationship between parameter choices and simulation behavior.

In this talk, we will provide an overview of the MESHFREE software and outline our ML-optimized approach. We will discuss initial results by visually representing the impact of various input combinations on output parameters such as drag and lift coefficients as well as convergence time. Additionally, we will highlight the initial performance of our ML algorithms in predicting simulation outputs based on specific input combinations.

Neural network simulation for stiff ODEs representing chemical mechanisms

Giorgio Taverna

Computational efforts for the calculation of chemical reactions are about 30% of the total resource requested to run simulations involving climate models. Finding alternatives to speed up the calculation of the chemistry module is then a crucial task. Recent studies show that the calculation of the Jacobian is the most computationally demanding part of the related ODEs and then solutions have been sought to overcome this problem. In this poster results from Kinetic Pre-Processor (KPP) solver and Icosahedral Nonhydrostatic (ICON) atmospheric Model (in a box model version) for the stiff H2O2 chemistry and the air-pollution Verwer systems, compared with neural network corresponding results are shown. The H2O2 chemistry mechanism consists of 4 reactions (3 species), while the Verwer system is made of 25 reactions (21 species). The simulations have been initialized with a fixed and a random set of values. These results form the basis to subsequently train the neural network.

Spatial Statistics, Machine Learning and Forecasting

Room 0.14

Chair: Friederike Becker

Spatial representation learning for ensemble weather simulations using invariant variational autoencoders

Jieyu Chen

Weather forecasts today are typically issued in the form of ensemble simulations based on multiple runs of numerical weather prediction models with different perturbations in the initial states and the model physics. In light of the continuously increasing spatial resolutions of operational weather models, this results in large, high-dimensional datasets that nonetheless contain relevant spatial and temporal structure, as well as information about the predictive uncertainty. We propose invariant variational autoencoder (iVAE) models based on convolutional neural network architectures to learn low-dimensional representations of the spatial forecast fields. We specifically aim to account for the ensemble character of the input data and discuss methodological questions about the optimal design of suitable dimensionality reduction methods in this setting. Thereby, our iVAE models extend previous work where low-dimensional representations of single, deterministic forecast fields were learned and utilized for incorporating spatial information into localized ensemble postprocessing methods based on neural networks, which were able to improve upon model utilizing location-specific inputs only. By additionally incorporating the ensemble dimension and learning representation for probability distributions of spatial fields, we aim to enable a more flexible modeling of relevant predictive information contained in the full forecast ensemble. Additional potential applications include data compression and the generation of forecast ensembles of arbitrary size.

We illustrate our methodological developments based on a 10-year dataset of gridded ensemble forecasts from the European Centre for Medium-Range Weather Forecasts of several meteorological variables over Europe. Specifically, we investigate alternative model architectures and highlight the importance of tailoring the loss function to the specific problem at hand.

Generating Synthetic Rainfall Fields by R-vine Copulas Applied to Seamless Probabilistic Predictions

Peter Schaumann

Many post-processing methods improve forecasts at individual locations but remove their correlation structure. However, this information is essential for forecasting larger-scale events, such as the total precipitation amount over larger areas like river catchments, which are relevant for weather warnings and flood predictions. We propose a method to reintroduce spatial correlation into a post-processed forecast using an R-vine copula fitted to historical observations. This method works similarly to related approaches in the literature, like the Schaake shuffle and ensemble copula coupling, by rearranging the predictions at individual locations. It ensures that the predictions at each location still exhibit the post-processed marginal distribution and allows spatial correlation to be reintroduced. Here, the fitted copula serves as a measure of how well a given arrangement compares with the observed distribution of precipitation in the historical data, where no close relationship is required between the post-processed marginal distributions and the spatial correlation source. This is an advantage compared to Schaake shuffle and ensemble copula coupling, which rely on a ranking with no ties at each considered location in their source for spatial correlations. However, weather variables such as the precipitation amount, whose distribution has an atom at zero, tend to have rankings with ties. To evaluate the proposed method, it is applied to a precipitation forecast produced by a combination model with two input forecasts that deliver calibrated marginal distributions but without spatial correlations. The obtained results indicate that the calibration of the combination model carries over to the output of the proposed model, i.e., the evaluation of area predictions shows a similar improvement in forecast quality as the predictions for

individual locations. Additionally, the spatial correlation of the forecast is evaluated with the help of object-based metrics, for which the proposed model also shows an improvement compared to both input forecasts.

Enhanced Universal Kriging for Uncertainty Quantification and Parameter Optimization: Application to West African Monsoon Simulations

Matthias Fischer

In the scientific discipline of uncertainty quantification (UQ), model input quantities (e. g. parameters of a computational model) are often described by probability distributions. In many applications, the propagation of uncertainty of input quantities to certain output quantities, i.e. Quantities of Interest (QoI), is to be determined. If computational models are expensive, surrogate models are preferably used which provide information about the relationship between input and output quantities.

For the construction of surrogate models, space-filling designs are generated in the input space to define training points, and evaluations of the computational model at these points are then conducted. However, the physical parameter space is often initially transformed into an i.i.d. uniform input space in order to apply space-filling training procedures in a sensible way. Due to this transformation surrogate modeling techniques tend to suffer with regard to their prediction accuracy. Therefore, a new method is proposed and assessed where input parameter transformations are considered for the definition of basis functions for universal kriging. The proposed method is then applied to a meteorological model to investigate uncertainty contributions in West African monsoon (WAM) simulations. For this purpose, the ICON model of the German Weather Service is run in a nested limited-area mode where the influence between selected model parameters and QoIs (e.g. characteristics of the African and Tropical easterly jets or the Saharan heat low) is investigated with the use of surrogate models and sensitivity studies. In a second step, the surrogate models are used to employ multivariate parameter identification studies by including ERA5-reanalysis as reference data. Results reveal the complex nature of the WAM system and indicate for which model parameters uncertainties need to be reduced to lower the spread in the outputs, and which model parameters need to be tuned for a better approximation of reanalysis data.

Deep Learning for Spatial Statistics via Neural Tangent Kernels

Ghulam Qadir

The traditional spatial statistics has been mostly centralized on stochastic process models, typically, the Gaussian process models, which are well studied and understood in terms of inference and predictions. While so far the stochastic process models have been the leading focus in spatial statistics, the deep learning methods are now also receiving notable heed from spatial statisticians. In this paper, we explore the use of deep learning for spatial statistics by using the theoretical framework of the Neural Tangent Kernel (NTK) which investigates the training dynamics of deep learning models in the infinite-width limit. In our work, we study some recently developed deep learning variants for spatial statistics against the Gaussian process regression through multiple simulation studies and data applications. Through our case studies, we provide some crucial guidelines for developing the appropriate deep learning models in the context of spatial data modeling.

Aggregating distribution forecasts from deep ensembles

Benedikt Schulz

The importance of accurately quantifying forecast uncertainty has motivated much recent research on probabilistic forecasting. In particular, a variety of deep learning approaches has been proposed over the past years, with forecast distributions obtained as output of neural networks. These neural network-based methods are often used in the form of an ensemble based on multiple model runs from different random initializations, resulting in a collection of forecast distributions that need to be aggregated into a final probabilistic prediction. With the aim of consolidating findings from the machine learning literature on ensemble methods and the statistical literature on forecast combination, we address the question of how to aggregate distribution forecasts based on an ensemble of deep neural networks. Using theoretical arguments, simulation experiments and a real data study on probabilistic wind gust forecasting, we systematically compare aggregation methods on the scale of probabilities and quantile functions for three variants of neural network-based approaches to probabilistic forecasting with different forecast distribution types as output. Our results show that combining forecast distributions can substantially improve the predictive performance. We propose a general quantile aggregation framework for deep ensembles which shows superior performance compared to a linear combination of the corresponding forecast densities. Finally, we

investigate the effects of the ensemble size and derive recommendations of aggregating distribution forecasts from deep ensembles in practice.

Testing components of Mincer-Zarnowitz-regression based score decomposition

Marius Puke

Researchers often utilize regression-based techniques, such as those developed by Mincer and Zarnowitz (1969, MZ), to evaluate forecasts for real-valued outcomes. Recent advancements in this field propose non-parametric MZ counterparts, reliability diagrams, and exact decompositions of strictly proper scoring rules into the interpretable components assessing (mis)calibration, discrimination, and uncertainty. A notable limitation of these components is that there are no objective measures for how large or small the terms should be. In this presentation, we introduce asymptotic tests for these components based on (linear) MZ regressions. We relate tests for the miscalibration component to backtesting exercises for risk measures and demonstrate that backtests only assess calibration while entirely ignoring a forecast's discriminating ability. Intuitively, this corresponds to ignoring the forecasts' ability to discriminate between periods of lower and higher. As a consequence, we propose the practical use of score decompositions that, additional to backtests, reveal information on the overall predictive ability and the hitherto unexploited information on discrimination and hence provoke more informative insights in applications.

Wednesday 27th September

17:30 – 20:00

Poster Session

Numerical optimization of a micromixer

Julius Jeßberger

The mixing performance of a micromixer can be significantly increased by the application of external energy sources, leading to a non-static flow and mixing process. In this work, a T-shaped micromixer with a meandering channel is considered. A periodic pulse function for the inlet pressure is numerically optimized w.r.t. frequency, amplitude and shape. Therefore, fluid flow and particle concentration are simulated three-dimensionally with the Lattice Boltzmann method (LBM). Forward Automatic Differentiation (AD) allows a generic application of fast gradient-based optimization schemes which is not bound to a specific application. The mixing quality could be increased by 21.9% in comparison to the static, passive execution. Methodically, the results confirm the suitability of the novel combination of LBM and AD to solve process-scale problems.

Large-Scale Statistical Inverse Problems Governed by PDEs

Maximilian Kruse

Mathematical models governed by partial differential equations (PDEs) play an essential role in science, engineering and economics. To generate meaningful predictions, PDEs need to be equipped with possibly uncertain initial, boundary or coefficient functions. The determination of these functions is facilitated by the vast amount of observational data that is typically available for the systems under consideration.

In this work, we employ a Bayesian approach to determining the unknown constituents of PDE models from potentially noisy data of the system output. Beyond point estimates, the Bayesian framework allows for uncertainty quantification in the inferred variables. Thus, we can measure the reliability of our estimates under the umbrella of probability theory. Bayesian inference further guides the choice of norms and regularization terms that need to be established in a -to some extent- ad hoc fashion for deterministic inverse problems.

We present a theoretical setup for Bayesian inverse problems on function spaces, which defers discretization to the latest possible moment. This paradigm guides the development of solution algorithms whose performance does not deteriorate for large-scale problems. We further discuss such algorithms, namely optimization- and sampling-based inference procedures. Lastly, we present computational results for some exemplary applications.

Monotonicity in inverse scattering for Maxwell's equations

Annalena Albicker

We consider an inverse scattering problem for time-harmonic Maxwell's equations in unbounded free space. The goal is to recover the position and shape of scattering objects by means of far field observations of the scattered electromagnetic waves. The media are supposed to be penetrable, non-magnetic and non-absorbing but the electric permittivity may be inhomogeneous inside the scattering objects. First, we establish monotonicity relations for the eigenvalues of the far field operator which maps superpositions of plane wave incident fields to the far field patterns of the corresponding scattered waves. In addition, we discuss the existence of localized vector wave functions that have arbitrarily large energy in some prescribed region whereas at the same time having arbitrarily small energy in some other prescribed region. Combining the monotonicity principle and the localized vector wave functions leads to rigorous characterizations of the support of the scattering objects. Finally, we present shape reconstruction algorithms and give numerical examples to illustrate the reconstruction procedure. This poster is based on a joint work with Roland Griesmaier.

Stable finite element approximations for cardiac elastomechanics

Laura Stengel

Computer models of the human heart are used for a better understanding of the cardiac function. Since the objective of these models is to be used in a clinical setting a compromise between computational cost and numerical accuracy is needed. Due to the high mathematical complexity of the underlying model, the finite element discretization commonly used is insufficient to obtain a good compromise between efficiency, reliability and accuracy.

Thus, we investigate three different spatial discretization approaches, namely the Conforming Galerkin, Discontinuous Galerkin and Enriched Galerkin method. For our computations we solve a commonly used benchmark problem in mechanical cardiac modelling.

We use an idealized left ventricle geometry with the base plane fixed in all directions and a pressure boundary condition applied on the endocardial surface. The passive mechanical behaviour is described by an isotropic hyperelastic and nearly incompressible material model. We compare degrees of freedom, the corresponding computational time and the displacement of the apex location for four different mesh resolutions using linear tetrahedral elements for all approaches, in addition to quadratic elements for the Conforming Galerkin discretization.

We show that the Conforming Galerkin method leads to the occurence of the locking phenomenon for coarse mesh resolutions. The Discontinuous Galerkin approach results in a higher number of degrees of freedom and computational time.

The Enriched Galerkin discretization shows a similiar robustness as the Discontinuous Galerkin method as well as less occurence of the locking phenomenon than in the Conforming Galerkin method.

In conclusion, the Enriched Galerkin approach offers a good compromise between computational cost and numerical robustness.

Mimicking Cochlea Processing using Critically Coupled MEMS Sensors

Folke Rolf

A thermally actuated MEMS sensor with a real time feedback loop is a potential candidate for a bio-inspired acoustic sensor. This comes form the fact, that by feeding back the velocity the damping is changed. Hence, by assigning the feedback strength accordingly two different Hopf bifurcations can be induced. Particularly, this type of bifurcation is assumed to be the essential nonlinearity of the cochlea leading to its remarkable sensing properties, i.e., the response of a system exhibiting a Hopf bifurcation is close to its critical point compressive and frequency selective to an external input. Yet, both Hopf bifurcations have a constant resonance frequency. Therefore, uncoupled MEMS sensors cannot be used to mimic the cochlea processing. However, it is known that the resonance frequency of coupled Hopf oscillators can be tuned by assigning the damping accordingly. Hence, the aim of this work is to analyze the dynamics of two coupled MEMS sensors in terms of the tunability of their resonance frequencies. For this the Hopf bifurcations of this system with respect to the smallest eigenvalue of its adjacency matrix are investigated. It turns out that the system has three Hopf bifurcations, where two bifurcations have a positive bifurcation parameter. Herein, only one of these two bifurcations has a tunable resonance frequency. The theoretical results are confirmed by experimental results.

The Finite Element Library M++

Niklas Baumgarten

On this poster, we present the latest version of the open-source parallel finite 5 element software M++ (Multigrid, Meshes and More) which has been developed within the last 6 15 years at the Karlsruhe Institute of Technology (KIT) by the group of Christian Wieners. As a 7 research code for various applications like cardio-vascular simulations, gas dynamic simulations 8 for carbon capturing, dislocation dynamics, computer assisted proofs and full waveform 9 inversion, it has grown a large array of features. This includes parallel preconditioning, space10 time discretizations, uncertainty quantification and a tutorial on scientific computing for 11 porous media model problems. It has been a central piece in many doctoral theses, serves as a 12 teaching tool for scientific computing and as project code for a practicum on software engineering.

Optimal control of elliptic PDEs under uncertainties using SGD and ADAM

David Schneiderhan

We present the application of the ADAM algorithm for solving an optimal control problem subject to elliptic partial differential equations (PDEs) under uncertainties. In particular, we use a stochastic gradient descent (SGD), similar to the one introduced in the literature and compute individual adaptive learning rates for different parameters from estimates of first and second moments of the stochastic gradient. We compare the results with the SGD and a Monte Carlo based gradient estimation. Therefore, we will take a look onto the convergence in dependency of the computational cost and number of iterations.

Pinning in an extended Lugiato-Lefever model

Lukas Bengel

In applications, locking of the repetition rate of a Kerr soliton comb inside a microresonator by pumping two modes is of particular interest. Mathematically this can be described by a new variant of the Lugiato-Lefever equation (LLE) given by:
$iu_t = -du_{xx} + iV(x)u_x + (\zeta - i)u - |u|^2u + if$, which is a damped and driven nonlinear Schrödinger equation with an additional potential V (x). In the rst part we discuss the existence of nontrivial stationary 2π-periodic solutions of the LLE using bifurcation theory and show

that localized solitons can be found if the potential V (x) has a sign change. In the second part we discuss stability properties of these solutions and show numerical simulations with pde2path that complement our analytical findings.
This is based on a joint paper with Dmitry Pelinovsky (McMaster University) and Wolfgang Reichel (KIT).

Asymptotic-Preserving Dynamical Low-Rank Approximation for Simulation of Marshak Waves

Chinmay Patwardhan

When radiation from a hot source penetrates into a cold material, it gives rise to a wave of thermal energy which propagates into it and travels as radiation heat fronts called Marshak waves. Several phenomena, like supernova explosion or radiation emitted from a hohlraum striking a fusion target, involve the formation of such heat fronts. Mathematically, this process can be modelled by the thermal radiative transfer equations which consist of coupled equations governing the transport of particles and the resulting change in temperature of the material. In several situations, this system is well approximated by a nonlinear diffusion-type equation, known as the Rosseland approximation. This can be obtained as the asymptotic limit of the scaled thermal radiative transfer equations with scaling parameter ε (collision length of particles), i.e. as $\varepsilon \to 0$ the system of equations asymptotically tend to the Rosseland approximation. Simulation of Marshak waves using the scaled equations pose several computational and numerical challenges. First, to resolve the high-dimensional phase space of the problem one requires large memory and computational resources and second, to perform multi-scale simulations stable numerical schemes need to be developed which capture the correct asymptotic limit of the system. In this work we propose to use an asymptotic-preserving (AP) dynamical low-rank approximation (DLRA) scheme based on macro-micro decomposition of the particle density to simultaneously deal with both the challenges. The macro-micro decomposition facilitates the construction of stable AP schemes which correctly captures the dynamics of the system in diffusive ($\varepsilon \ll 1$) and kinetic regimes ($\varepsilon \sim O(1)$). On the other hand DLRA evolves the solution on a low-rank manifold while never computing the full solution which significantly reduces memory and computational requirements. We plan to extend the existing work on AP DLRA schemes for radiation transport to simulate Marshak waves and provide stability results for our new numerical scheme.

Map of transmission coefficients for open bent waveguides with constant curvature

Mariia Sukhova

A free-form waveguide, also called a photonic wire bond, transmits light between different components assembled into a single photonic integrated circuit. Optimization of its shape is necessary to minimize signal losses, and the calculation of the transmission is an essential element in this task. The solution of the complete 3D Maxwell system in a free-formed waveguide requires a lot of computational effort. Therefore, simplified methods are considered to find an effective way to evaluate the transmission. One such method is the multimode approximation, an extension of the fundamental mode approximation. This approach essentially divides the photonic wire bonds into tiny sections. Each section is characterized by a propagation loss because of the finite curvature, and at the interface between consecutive sections, we encounter transmission losses. Tracing the fraction of light that propagates through the free-form waveguide allows for the fast computation of the light transmission. In this work, we present a calculation of transmission coefficients for an interface between two bent waveguide sections of various radii of curvature using semi-analytic solutions. We consider a 2D slab waveguide that supports two guided modes. At the junction of two waveguide sections with different radii of curvature, R_L (left) and R (right), a scattering problem arises, since the guided modes are directly transmitted and coupled to each other. Our goal was to calculate the transmission coefficients t_{11}, t_{22}, t_{12}, and t_{21} for these modes. This calculation was done for pairwise combinations of the radii of the curved segments in a range between 7 µm and 1000 µm. Since the waveguide segments have a constant curvature, we could find a semi-analytic solution following. As a result, we obtained a pre-calculated database of transmission coefficients. The advantage of the semi-analytic approach lies in the sufficient accuracy of the obtained transmission coefficients, which allows the transmission approximation of a free-formed waveguide. The finite element method is used as a reference solution for evaluating the transmission of waveguides with varying curvature.

Simulation of the Deformation for Cycling Chemo-Mechanically Coupled Battery Active Particles with Mechanical Constraints

Raphael Schoof

One of the key technologies for storing energy in our modern world are lithium-ion batteries due to their properties of higher energy density and longevity. However, mechanical degradation is one crucial aging

mechanism. For example, there is a volume change of around 10 % for graphite, but for silicon there is a volume change up to 300 %. Especially, the occurring stresses are critical if the electrode particle is restricted to a limited surrounding, e.g., due to the material structure or the current collector. This can end in particle fracture if the mechanical stresses are too large. Coupling lithium diffusion and large deformations the particle model is based on a thermodynamically consistent transport theory with a common free energy density. A solid solution approach models the diffusion and a finite deformation theory characterizes the displacements for cycling a representative battery active particle. This model is extended by an obstacle contact to incorporate the restricted swelling. The resulting model approach features a variational inequality for the displacement. Therefore, we use the concept of the primal-dual active set algorithm to deal with the particle contact. An efficient adaptive numerical solution algorithm in space and time is used overcoming the limits for application cases. In addition, a parallel distributed memory implementation offers the possibility to examine a larger range of electrode particle shapes. In the end, physical and numerical aspects of the model and the solver for different battery active particles like graphite or silicon are studied and compared. The different properties of cathode particles and different shaped obstacles lead to various interrelation between the host material and the mechanical constraints. The efficient adaptive solution algorithm as well as the parallel distributed memory implementation allow further the investigation of computationally intensive parameter regimes and two and three-dimensional particle geometries.

Fully 3D spatio-temporal resolved models of virus replication evaluated at realistic reconstructed cell geometries

Markus M. Knodel

Virus pandemics and endemics cause enormous pain and costs. Major processes of the intracellular Hepatitis C virus (HCV) viral RNA (vRNA) replication cycle are restricted to the 2D Endoplasmatic Reticulum (ER) manifold, while others take place in the 3D cytosol volume. Modeling the interplay of the major components of the vRNA replication cycle with partial differential equations (PDEs), we establish a system of surface PDEs (sufPDEs) for effects restricted to manifolds coupled to PDEs describing volume effects. Using the diffusion coefficient of viral proteins which we estimated based on experimental data, we discretize the populationdynamics inspired nonlinear diffusion-reaction equation PDE/sufPDE system with the aid of a vertex-centered Finite Volume scheme and evaluate it at unstructured grids representing data based realistic reconstructed cell geometries. We describe the numerical techniques applied and demonstrate the numerical robustness of our simulations. Our framework might contribute to efficient development of antiviral drugs and potent vaccines.

A Machine learning algorithm for Rift Valley fever outbreaks prediction and classification in Kenya

Damaris Mulwa

Rift Valley Fever (RVF), one of the most devastating climate sensitive zoonosis has been reported in kenya in the last four years. A data bank maintained by the International Livestock Research Institute (ILRI) in Kenya has information that can be utilized to forecast the occurrence of Rift Valley Fever using machine learning methods. No research has been done utilizing machine learning to simulate the prediction of an RVF outbreak in kenya, according to literature reviewed. This research used five machine learning models to model the outbreak of RVF using climate data from the year 1981 to 2010. The machine learning techniques used were Naive Bayes (NB), Support Vector Machine (SVM), Logistic regression, Random Forest and Artificial Neural Network. The results of the research showed that Random Forest had the best accuracy on the testing data set of 89.80% and thus Random Forest is the best model to predict RVF outbreak considering the data in question, SVM with polynomial kernel is the second best model with an accuracy of 88%, Logistic regression was the third best model with an accuracy of 85.7%, Naive Bayes was the fourth best model with an accuracy of 84.7% and ANN was the fifth best model with an accuracy of 83.7%. The accurate prediction of RVF outbreak in a county that has had past severe outbreaks of RVF will have a great help in the optimizing the disease management. The proposed model can assist the decision making by the government of kenya and other countries at large by early prediction of when an outbreak can happen.

Uncertainty quantification for data-driven weather models

Christopher Bülte

Data-driven machine learning methods for weather forecasting have experienced a steep progress over the last years, with recent studies demonstrating substantial improvements over physics-based numerical weather prediction models. Beyond improved forecasts, the

major advantages of purely data-driven models are their substantially lower computational costs and faster generation of forecasts once a model has been trained. However, in contrast to the now widely-used ensemble forecasts from physical weather models, most efforts in data-driven weather forecasting have been limited to deterministic, point-valued predictions only, making it impossible to quantify forecast uncertainties which is crucial in research and for optimal decision making in applications. Our overarching aim is to evaluate and compare methods for creating probabilistic forecasts from neural networkbased weather models. Specifically, we compare approaches for quantifying forecast uncertainty based on generating ensemble forecasts from data-driven weather models via perturbations to the initial conditions, as well as applying statistical post-hoc uncertainty quantification methods, using data-driven forecasts from Nvidia's FourCastNet model as a case study. In addition to generating probabilistic predictions, such approaches further allow for investigating optimal "hybrid" combinations between physical and machine learning models for weather prediction.

Study of random w-trees and automaton synchronization

Attila Genda

This work focuses on examining the synchronization properties of repeated words of length k on deterministic finite automata of size n, utilizing both numerical and analytical approaches. We introduce a polynomial algorithm ($O(n^2)$) that leverages w-trees to identify short synchronizing words. Our algorithm can find synchronizing words of lengths proportional to $\sqrt{n} \log n$, even for automata with several hundred thousand states. Additionally, we present experimental results on the height of w-trees, revealing that the average tree height follows a pattern of $O(\sqrt{n}/k)$. Moreover, this study incorporates modeling the random DFA synchronization process using Markov chains. We provide empirically justified estimates for the mean shortest synchronizing word length. These estimates indicate a proportional relationship between the shortest resetting word length and the square root of the automaton size.

We confirm the theoretical results from the literature on the height of w-trees $H(n, k)$ by fitting experimentally obtained data on the median tree height. When $k = 1$, this result shows a good agreement with the theoretical result on the mean height of labeled trees $E(H(n, 1)) \sim 2.50663\sqrt{n}$.

Furthermore, we demonstrate by experimental means that for large n synchronization of uniform random automata by consecutive application of random letters does not depend significantly on the size of the underlying alphabet. This observation allows us to effectively approximate the shortest synchronizing word length by a Markov chain-based, semi-analytic model.

Analysis of Earthquake Forecasting in Italy

Kristof Kraus

We evaluate individual and ensemble model forecasts submitted to the Italian experiments of the Collaboratory for the Study of Earthquake Predictability (CSEP). The models produce forecasts for the mean number of earthquakes in a collection of grid cells during the subsequent seven-day period. The comparison is based on consistent scoring functions for means, which are widely used, theoretically principled tools for forecast evaluation. In combination with isotonic regression, we provide both quantitative and qualitative (graphical) assessments of the forecasts' strengths and weaknesses in terms of calibration and discrimination. In particular, we show where and how models outperform their competitors.

TEEMLEAP - A new TEstbed for Exploring Machine LEarning in Atmospheric Prediction

Jannik Wilhelm

The TEEMLEAP project is fostering the collaboration between scientists from the KIT centers Climate and Environment (ZKU) and Mathematics in Sciences, Engineering, and Economics (MathSEE). Recently, the researchers have established a first version of an idealized – yet realistic – testbed for exploring Machine Learning (ML) in weather forecasting.

Numerical weather prediction (NWP) models still exhibit systematic errors caused by simplified representations of physical processes, assumptions about linear behavior and the challenging task to integrate all available observational data. In contrast to weather services, which naturally focus on improvements of NWP models in their full complexity, with the testbed TEEMLEAP intends to provide a platform for evaluating application possibilities and potential benefits of ML along the entire process chain of weather forecasting. The testbed currently consists of the following elements: (1) Pseudo-radiosounding observations generated from ERA5 reanalysis data (vertical profiles of air temperature, humidity, pressure and wind) (2) Data assimilation coding environment (DACE) of the German Weather Service (DWD) (3) Icosahedral nonhydrostatic (ICON) modelling framework of DWD (4) Innovative statistical and ML-based methods for post-processing.

The researchers investigate in the first pilot experiments, whether weather forecasts were more skillful, if radiosounding sensors would measure more precisely or if more radiosoundings were regularly launched over the entire globe. The influence of the ICON model resolution and assimilation frequency (How often does ICON get information from the radiosoundings?) is studied as well. In addition, post-processing techniques will be employed to examine the potential for reducing forecast errors a posteriori.

TEEMLEAP aims to provide guidance and advice to weather services by developing a measure for the cost-benefit ratio of the different experiment forecasts, and by exploring to which parts of the forecast chain the forecast skill is most sensitive.

We will show and discuss experiment results, and illustrate ideas and possibilities for further testbed applications.

Bayesian inference for functional extreme events defined via partially unobserved processes

Max Thannheimer

In order to describe the extremal behaviour of some stochastic process X approaches from univariate extreme value theory are typically generalized to the spacial domain. Besides max-stable processes, that can be used in analogy to the block maxima approach, a generalized peaks-over-threshold approach can be used, allowing us to consider single extreme events. These can be flexibly defined as exceedances of a risk functional ℓ, such as a spatial average, applied to X. Inference for the resulting limit process, the so called ℓ-Pareto process, requires the evaluation of $\ell(X)$ and thus the knowledge of the whole process X. In practical application we face the challenge that observations of X are only available at single sites. To overcome this issue, we propose a two-step MCMC-algorithm in a Bayesian framework. In a first step, we sample from X conditionally on the observations in order to evaluate which observations lead to ℓ-exceedances. In a second step, we use these exceedances to sample from the posterior distribution of the parameters of the limiting ℓ-Pareto process. Alternating these steps results in a full Bayesian model for the extremes of X.

Robust Data-Driven Coarse-Graining for Surrogate Modeling

Jaroslav Borodavka

In many applications of the natural sciences, models are employed which are based on processes occurring across different length and time scales. While these multiscale systems may be constructed and modeled in several ways, an important class are those described by (random) dynamical systems, in particular stochastic differential equations. For such multiscale systems it is possible to rigorously derive a so-called surrogate (or effective) model, a simplified reduced order model that captures the system's most dominant features. However, oftentimes it is not feasible to derive closed-form expressions for the drift and diffusion coefficient of the surrogate model analytically, because of the complexity of the underlying multiscale system or simply because the full model is not completely known. In this case one would resort to a data-driven modeling strategy in order to estimate the drift and diffusion coefficient of the surrogate model from observations of the multiscale system.

It has been shown that standard statistical learning techniques fail to provide consistent estimates when confronted with such observations. The maximum likelihood estimator is an example of a well-established statistical learning estimator that fails to converge for multiscale observations. In order to overcome these recent drawbacks, we are, in this project, mainly concerned with the development of novel unbiased and effective data-driven training strategies for the identification and analysis of surrogate models for complex multiscale stochastic differential equations. To tackle this problem, we will opt for different approaches in different settings, such as sparsity-constrained semi-parametric inference; data-subsampling regularization techniques for the MAP estimator in a hierarchical Bayesian framework; or a non-parametric Bayesian framework in a function space setting where we aim to develop an effective regularization for the prior measure of the drift function so that the posterior measure converges under multiscale observations in a suitable sense.

MS/MS Prediction in Metabolomics with Kernels

Nils Koster

We introduce a novel and flexible approach to predict the fragmentation spectra of small-molecule metabolites. This task is essential in metabolomics as it allows for much faster identification of a given compound while heavily reducing the cost of analysis with expensive hardware. While the direct approach, predicting the compound given some mass spectrum is well-studied, we tackle the reverse problem. First, we probabilistically predict the respective spectrum given each likely compound, which are encoded in a commonly used embedding. Second, given all predicted

spectra, we select the k most similar to the observed one. This allows us to solve a variety of different tasks, including fragmentation simulation, spectrum annotation and search for a given molecule. Recent advances in kernel methods allow us to efficiently harness great probabilistic predictive power and interpretability.

Generalized polynomial chaos based Lattice Boltzmann method

Mingliang Zhong

Computational fluid dynamics (CFD) already shows great achievement in the industry via the deterministic method. However, uncertainty still exists between the fluid mechanic model and real physics. It generally comes from three aspects: measurement errors, physical models, and computational errors. The non-intrusive method, which uses the developed model as the deterministic method, is the most straightforward way to quantify the essence and influence of uncertainty. After sampling the uncertain parameters and substituting them into the model for numerous simulations, the results are statistically analyzed to determine the quantity of interest. The most well-known nonintrusive method is the Monte Carlo method, however, it is also too expensive to apply to the CFD. In comparison, the generalized polynomial chaos (gPC)-based method can achieve comparable accuracy at a significantly lower cost. In this study, the Lattice Boltzmann method (LBM) is selected as the deterministic method, and we use the gPC-based stochastic collocation method to estimate the uncertainty. We also first propose an intrusive stochastic Galerkin (SG) gPC-based method on LBM. The CFD benchmark test cases, lid-driven cavity flow and flow past a circular cylinder are selected. Our research's outcomes are more effective than those obtained using the Monte Carlo method, with the same accuracy.

A Wasserstein perspective of Vanilla GANs

Lea Kunkel

In recent years the empirical success of Generative Adversarial Networks (GANs) caused an increasing interest in theoretical research. The statistical literature is mainly focused on Wasserstein GANs and generalizations thereof, which especially allow for good dimension reduction properties. However, statistical results for Vanilla GANs, the original optimization problem, are still rather limited and require assumptions such as smooth activation functions and equal dimensions of latent and ambient space. To bridge the gap, we draw a connection from Vanilla GANs to the Wasserstein distance. By doing so, problems caused by the Jensen-Shanon divergence can be avoided and existing results for Wasserstein GANs can be extended to Vanilla GANs. In particular, we obtain an oracle inequality for Vanilla GANs in Wasserstein distance.

Thursday 28th September

11:00 – 12:00

Parallel sessions

Shapes, Approximations and Optimisation I
Room 0.016
Chair: Christian Füllner

Efficient A-Optimal Bayesian Experimental Design using Projection-Based Conditional Expectation Approximation (PACE)
Vinh Hoang

We address the computational efficiency of the A-optimal Bayesian design of experiments based on computationally expensive partial differential equations. A-optimality is a widely used criterion in Bayesian experiment design, aiming to minimize the expected conditional variance and find the optimal design. We propose a novel likelihood-free method for the A-optimal experiment design that does not require sampling or approximating the Bayesian posterior distribution, avoiding issues with posterior intractability. Our approach leverages two principle properties of the conditional expectation: the law of total variance and the orthogonal projection property. By utilizing the law of total variance, we obtain the expected conditional variance through the variance of the conditional expectation. Furthermore, we exploit the orthogonal projection property to approximate the conditional expectation using regression, eliminating the need for likelihood function evaluation. To implement our approach, we employ deep artificial neural networks (ANN) for approximating the nonlinear conditional expectation. Particularly for continuous experimental design parameters, we integrate the minimization of the expected conditional variance into the training process of the ANN-based approximation. This integration is enabled by the shared objective function, leading to improved algorithm efficiency. Through numerical experiments, we demonstrate that our method significantly reduces the number of computationally expensive forward-model evaluations compared to common likelihood-based approaches, effectively overcoming a significant bottleneck.

On the Uniqueness of Equilibrium Prices in a Bayesian Assignment Game
Damián-Emilio Gibaja-Romero

In the Assignment Game, introduced by Shapley and Shubik (1971), most solution concepts yield a multiplicity of solutions under which comparative statics are not naturally developed. To guarantee the uniqueness of equilibrium, we study a Bayesian Assignment Game where neither buyers nor sellers know the valuation of other players, sellers set prices after observing their valuations, and goods are allocated whenever a buyer pays the price. So, the expected utility of each seller is invariant concerning the buyer who gets her good. Based on the Intermediate Value Theorem for Improper Integrals, we derive conditions on the distribution of valuations to demonstrate that each seller's best response is independent of other sellers' decision rules since the probability of goods being individually rational is proportional to the probability of being ranked at any position in the buyers' preference list. Moreover, the seller's best responses are fixed points of the reverse hazard rate function. So, the equilibrium price vector is unique when the reverse hazard rate is a contraction.

Consequently, comparative statistics are naturally developed. As expected, for example, the relationship between equilibrium prices and valuations is positive. Finally, we provide a closed-form equilibrium price vector when valuations follow an exponential distribution. In this setting, prices have a negative relation with respect to the parameter's distribution.

Exploring Challenges and Advancements in Absolute Value Equations
Hossein Moosaei

Absolute value equations (AVE) are seemingly straightforward yet pose significant computational challenges as they are NP-hard and non-differentiable problems. Over the past few decades, researchers have increasingly focused on studying AVE. The study of AVE has gained prominence due to its inherent complexities. Researchers have investigated various aspects of AVE, including theoretical foundations, solution methodologies, and practical implications. Despite the progress made, several challenges remain unaddressed, and open problems persist in the field of AVE. These challenges and open problems serve as catalysts for future research, encouraging scholars to delve deeper into the complexities of AVE and propose innovative solutions. This talk offers a comprehensive overview of the related works in this field. By identifying challenging issues and highlighting open problems, this presentation sets the stage for future research directions, and researchers can pave the way for further progress in solving these complex equations.

Simulation of lithium ion batteries
Room 2.066
Chair: Fabian Castelli

Efficient Simulation of Chemo-Elastic-Plastically Coupled Battery Active Particles

Raphael Schoof

Next-generation lithium-ion batteries with anode materials such as silicon are preferred due to a higher energy density. However, this benefit comes at the cost of volume expansions up to 300% and large mechanical stresses that lead to plastic deformation of the material. This is especially crucial for fast charging of the battery at higher C-rates since fast charging results in larger stresses and therefore in an earlier starting of plastic deformation changing the material behavior. We build on a thermodynamically consistent continuum model approach considering chemical, elastic and plastic effects during charging and discharging of a representative battery active particle. Due to the large volume increase of silicon, a finite deformation approach is reasonable. The plastic modeling compares ideal plastic and viscoplastic behavior as well as linear isotropic hardening. Plastic material behavior results in solving the corresponding classical loading and unloading conditions expressed via the Karush–Kuhn–Tucker (KKT) conditions. Since accurate one-dimensional simulations already need high computational costs, higherdimensional geometrical setups and long-term studies of a few cycles of charging and discharging are not feasible with reasonable effort. With an efficient finite element approach, an adaptive solution algorithm from the literature and the used concept of static condensation for the plasticity treatment, we are able to overcome this limitation. The usage of parallel programming capacities for a further simulation speedup enables the study on the effect of plastic behavior in long-term cyclings in different two- and three-dimensional examples and computationally demanding parameter regimes within a reasonable simulation time.

A PINN-based LOD for the solution of multiscale problems

Mehdi Elasmi

Several real world applications have a multiscale nature, meaning that their overall behavior is typically determined through an interplay of different effects stemming from multiple length and/or time scales. The numerical simulation of such problems using standard (monoscale) methods requires resolving the characteristic features on the finest relevant scale, which is computationally either not feasible or very expensive. Nevertheless, various multiscale methods have been developed to effectively simulate the global behavior for this kind of problems with a coarse mesh. These methods rely on homogenization techniques, which can be either numerical or analytical, i.e., based on homogenization theory provided some additional structure such as periodicity and scale-separation is available. For the sake of generality, we opt for a numerical homogenization approach. In particular, we consider the Localized Orthogonal Decomposition (LOD), which relies on the decomposition of the exact solution into macroscopic and microscopic contribution. To this end, the resolution of several localized sub-problems, called correction problems, is required. Obviously, this could also pose a computational challenge in the presence of rough and unstructured materials. In this work, we intend to enhance and accelerate the LOD method by using deep learning techniques to compute the local correction problems. In particular, we employ for this Physics-Informed Neural Networks (PINNs). A PINN extends the data-based black box approach of classical neural networks to a gray box approach by incorporating the governing equations of a problem into the loss function. This allows the reduction of the amount of data needed for the training procedure, and guarantees physically and mathematically consistent results. Overall, we observe through various examples that the coupling of LOD with PINNs in an online-offline scheme reveals to be a promising alternative and should be further investigated.

Microstructure Simulation of Lithium-Ion Battery Degradation due to Solid Electrolyte Interphase Growth

Falco Schneider

Lithium-ion batteries are currently a key technology for energy storage solutions. They can be used as stationary storage for renewable energies, but also as a power source in battery electric vehicles and consumer electronics, due to their relatively high energy and power density. While lithium-ion batteries have been extensively studied and developed over the last decades, the exact causes and relations of physical degradation effects inside the batteries are still an area of active research.

In this work we consider a detailed physical model which characterizes the electrochemical transport on the spatially resolved three-dimensional electrode microstructures within a lithium-ion battery cell. The model is given as a coupled system of nonlinear partial differential equations which describe the evolution of the lithium concentration and the Maxwell potential

inside the battery. In order to account for cell degradation, a model extension is considered which captures the growth of the solid electrolyte interphase (SEI), a thin layer coating the anode surface and one of the major degradation effects causing capacity and power fade of the cell over its lifetime. This introduces additional computational variables for the local SEI thickness and current density along the anode surface area. The growth of the SEI is characterized by ordinary differential equations, while the local current densities are given implicitly through algebraic equations, further increasing the complexity of the mathematical system to solve.

This model extension poses a challenge for common monolithic solution approaches, due to the addition of a slow characteristic time scale and a saddle-point structure. We address this issue, by deploying a semi-implicit solution scheme for the coupled model of cell transport and degradation. Finally, we will present some exemplary simulation results.

Forecast Evaluation: Theory
Room 2.058
Chair: Fabian Krüger

Characterization of translation invariant MMD on R^d and connections with Wasserstein distances

Clement Dombry

Kernel mean embeddings and maximum mean discrepancies (MMD) associated with positive semi-definite kernels are important tools in machine learning that allow to compare probability measures and sample distributions. Two kernels are said equivalent if their associated MMDs are equal. We characterize the equivalence of kernels in terms of their variogram and deduce that MMDs are in one to one correspondence with negative semi-definite functions. As a consequence, we provide a full characterization of translation invariant MMDs on R d that are parametrized by a spectral measure and a semi-definite symmetric matrix. Furthermore, we investigate the connections between translation invariant MMDs and Wasserstein distances on R d . We show in particular that convergence with respect to the MMD associated with the Energy Kernel of order $\alpha \in (0, 1)$ implies convergence with respect to the Wasserstein distance of order $\beta < \alpha$. We also provide examples of kernels metrizing the Wasserstein space of order $\alpha \geq 1$.

Quantile-based approximation and decomposition of the Cramér distance

Johannes Resin

The Cramér distance (CD), also referred to as the integrated squared distance, is a commonly used distance between probability distributions. In the context of probabilistic forecasting, it can be used both to assess the similarity between different forecast distributions and to compare a posited distribution with the empirical distribution of a sample. We investigate a quantile-based representation of the CD, which is useful in two ways. Firstly, the representation gives rise to a quantile-based approximation of the CD, which can be used if forecast distributions are provided as quantiles at pre-specified levels and has the desirable property of being a k-proper divergence. Secondly, the alternative representation can be decomposed into four components, which capture shifts and differences in dispersion between the two distributions. We demonstrate the merits of the quantile-based approximation and its decomposition in applications from climatology, epidemiology and economics.

Asymptotics and Asymmetries of the Coefficient of Predictive Ability (CPA): Bridging Correlation and Discrimination Ability

Andreas Eberl

The Receiver Operating Characteristic (ROC) curve and the area underneath it (AUC) are popular tools to evaluate the discrimination ability of binary probability forecasts. Gneiting and Walz (2022) have recently proposed the coefficient of predictive ability (CPA) as a generalization of the AUC beyond the case of a binary predictand. In the case of non-tied observations, the CPA is equivalent to Spearman's rank correlation between forecasts and realizations. This talk discusses population versions of the empirical CPA. Two different, irreconcilable versions are obtained depending on whether the underlying distribution is continuous or discrete. While the continuous version is again equivalent to Spearman's rank correlation, the discrete version is asymmetric and reduces to the highly asymmetric AUC as a special case. Considering distributions that fall in between the two extremes of continuous and binary generates insights on how discrimination ability turns into correlation, and how asymmetry turns into symmetry.

Health Statistics
Room 2.059
Chair: Johannes Bracher

A stochastic hierarchical model for low grade glioma evolution

Amira Meddah

A stochastic hierarchical model for the evolution of low grade gliomas is proposed. Starting with the description of cell motion using a piecewise diffusion Markov process (PDifMP) at the cellular level, we derive an equation for the density of the transition probability of this Markov process based on the generalised Fokker–Planck equation. Then, a macroscopic model is derived via parabolic limit and Hilbert expansions in the moment equations. After setting up the model, we perform several numerical tests to study the role of the local characteristics and the extended generator of the PDifMP in the process of tumour progression. The main aim focuses on understanding how the variations of the jump rate function of this process at the microscopic scale and the diffusion coefficient at the macroscopic scale are related to the diffusive behaviour of the glioma cells and to the onset of malignancy, i.e., the transition from low-grade to high-grade gliomas.

Extended Excess Hazard Models for Spatially Dependent Survival Data

André Victor Ribeiro Amaral

Relative survival represents the preferred framework for the analysis of population cancer survival data. The aim is to model the survival probability associated to cancer in the absence of information about the cause of death. Recent data linkage developments have allowed for incorporating the place of residence or the place where patients receive treatment into the population cancer data bases; however, modeling this spatial information has received little attention in the relative survival setting. We propose a flexible parametric class of spatial excess hazard models (along with inference tools), named “Relative Survival Spatial General Hazard” (RS-SGH), that allows for the inclusion of fixed and spatial effects in both time-level and hazard-level components. We illustrate the performance of the proposed model using an extensive simulation study, and provide guidelines about the interplay of sample size, censoring, and model misspecification. We present two case studies, using real data from colon cancer patients in England, aiming at answering epidemiological questions that require the use of a spatial model. These case studies illustrate how a spatial model can be used to identify geographical areas with low cancer survival, as well as how to summarize such a model through marginal survival quantities and spatial effects.

Collaborative nowcasting of COVID-19 hospitalization incidences in Germany

Daniel Wolffram

Real-time surveillance is a crucial element in the response to infectious disease outbreaks. However, the interpretation of incidence data is often hampered by delays occurring at various stages of data gathering and reporting. As a result, recent values are biased downward, which obscures current trends. Statistical nowcasting techniques can be employed to correct these biases, allowing for accurate characterization of recent developments and thus enhancing situational awareness. In this paper, we present a preregistered real-time assessment of eight nowcasting approaches, applied by independent research teams to German 7-day hospitalization incidences during the COVID-19 pandemic. This indicator played an important role in the management of the outbreak in Germany and was linked to levels of non-pharmaceutical interventions via certain thresholds. Due to its definition, in which hospitalization counts are aggregated by the date of case report rather than admission, German hospitalization incidences are particularly affected by delays and can take several weeks or months to fully stabilize. For this study, all methods were applied from 22 November 2021 to 29 April 2022, with probabilistic nowcasts produced each day for the current and 28 preceding days. Nowcasts at the national, state, and age-group levels were collected in the form of quantiles in a public repository and displayed in a dashboard. Moreover, a mean and a median ensemble nowcast were generated. We find that overall, the compared methods were able to remove a large part of the biases introduced by delays. Most participating teams underestimated the importance of very long delays, though, resulting in nowcasts with a slight downward bias. The accompanying prediction intervals were also too narrow for almost all methods, but incorporating un- certainty quantification using past real-time nowcast errors proved advantageous when compared to the standard model-based uncertainty intervals. Averaged over all nowcast horizons, the best performance was achieved by a model using case incidences as a covariate and taking into account longer delays than the other approaches. For the most recent days, which are often considered the most relevant in practice, a mean ensemble of the submitted nowcasts performed best. We conclude by providing some lessons learned on the definition of nowcasting targets and practical challenges.

Thursday 28th September

15:45 – 17:05

Parallel sessions

Shapes, Approximations and Optimisation II
Room 0.016
Chair: Markus Gabl

Maximizing the electromagnetic chirality for metallic nanowires in the visible spectrum
Marvin Knöller

Electromagnetic chirality describes differences in the interaction of scattering objects with electromagnetic fields of different helicity. If the scattering behavior of an object with respect to incident waves of one helicity cannot be reproduced with incident fields of the opposite helicity, then the object is said to be electromagnetically chiral (emchiral), otherwise it is called em-achiral. Em-chirality can be quantified by chirality measures that attain the value 0 for an em-achiral object and the value 1 for a maximally em-chiral object. We study a shape optimization problem, where the goal is to construct thin metallic nanowires that exhibit large measures of em-chirality at a given frequency. We present a gradient based optimization method, based on an asymptotic representation formula for approximating scattered fields due to thin metallic scattering objects. In the visible range, the metallic nanowires obtained by our optimization scheme, exceed the chirality values attained by traditional metallic helices.

Optimal design of obstacles with respect to their electromagnetic chirality
Raphael Schurr

We consider the scattering of time harmonic electromagnetic waves by perfectly conducting or penetrable objects. Such an object is called electromagnetically chiral if the scattering response from incident fields with one pure helicity (direction of circular polarization) cannot be reproduced with incident fields of the opposite helicity. The complete scattering response of a scatterer can be described by the far field operator which can in turn be split into operators describing the contributions for each incoming and outgoing helicity. The goal of our research is to develop methods that optimize the shape of the scatterer such that its electromagnetic chirality becomes maximal. Such methods typically involve derivatives of the far field operator. We hence prove its Fréchet differentiability. In the numerical experiments we restrict the observation to either starshaped or to tube-like objects. We obtain higher electromagnetic chirality from the latter, however, the numerical approach is much more costly.

Concave tents: a new tool for optimizing nonlinear convex functions over nonconvex sets
Markus Gabl

Optimizing a nonlinear, convex function over nonconvex sets is challenging since solving convex relaxations where the nonconvex set is approximated by its convex hull may produce substantial relaxation gaps and infeasible solutions, which have to be "rounded" to a feasible one, often with uncontrollable losses in performance. For this reason the aforementioned convex hulls are especially useful if the objective function is linear or even concave, since concave optimization is invariant to taking the convex hull of the feasible set. We propose the notion of concave tents, which are concave overestimators of the convex objective function that agree with the objective function on the feasible set, that allow for concave reformulations of the problem. We derive ways to construct these concave tents under very mild assumptions as the optimal value function of conic optimization problems. Hence, evaluating our concave tents requires solving a conic problem. Interestingly, we can find super-derivatives by solving the conic dual problem, so that differentiation is of the same complexity as evaluation. For feasible sets that are contained in the extreme points of their convex hull we construct these concave tents in the original space of variables. For general feasible sets we propose a double lifting strategy, lifting hte optimization problem into a higher dimensional space in which the concave tent can be constructed just as easily. The construction of the concave tents as well as the double lifting strategy exploit copositive optimization techniques so that our exposition establishes a connection between copositive optimization and nonlinear convex optimization and expands the applicability of the copositive optimization paradigm substantially. Preliminary applications and numerical experiments show that these concave tents can be useful e.g. in global optimization where they allow us to use techniques like Frank-Wolfe algorithms, in areas where they have so far not been applicable.

Experiments in small scale fluid dynamics

Room 2.066
Chair: Bettina Frohnapfel

Phase-Sensitive, Active Microrheology via Probe-Free Application of Thermoviscous Flows

Iliya Stoev

We recently found how thermoviscous expansion phenomena give rise to a new, contactless particle trap that is characterised by a linear force-extension relationship and can therefore be employed in non-invasively measuring femtonewton forces with thermally limited sensitivity. Our new forcemeasurement method is based on optically generated flows, thereby lifting prerequisites related to the probe material and resulting in only moderate heating at the position of the micromanipulated object. This methodology offers an appealing alternative to the use of optical tweezers in highly delicate samples and living systems. Next, we asked the question if our thermoviscous flows can be used to obtain more quantitative data and possibly demonstrate the equivalence between flow-driven and force-driven rheology in their ability to extract phase angles as a measure of relative mechanics. With our new flow-based and phase-sensitive microrheology, we provide access to the mechanics of highly viscous media, tenuous gels and even cellular cytoplasm. Further refinements of the method aim at multiplexing and removing the need for using fluorescent tags.

Simulation of 3D Interferometric Particle Imaging Experiments for the Measurement of Multi-Phase Flows

Christian Sax

The investigation of bubbly flows is of great importance for research areas like fuel cells, electrolysis, cavitation and boiling. A widely used technique for sizing spherical particles is interferometric particle imaging (IPI), which is also utilized to characterize bubbly flows. The technique uses the interference patterns generated by the scattered light at particles to determine their size, and more recently their eccentricity and orientation in space. Current progress focuses on the development of a measurement system that provides information on the flow field of both the liquid and the dispersed phase. However, the optical transfer function describing the scattering of the light at the particles and the formation of the interference patterns is complex and highly non-linear. Consequently, the inverse problem is not easy to formulate. Measurement methods must derive information in the inverse direction. Such algorithms must be able to detect particles, distinguish different types of particles (corresponding to different phases) and analyzing them.

For the development of such algorithms large amounts of test data are required. Test data cannot be obtained experimentally in large quantities, because it requires manual labelling to capture groundtruth information. Instead, a digital twin of the experimental setup is created to obtain synthetic images with known ground-truth properties. The presented simulator builds upon the Debye-series expansion of the Mie-theory and uses the generalized Hyugens-Fresnel integrals to compute the resulting interference patterns. The model is an expansion of previous simulators and uses the linear 1 character of the solution of the Hyugens-Fresnel integrals for the given system. As such, different features from two models can be combined by superposition of the solutions. Further features can likewise be added, which are e.g. several particle types (for multiple phases) and the extension of the previously two-dimensional models to three-dimensionally distributed particles in the test volume.

Modeling flow and slip over superhydrophobic and liquid-infused surfaces via a constant-shear boundary condition

Clarissa Schönecker

Superhydrophobic and liquid-infused-surfaces (LIS) have been widely explored for their ability to reduce drag or to repel aqueous liquids. They rely on a second fluid (mostly air or oil) that is enclosed in the roughness features of a surface, which provides a slip boundary condition to the fluid flowing over the surface. In theoretical models, the interfaces between the main and the secondary fluid are commonly modeled via a Navier slip boundary condition, which relates the fluid velocity to its gradient normal to the surface via a material parameter. This material parameter is called the local slip length and typically assumed to be constant.

Here, we present that assuming a constant-shear boundary condition instead of a constant slip length yields more physical results, especially for higher-viscosity secondary fluids. At the same time, the constant shear can still be expressed as a slip length, such that the derived equations can be intuitively employed. Additionally, the constant-shear approach provides the possibility to derive a variety of new solutions for flows over slippery surfaces via a straightforward superposition approach. As examples of such solutions, we present analytical equations for the flow field and the effective slip length of slippery tubes and annuli.

Modeling flow through slippery pipes – A modernized approach to Philip's classic solution

Sebastian Zimmermann

In 1972, Philip introduced the classical formula for the analytical description of pressure-driven axial pipe flows with mixed no-slip and no-shear boundary conditions. This formula has since become the cornerstone for understanding and modelling various applications, including flow in porous media and flow along superhydrophobic surfaces of circular geometry. In this contribution, we present an alternative derivation and formulation for Philip's solution using the powerful tools of complex analysis, specifically conformal mapping. Central to this novel approach are so-called prime functions, acting as fundamental building blocks of our approach. They generally play a crucial role in solving problems involving multiply connected domains, but receive relatively little attention.

The presented result not only provides a new perspective on modelling pressure-driven flows in circular geometries but also holds the potential for extending these analytical findings to multiply connected domains, such as axially traversed annuli and more. By utilizing the insights gained from our approach, we aim to unlock new possibilities and enhance our understanding of fluid dynamics in circular geometries with heterogeneous boundaries.

Forecast Evaluation: Methods and Applications

Room 2.058

Chair: Marc Pohle

Assessing the calibration of multivariate probabilistic forecasts

Sam Allen

When predicting future events, it is common to issue forecasts that are probabilistic. For probabilistic forecasts to be useful, they must be calibrated, in the sense that they align statistically with the corresponding outcomes. However, while checks for calibration are well established when evaluating univariate forecasts, it is relatively rare to assess forecast calibration in multivariate applications. In this work, we adapt existing definitions of multivariate calibration to generate simple and interpretable checks for calibration that facilitate a more comprehensive understanding of how multivariate forecasts perform. This leads to multivariate rank and PIT histograms that target particular aspects of the multivariate forecasts. We present examples of this in the case of probabilistic spatial field forecasts. We then discuss how we can monitor multivariate calibration over time using e-values. E-values are nonnegative random variables that can be combined multiplicatively to form a test martingale that is suitable for hypothesis testing in sequential settings. We demonstrate the practical utility of this framework by employing these tools to sequentially assess the calibration of probabilistic forecasts for spatial weather fields.

Uncertainty Quantification in Forecast Comparisons

Tanja Zahn

Comparing competing forecasting methods via expected scores is the cornerstone of forecast evaluation. Skill scores or relative expected scores enhance interpretability in that they indicate the relative improvement of a forecasting method over a competitor. At the moment, statistical inference in forecast comparisons is usually restricted to forecast accuracy tests for single forecast horizons, single variables and single locations. We introduce simultaneous confidence bands for skill scores (as well as relative expected scores and score differences) to quantify sampling uncertainty in forecast comparisons. The confidence bands are a simple tool to characterize and represent sampling uncertainty graphically. Further, they can be used for a single variable over multiple forecast horizons or multiple locations or for multiple variables and as such avoid multiple comparison problems. They are applicable for any type of forecast, from mean over quantile to distributional forecasts, and are implemented via a moving block bootstrap. The validity of the bands is ensured by an assumption that is akin to the classical Diebold-Mariano assumption for forecast accuracy tests. We illustrate our methodology in applications to economic and meteorological forecasts, also reinforcing the perils of ignoring sampling uncertainty and the usual multihorizon, multi-location or multi-variable nature of forecast evaluation.

Direction Augmentation in the Evaluation of Armed Conflict Predictions

Lotta Rüter

In many forecasting settings, there is a specific interest in predicting the sign of an outcome variable correctly in addition to its magnitude. For instance, when forecasting armed conflicts, positive and negative log-changes in monthly fatalities represent escalation and de-

escalation, respectively, and have very different implications. In the ViEWS forecasting challenge, a prediction competition on state-based violence, a novel evaluation score called targeted absolute deviation with direction augmentation (TADDA) has therefore been suggested, which accounts for both for the sign and magnitude of log-changes. While it has a straightforward intuitive motivation, the empirical results of the challenge show that a no-change model always predicting a log-change of zero outperforms all submitted forecasting models under the TADDA score. We provide a statistical explanation for this phenomenon. Analyzing the properties of TADDA, we find that in order to achieve good scores, forecasters often have an incentive to predict no or only modest log-changes. In particular, there is often an incentive to report conservative point predictions considerably closer to zero than the forecaster's actual predictive median or mean. In an empirical application, we demonstrate that a no-change model can be improved upon by tailoring predictions to the particularities of the TADDA score. We conclude by outlining some alternative scoring concepts.

Mathematical Statistics and Stochastic Processes
Room 2.059
Chair: Andreas Eberl

Multilevel Monte Carlo methods for parametric expectations: distribution and robustness measures

Sebastian Krumscheid

The multilevel Monte Carlo (MLMC) method is an efficient sampling method for the approximation of expected system outputs and is applicable to a wide range of applications. However, its use for quantities of interest that cannot be expressed as expected values is not straightforward. In this talk, we will discuss recent advances that allow for a more informative characterization of a system output's distribution using the MLMC method. Specifically, we will introduce MLMC techniques for approximating generic parametric expectations, that is, expected values depending on a parameter. The resulting MLMC estimator for functions allows for the derivation of efficient approximations to further characterize a system output's distribution. We will outline a procedure for constructing MLMC estimators for robustness indicators, focusing on those quantifying "tail" risks using quantiles (value-at-risk) or conditional values-at-risk. While these techniques offer near-optimal computational complexity, their direct application may be hindered in practice when relying on the theoretical a priori error estimates. To address this gap, we will present novel computable error estimators for optimally tuning the MLMC methods, leading to an efficient and robust continuation type adaptive algorithm. This is joint work with Q. Ayoul-Guilmard, S. Ganesh, and F. Nobile (EPFL).

Statistical guarantees for stochastic Metropolis-Hastings

Maximilian Steffen

Uncertainty estimation is a key issue when considering the application of deep neural network methods in science and engineering. To this end, numerous Bayesian neural network approaches have been introduced where the main challenge is to construct an algorithm which on the one hand is applicable to the large sample sizes and parameter dimensions of modern applications and which on the other hand admits statistical guarantees. We introduce a version of a stochastic Metropolis-Hastings MCMC sampler which allows for large sample sizes due to the stochastic Metropolis-Hastings step and which can be applied to large parameter dimensions due to a directional noise in the proposal distribution. The statistical properties of the resulting Gibbs posterior distribution are studied in a nonparametric regression setting. We prove a PAC-Bayes oracle inequality which yields optimal contraction rates. Moreover, we analyze the diameter and show high coverage probability of the resulting credible sets.

Continuous-time Mean Field Markov Decision Models

Sebastian Höfer

For many Markovian decision problems, it is reasonable to consider several statistically equal decision makers operating simultaneously on the same state space and interacting with each other (e.g., maintenance of identical machines in a production site, population of potentially infected persons). Depending on the model, the state transition and the profit of the individual may also depend on the empirical distribution of the decision makers across the states. In the limiting case, as the number N of decision makers tends to infinity, we show that the resulting mean-field model describes a classical deterministic control problem, for which the limit state process is characterized by a controlled ordinary differential equation. We show that an optimal control of the mean-field model yields an asymptotically optimal control for the model with N decision makers. In the end when time allows we discuss some applications. The talk is based on a joint work with N. Bäuerle.

Friday 29th September

11:00 – 13:00

Parallel sessions

Shapes, Geometry, Number Theory and Algebra II
Room 2.058
Chair: Andreas Ott

Geodesic Least Squares: Robust Regression Using Information Geometry
Geert Verdoolaege

Geodesic least squares (GLS) is a regression technique that operates in spaces of probability distributions. Based on minimization of the Rao geodesic distance between two probability models of the response variable, GLS is robust against outliers and model misspecification. The method is very simple, without any tuning parameters, owing to its solid foundations rooted in information geometry. In this contribution, we illustrate the robustness properties of GLS using various applications in the fields of magnetic confinement fusion and astrophysics. Additional interpretation is gained from visualizations using several models for the manifold of Gaussian probability distributions. Finally, GLS is shown to compare favorably to other robust regression methods, including minimum distance estimation techniques based on alternative similarity measures.

Capturing Spatiotemporal Signaling Patterns in Cellular Data with Geometric Scattering Trajectory Homology
Dhananjay Bhaskar

Cell signaling plays a critical role in orchestrating the complex interactions and processes necessary for the proper functioning and survival of organisms. This intricate communication system allows cells to perceive and respond to their ever-changing environment by transmitting and processing information through a series of biochemical reactions. Although many signaling molecules and pathways have been identified, the dynamics of signaling processes, including their initiation, propagation, termination, and adaptation, are not yet fully understood. To facilitate quantitative understanding of complex spatiotemporal signaling activity, we developed Geometric Scattering Trajectory Homology (GSTH), a general framework that integrates geometric scattering and topological data analysis (TDA) to provide a comprehensive understanding of complex cellular interactions. This combination allows for the effective capture of both local and global patterns, as well as a robust analysis of the underlying topology. By accounting for the multi-scale nature of cellular interactions and the temporal fluctuations of signaling events, GSTH uncovers the intricate mechanisms that govern cellular communication and coordination. We tested this framework using a variety of computational models and experimental data. Our findings demonstrate that the GSTH-generated trajectory is related to the degree of synchrony, speed, and quasi-periodicity of the underlying signaling pattern. We recovered model parameters and experimental conditions by training neural networks on the trajectory, showing that our approach preserves information that characterizes various cell types, tissues, and drug treatments.

Intersection properties of Brownian motion
Fanqi Meng

Based on the original study started by Lévy, Kakutani, Taylor, Dvoretzky and Erdös, we talk about new way using Hausdorff dimension from fractal geometry and fractal percolation to estimate existence problem of shared common points by independent two or more Brownian motion paths and self-intersection problem of Brownian motion, under the condition of different space dimensions.we show that only if dimension $d \leq 3$, intersection of two Brownian motions is nonempty almost surely and only in case $d = 2$, the intersection of any finite number greater or equal 3 of independent Brownian paths is nonempty almost surely. Since Brownian bridges share intersection properties in common with Brownian motions due to the mutually absolute continuity and intersection equivalence, we can convert self-intersection problem of one Brownian motion path into intersection problem of separated independent Brownian bridges. Moreover we talk about potential application of notions above in intersection properties of random walks.

Inverse Problems
Room 2.066
Chair: Lukas Pieronek

Approximation methods for fast calculation of transmission in multimode waveguides
Maria Paszkiewicz

Approximation methods are favourable for the fast modelling of large optical structures, for which a numerical solution to Maxwell's equations is no longer feasible. In this work, we present a fundamental mode approximation (FMA) based on the literature and its extension to multi-mode approximation (MMA) to describe the light propagation in curved waveguides. In spatial regions with a sudden change in the radius of curvature, light is coupled with a notable amplitude to the higher-order modes, which affects the transmission of the fundamental mode. The latter approximation method intends to overcome limitations of the fundamental mode approximation when the waveguides support multiple modes. The approximation methods reduce computation time from the range of hours to milliseconds. In this talk we will present few examples of curved planar waveguides, for which we computed the approximated transmission and compared the results to numerical simulations performed in the time domain solver CST Microwave Studio, based on Finite Integration Technique (FIT).

Inverse design of polariton cavities

Oliver Kuster

Exciton-polaritons describe a coherent state of strongly coupled excitons and photons inside a semiconductor microcavity. By increasing the density of polaritons a transition into a macroscopically occupied state, the condensate, is possible. This exciton-polariton condensate represents a coupled light-matter state, which is interesting due to its opto-electronic properties. The particular nature of the condensate can generally be described by a non-linear Schroedinger equation, the so called Gross-Pitaevskii equation. As the potential of the Gross-Pitaevskii equation can be mapped to the topography of the microcavity hosting the exciton-polariton condensate, it is possible to design polaritonic devices with a particular functionality. To design these devices we look at a gradient based inverse design method called topology optimisation. The desired functionality of the cavity is encoded into a figure of merit, which is then optimised. Using the gradients of the figure of merit, a local minima is found which represents a particular microcavity design. Here, we present four different exciton-polariton devices which were conceived using topology optimisation: A flat top surface, a phase vortex, a lense and a non-linear beam splitter.

Solving inverse problems posed by laser and particle accelerator diagnostics – what we can and what we need – an application-centered perspective

Erik Bründermann

Real-time diagnostics of electron bunches at near-light speeds in particle accelerators, of the field strengths in accelerator magnets, and of laser properties is key to understanding of the underlying physics and dynamics. It is also the key to performance enhancement and efficient use of particle and photon beams in a wide range of fields in physics, materials and life sciences, medicine and industrial applications. With signal lengths in the picosecond to attosecond range, particle and photon sources now offer signal repetition rates in the MHz and GHz range. A seemingly simple task such as "characterize this beam" in time and space, in polarization and spectral domain, at high repetition rate, over a wide dynamic range and for different time scales, quickly becomes extremely complex. These days, we collect a lot of data very quickly. However, the data is still sparse, mainly because we need to diagnose in real time to avoid missing any of the signals generated. At KIT's MathSEE center, we have started a cooperation with mathematicians for the efficient and, above all, faster solution of inverse problems. We also meet this challenge from the SEE-side by developing ultra-fast, high-throughput diagnostic methods and adapting them for use with multi-dimensional tomography, multi-spectral analysis, synchronous networks of different diagnostic modalities and machine learning. From an application-centered perspective, this presentation will give some examples of inverse problems that we face at particle accelerators and lasers.

Full Waveform inversion and mathematical challenges

Lukas Pieronek

Full Waveform inversion (FWI) is a state-of-the-art geophysical imaging method that exploits seismic measurements to reconstruct shallow earth parameters. Mathematically, this translates into a non-linear inverse problem where the seismic measurements are modeled as solutions to a wave-type system and the searched-for parameters are (some of) the coefficients. In order for numerical solutions to be successful, both the parameter and measurement spaces need to be selected carefully: For instance, the reconstruction of sharp material interfaces requires non-smooth parameter spaces which are numerically difficult to cope with. Likewise, to minimize artifacts and spurious reconstructions, the resulting non-linear objective functional should be as convex as possible, which thus constraints the choice of metrics for the seismic measurements. In this talk, we present novel ideas and solutions regarding these challenges in FWI.

Linear seismic imaging and approximate inversion

Kevin Ganster

In seismic imaging one seeks subsurface material parameters of the earth from measurements of reflected waves. The data is obtained by exciting shockwaves at certain source-positions and record their reflections by receivers. Mathematically we need to solve an inversion problem for the acoustic wave equation and consider a linearization around an a-priori known background velocity. In this talk, we want to provide an overview of the involved steps of the inversion algorithm and present a first application to real-world data.

Enabling Uncertainty Quantification in Scientific Applications

Linus Seelinger

We present a new way to design scientific software, making advanced uncertainty quantification methods available to complex numerical models. Uncertainties arise in many applications in science and engineering, for example due to measurement errors or incomplete knowledge. Quantitatively assessing their impact on model predictions or inferences is crucial in many cases. Solving such uncertainty quantification (UQ) problems often requires combining advanced UQ methods with efficient numerical model solvers, and possibly even moving to high performance computing resources. The resulting technical complexity is currently holding back many interesting applications. UM-Bridge provides an easy to use, language-agnostic link between advanced UQ software packages and numerical models. Due to separation of concerns between UQ experts and model experts, performing UQ on complex models becomes feasible at a fraction of the usual effort. UM-Bridge support in a number of established UQ frameworks offers a wide variety of tools to model experts. Further, UM-Bridge enables the first library of UQ benchmark problems, built by > 15 contributors across > 10 institutions. Beyond linking fields in academia, early industry adoption of UM-Bridge shows that it allows bringing state-of-the-art research closer to real-world applications. In this talk, we give an overview of UM-Bridge and show a number of successful applications. We openly invite further discussion and offer active support in linking fields across MathSEE via UM-Bridge.

Analysis of nonlinear physical systems

Room: 2.067

Chairs: Ivan Fernandez-Corbaton and Nasim Shafieeabyaneh

A Scalar Product for Computing Fundamental Quantities in Matter

Ivan Fernandez-Corbaton

In classical electrodynamics, there exists a convenient and general way to compute the amounts of fundamental quantities such as linear and angular momentum contained in a given dynamic electromagnetic field. The approach exploits the tools of Hilbert spaces. The quantities are computed “a la Dirac” as sandwiches $\langle f|G|f\rangle$, where $|f\rangle$ is the ket representing the field and G is the Hermitian operator representing the quantity of interest, e.g., an angular momentum operator, and the scalar product $\langle f|g\rangle$ is the only one that is invariant under all the transformations in the largest group of invariance of Maxwell equations, the 15-parameter conformal group.

In my talk, I will explain how the algebraic approach can be extended to static material systems, allowing one to compute the amounts of fundamental quantities such as helicity and angular momentum contained in static matter, given its charge and magnetization densities. The extension is achieved by finding a scalar product expression invariant under the 10-parameter static conformal group. Such group is obtained by removing from the 15-parameter version the transformations that are incompatible with the static setting.

We foresee that the methodology will in particular be useful for the design and analysis of experiments involving the switching between stable states of a material system, such as for example when using circularly polarized light for switching the magnetization direction in magnetic films, which indicates a path towards much faster and energy efficient computer memories, and whose underlying mechanisms are under intense scrutiny

Polychromatic T-Matrix: Group-theoretical Perspective and Applications

Maxim Vavilin

As was discovered by Eugene Wigner, physical fields can be classified according to their transformation properties under isometries of space-time: rotations, translations, and Lorentz boosts, which together constitute the Poincare group. The classical free electromagnetic field falls into the zero mass and helicity $\lambda = \pm 1$ class: it can be decomposed as a sum of parts that transform according to such massless unitary irreducible representations of the Poincare group. The coefficients of this decomposition, which are complex scalar functions,

belong to a Hilbert space with a certain scalar product dictated by the representation theory.

Light-matter interactions can be described by means of the scattering operator (S-matrix), or equivalently the transition operator (T-matrix), which maps such Hilbert space onto itself. Recent advances allow one to numerically compute the T-matrices of objects such as molecules, nanoparticles, metasurfaces, and 3D-printed materials. Computations based on the T-matrix produce efficient and accurate predictions of the electromagnetic responses of complicated practical systems, such as for example nano-structured coatings for suppressing light reflection in solar cells, or optical cavities for the enhanced sensing of molecules.

Many theoretical aspects behind the T-matrix method, however, have been limited to monochromatic scattering. In my talk I will show how representation theory can be applied to the T-matrix formalism in order to guide its rigorous extension to the polychromatic domain. I will demonstrate how this allows one to formulate and answer questions such as: given a time-dependent light pulse, how much momentum, angular momentum and energy are transferred to an object hit by that pulse? And: knowing the light-matter interaction properties of an object at rest, what are its optical properties when it moves with relativistic speed? These questions are relevant for the optical manipulation of small objects with pulsed lasers, and for the understanding and engineering of light sails, respectively.

Cross-Correlation and Averaging: An Equivalence Based on the Classical Probability Density

Attila Genda

In nonlinear differential equations, the averaging method is commonly used to effectively reduce systems with "fast" oscillations superimposed on "slow" drift. Averaging involves the calculation of an integral, which may be straightforward in some cases but can also require simplifications like series expansions. Our proposal offers an alternative approach that leverages the classical probability density (CPD) of the "fast" variable. The CPD is a function that describes the likelihood of finding a moving particle at any possible position along its trajectory g(t), with the probability being proportional to the time spent in the vicinity of that position. We establish the equivalence between the averaging integral and the cross-correlation product of the CPD and the target function. This equivalence simplifies handling many problems, particularly those involving piecewise-defined target functions. To calculate the averaged function effectively, we present a numerical method that exploits the well-known mathematical properties of cross-correlation products. Main result. We consider the averaging of a scalar-valued function of the form $f(x_S + x_F)$ where the "slow" variable is denoted by x_S and the "fast" variable by x_F . We assume, furthermore, that the "fast" variable x_F can be given as a periodic function of the time g(t) with the time period T (for aperiodic functions, let $T \to \infty$). Hence, $x_F = g(t)$, thus, one has $f(x_S + g(t))$. We prove that the time average of this function is equivalent to the cross-correlation of f(x) and the CPD ρ(x) of the "fast" variable x_F (t). Using this equation, we develop alternative methods for calculating the average of analytic functions. These methods rely on the moments of the CPD, allowing us to use the corresponding moment-generating and characteristic functions. By doing so, we can derive an equation which expands the averaged function in terms of the CPD's moments and the original function's derivatives.

Computing the flow of a dusty fluid in a Circular pipe with a porous medium

Anju Saini

The erratic flow of an incompressible, viscous and dusty fluid via a circular conduit in a porous material is examined in this work. Both a consistent magnetic field with a perpendicular direction to the flow pattern and a steady state gradient in the axial direction are used. It is anticipated that the particle phase will act like a viscous fluid. Through numerical analysis, it is determined how the porosity of the medium and the particle-phase viscosity affect the particle-phase and fluid velocities. In order to analyse the velocity distributions of the dust and fluid phases, it is important in this study to construct solutions for an electrically conducting dusty fluid moving in a circular pipe that is constrained by the thickness of the deposition on the wall. In this study, it is examined whether lowering the fluid and particle velocities results from increasing the porosity parameter.

Application of fully implicit Nested Newton solvers to multicomponent multiphase flow in porous media and to elastoplastic deformations of biological tissue

Markus M. Knodel

Advanced models of complicated physical and biological processes incorporate huge equation systems which combine partial differential equations (PDEs), ordinary differential equations (ODEs), and algebraic equations

(AEs). The application of nested Newton solvers allows to shift a substantial part of the nonlinear computations to the so-called local system containing only non-spatially coupling equations (ODEs, AEs). The global equations contain all PDEs. The local variables are coupled with the global variables by means of a so-called resolution function. The solution technique remains monolithic and fully implicit. The number of the local Newton steps (which can be performed with perfectly parallel scalability) displays an upper bound for the global Newton steps.
We present two examples of applications of a nested Newton algorithms which allow the efficient evaluation of the corresponding models: We simulate elastoplastic deformation of biological tissue with anisotropic structure in case of a highly nonlinear material model. Applying the BilbyKrönerLee (BKL) multiplicative decomposition of the deformation gradient into an elastic and a plastic part, a natural split into local and global system is achieved. Performing different numerical experiments of a monophasic model of fiber-reinforced tissues and comparing to another plasticity algorithm, we observe a strong improvement of the performance.

Further, we apply the globally fully implicit PDE reduction method developed 2007 by Kräutle and Knabner for one-phase flow extending the method to the case of an arbitrary number of gases in gaseous phase in order to study the efficacy of mineral trapping scenarios for CO2 storage behavior in deep layers. The chemistry of the multiphase multicomponent flow in porous media model includes both general kinetic and equilibrium reactions. Our applications demonstrate the potential of nested Newton procedures for efficient solution techniques in case of highly nonlinear models of complicated scenarios.

A high-order numerical method for solving non-periodic scattering problems in three-dimensional bi-periodic structures

Nasim Shafieeabyaneh

We consider scattering of non-periodic incident fields in three-dimensional bi-periodic structures. Such scattering problems, modeled by the Helmholtz equation, are challenging due to the unboundedness of the domain and the non-periodicity of the problem. To overcome these difficulties, we apply the Floquet-Bloch transform, which decomposes the problem posed in the unbounded domain into a family (indexed by the Floquet-parameter) of periodic problems in a bounded cell. The solution of the non-periodic scattering problem is obtained by the inverse Floquet-Bloch transform, which is the double integral of the solutions of the decomposed problems with respect to the Floquet-parameter. To solve these scattering problems, we present a high-order numerical method. We first analyze the regularity of the solutions of the decomposed problems with respect to the Floquet-parameter; their singularities are located on a finite number of circular arcs. Then, we propose a high-order tailor-made quadrature method adapted to these singularities. Finally, we prove that the proposed method is super-algebraically convergent.

Machine Learning for Weather and Climate Modelling

Room: 0.014
Chair: Julian Quinting

Machine Learning for High-Resolution Climate Projections: Generative Models Meet Proper Scoring Rules

Maybritt Schillinger

Future projections from physical climate models (global circulation models, GCMs) have a coarse spatial resolution, using grid cells with a length of about 100 km in the mid-latitudes. Regional climate models (RCMs) with higher spatial resolutions (e.g. around 10 km) are computationally costly. To tackle this issue, our work demonstrates how machine learning methods can predict the high-resolution RCM data from low-resolution GCM input. To this end, we combine generative models with statistical tools from forecast evaluation. In particular, we present a simple neural network architecture that predicts the Fourier coefficients of the high-resolution field, separately for each day and variable (temperature and precipitation). The loss function of our model is a proper scoring rule, measuring the discrepancy between the model's predictions and the true RCM's distribution, and is minimised if both distributions agree. Our experiments show promising results: the predictions have fine details, good visual quality and exhibit only small biases when averaged over time or space. However, the generative model still slightly underestimates the conditional variance, i.e. it generates too similar high-resolution outputs when applied to the same fixed low-resolution input several times. Additionally, we train the generative model on several GCM-RCM datasets and ensure consistency between the generated outputs. Further, we establish a model to generate observational data and use it to map the RCM's to the observational distribution. To summarise, our work presents a new machine learning method to generate high-resolution climate predictions which is fast to train and allows for

quick sample generation. Our generative model could also be of interest to other scientific disciplines.

Forecasting lightning probabilities derived from the Lightning Potential Index using neural networks

Manuel Baumgartner

Forecasting the occurrence of thunderstorms is a well-known challenge in weather prediction. Since a thunderstorm is by definition accompanied by at least one lightning, we aim to forecast the occurrence of at least one lightning within a pre-defined area and a pre-defined time-interval. Numerous prior research studies on forecasting and detecting lightnings provide a rich database of model diagnostics and observational data. One example of such a model diagnostic is the so-called (subgrid-scale) Lightning Potential Index (LPI), that was recently implemented in the operational ICON-model and is now available operationally, even in the ICON-EU ensemble. On the other hand, there are extensive observation networks that provide lightning observations, such as the Linet-network that provides lightning observations over Europe.

In our work, we use lightning observations from the Linet-network as ground truth and establish a translation from LPI to lightning probabilities. For this task, we trained neural networks to predict the desired lightning probabilities in a "global postprocessing mode", i.e. using the same network for the forecasts on the whole domain of ICON-EU, which is significantly larger than the domain of the Linet-network. We present the setup of the postprocessing method together with details of the training of the neural networks and show first results from its forecasts and their evaluation. In particular, these lightning probabilities outperform raw model probabilities as derived by counting the exceedance of a LPI-threshold and thereby avoid the need to even define such a threshold. We will also address aspects of producing stable operational forecasts by applying an ensemble of neural networks.

Comparison of Model Output Statistics and Neural Networks to postprocess wind gusts

Cristina Primo Ramos

Wind gust is one of the main relevant meteorological variables playing an important role in warning strategies of the national meteorological services, due to the high impact in society of its extreme values. In turn, wind prediction is quite challenging because it is affected by small-scale processes, influenced by the local characteristics. Meteorological centers are provided with ensemble prediction systems (EPS), that run ensembles of forecasts, rather than a unique deterministic one, to account for the different sources of uncertainty around the predictions. Probabilistic values like wind gust exceeding a threshold can then be derived from those ensembles. Nevertheless, these probabilistic forecasts still exhibit systematic errors inherent to the numerical models and post-processing techniques are essential to correct them.

Model Output Statistics (MOS) is a common operational postprocessing technique, however, more modern methods appeared in the research community, like neuronal networks, seem to be promising techniques in the wind gust postprocessing field. The transition from research to operations requires from a comparison of both techniques. Hence, this study aims to compare probabilistic wind gust forecasts coming from applying Ensemble-MOS, the postprocessing technique used by the German Meteorological Center consisting of linear and logistic regressions, and two neuronal networks proved in the literature to improve wind gust predictions, named distributional regression network and Bernstein Quantile Network. These three postprocessing techniques are applied to the direct model outputs of the German limited area model ensemble prediction system, COSMO-D2-EPS. Their performance is compared in terms of properties like accuracy, reliability or resolution.

Multivariate post-processing of sub-seasonal weather regime forecasts

Fabian Mockert

Reliable forecasts of quasi-stationary, recurrent, and persistent large-scale circulation patterns – so-called weather regimes – are crucial for various sectors of society, including energy, health, and agriculture. Despite steady progress, probabilistic weather regime predictions still exhibit significant biases and are not reliable beyond 15 days of lead time. Thus, this study aims to advance their predictions through ensemble postprocessing. Our approach is based on a year-round regime definition that distinguishes between four types of blocked regimes dominated by high-pressure situations in the North Atlantic-European region and three types of cyclonic regimes dominated by low-pressure situations. The manifestation of each regime can be expressed by a seven-dimensional weather regime index representing the projection of the 500-hPa geopotential height field onto the mean patterns of the seven weather regimes.

This index is calculated for ECMWF's sub-seasonal reforecast ensemble data valid in the period 1999 to 2020 and verified against ERA5 reanalyses. To improve

the accuracy and reliability of the multivariate probabilistic weather regime forecasts, we adjust the raw model outputs respective to their uncertainties and biases using a combination of Ensemble Model Output Statistics (EMOS) and Ensemble Copula Coupling (ECC). With EMOS, the year-round mean skill horizon (referring to the 0.1 level of the CRPSS compared to the climatological forecast) increases by 1.5 days compared to the current state-of-the-art weather regime forecast. We further replace the univariate EMOS method with a neural network-based distributional regression approach that provides greater flexibility in predictor intake.

Overall, our study reveals that statistical post-processing techniques are one way to improve weather regime forecasts, which can help plan and manage, reduce risks, and maximise societal benefits.

Combining physical knowledge and statistical models to forecast weather on subseasonal timescales

Selina Kiefer

For many practical applications, e.g. agricultural planning, skillful weather predictions on the subseasonal timescale are key for making sensible decisions. Since traditional numerical weather prediction models are often not capable of delivering such forecasts, we use an alternative forecasting approach combining both, physical knowledge and statistical models. Selected meteorological variables from ERA-5 reanalysis data are used as predictors for wintertime Central European mean 2- meter temperature and the occurrence of cold wave days at lead times of 14, 21 and 28 days. The forecasts are created by Quantile Regression Forests in case of continuous temperature values and Random Forest Classifiers in case of binary occurrence of cold wave days. Both model types are evaluated for the winters 2000/2001 to 2019/2020 using the Continuous Ranked Probability Skill Score for the continuous forecasts and the Brier Skill Score for the binary forecasts. As a benchmark model, a climatological ensemble obtained from E-OBS observational data is considered. We find that the used machine learning models are able to produce skillful weather forecasts on all tested lead times. As expected, the skill depends on the exact winter to be forecasted and generally decreases for longer lead times but is still achieved for individual winters and in the 20-winter mean at 28 days lead time. Since machine learning models are often subject to a lack of interpretability and thus considered to be less trustworthy, we apply Shapley Additive Explanations to gain insight into the most relevant predictors of the models' predictions. The results suggest that both Random-Forest based models are capable of learning physically known relationships in the data. This is, besides the capability of producing skillful forecasts on the subseasonal timescale, a selling point of the combination of physical knowledge and statistical models.

Deep learning for post-processing global probabilistic forecasts on sub-seasonal time-scales

Nina Horat

Sub-seasonal weather forecasts are becoming increasingly important for a range of socioeconomic activities. However, the predictive ability of numerical weather prediction models is very limited on these time-scales. We propose post-processing methods based on convolutional neural networks to improve sub-seasonal forecasts by correcting systematic errors of the numerical weather models. Since our post-processing models operate directly on spatial input fields, they are able to retain spatial relationships and to generate spatially homogeneous predictions.

The proposed post-processing models use forecast fields of multiple meteorological variables as input, and produce global probabilistic tercile forecasts for biweekly aggregates of temperature and precipitation for weeks 3-4 and 5-6. The model architectures and the training strategy are optimized to deal with the low signal-to-noise ratio in sub-seasonal forecasts and the limited amount of training data. Half of the tested architectures use the well-known UNet architecture specifically designed for image segmentation. The remaining architectures are based on a standard convolutional neural network architecture as typically used for image classification, with the difference that a set of basis functions is used to provide spatial predictions.

In a case study based on a public forecasting challenge organized by the World Meteorological Organization, our post-processing methods outperform the recalibrated forecasts from the European Centre for Medium-Range Weather Forecasts, and achieve improvements over climatological forecasts for all considered variables and lead times. We further demonstrate that all approaches lead to skilful and well-calibrated probabilistic forecasts.

Statistical Methods in Economics

Room 0.016

Chair: Lotta Rüter

Prediction intervals for economic fixed-event forecasts

Fabian Krüger

The fixed-event forecasting setup is common in economic policy. It involves a sequence of forecasts of the same ('fixed') predictand, so that the difficulty of the forecasting problem decreases over time. Fixed-event point forecasts are typically published without a quantitative measure of uncertainty. To construct such a measure, we consider forecast postprocessing techniques tailored to the fixed-event case. We develop regression methods that impose constraints motivated by the problem at hand, and use these methods to construct prediction intervals for gross domestic product (GDP) growth in Germany and the US.

Uncertainty Quantification for Macroeconomic Panel Forecasts

Friederike Becker

Real-time point forecasts for key macroeconomic indicators such as real GDP growth or inflation are ubiquitous in both academia and the media. They play an important role in many decision making contexts, for both the private and the public sector, but are rarely communicated alongside an assessment of their uncertainty. We quantify the uncertainty that is inherent in a panel data set of point forecasts for a large set of countries, where we construct individual distribution functions that exploit potential similarities between countries. Specifically, we derive a combined empirical cumulative distribution function estimator that minimizes the empirical CRPS, where combination weights for different units are either estimated directly or parametrized via a set of features that inform the similarity between units. We study this estimator theoretically, as well as its behavior on simulated data and on fixed-event forecasts issued bi-annually over the past 30 years by the World Economic Outlook (WEO). We perform calibration checks of the resulting distributional forecasts and compare the estimator's performance to a baseline specification. A central advantage of the method is that it is constructed only of the forecast-observation pairs and, optionally, a set of features selected by the user. It hence requires no access to the forecast-generating model or any information that informed it, facilitating its application in a potentially wide range of settings.

Wages and capital returns in a generalized Pólya urn

Stefan Großkinsky

The evolution of inequality and its underlying mechanisms is a widely discussed issue in research and public debates, not least due to the popular work of Thomas Piketty. Most studies consent that in industrial countries the empirical distribution of wealth exhibits a two-tailed structure with a power-law tail for the richest persons in an economy. We investigate the hypothesis that such distributions arise generically due to a feedback mechanism for capital returns. Generalized Pólya urns with non-linear feedback are an established probabilistic model to describe the dynamics of growth processes with reinforcement. Depending on the feedback function, it is well known that the model may exhibit monopoly, where a single agent achieves full market share. In the first part of the talk we summarize rigorous results for the asymptotics and large scale dynamics of such urn models. In the second part we present a modified version to model the dynamics of household wealth, incorporating wealth-independent wages as well as capital returns. From wealth and wage data we extract a fundamental relationship between the two main parameters of the model, the wage share and the feedback exponent. We show theoretically and numerically that heavy-tailed distributions arise naturally in such models from various generic initial conditions, and with realistic parameters and we get a good quantitative match with observed empirical distributions.

Compression and Simulation of Large Insurance Portfolios with New Business

Maximilian Diehl

We develop compression methods for large life insurance portfolios, where the insured collective is grouped into cohorts based on selected contract-related criteria. This allows us to simulate an extremely reduced number of representative contracts. We also show how to efficiently integrate new contracts into the existing insurance portfolio. Furthermore, we investigate the efficiency of the compression methods and their quality in approximating the uncompressed life insurance portfolio. In particular, we show how one can obtain bounds for the default probability of the life insurer as being part of conservative estimation procedures prescribed by regulating authorities. For the simulation of the insurance business, we devise a stochastic asset-liability management model. The incorporated balance sheet model is in line with the principle of double-entry bookkeeping as required in accounting. We provide a detailed modeling of the strategies for investing in the capital market and for financing the due obligations. Thereby, we take into account the complexity of managing a large insurance portfolio. In extensive simulation studies, we illustrate the short- and long-term behavior of our model and show impacts of different

business forms, the predicted new business, and possible capital market crashes on the profitability and stability of a life insurer.

On Mathematical Guarantees in Machine Learning for Safe Autonomous Driving

Philipp Geiger

Machine learning (ML) is a applied in more and more areas of society, and solves previously unsolved problems. But for deployment of ML in (safety-)critical systems, like using imitation learning (IL) for autonomous driving, we need strong validation arguments - ideally mathematically proven statements about an ML system's behavior during deployment. Obtaining such mathematical guarantees is difficult though, when trying to account for computational tractability and flexibility, as well as the inherent uncertainty about the deployment environment. This remains a fundamental challenge, in particular in notoriously intransparent deep learning.

In this presentation, I will start with a short overview over different approaches for obtaining mathematical guarantees about ML systems, in particular for safety. Then I will present our recent work on fail-safe adversarial generative imitation learning in multi-agent systems, with an application in autonomous driving.

Specifically, our work consists of theory and a modular IL method, with a safety layer that enables a closed-form probability density/gradient of the safe generative IL policy, end-to-end generative adversarial training, and worst-case safety guarantees. The safety layer maps all actions into a set of safe actions, and uses the change-of-variables formula plus additivity of measures for the density. The set of safe actions is inferred by first checking safety of a finite sample of actions via adversarial reachability analysis of fallback maneuvers, and then concluding on the safety of these actions' neighborhoods using, e.g., Lipschitz continuity. We provide theoretical analysis showing the robustness advantage of using the safety layer already during training (imitation error linear in the horizon) compared to only using it at test time (up to quadratic error due to distribution shift). In an experiment on real-world driver interaction data, we empirically demonstrate tractability, safety and imitation performance of our approach.