Berlin Mathematical School

Descriptions of available dissertation projects in MATH+

AA1-10: New methods for inhibiting Sars-Cov2 cell entry

In collaboration with experimentalists in Berlin and worldwide, we pursue the development of drug molecules that inhibit cell entry of SARS-CoV-2, the virus causing Covid-19. From the theoretical viewpoint we need to combine established methods for structure modeling, docking, molecular dynamics simulations and Markov state modeling with novel machine learning methods. Specifically, we want to develop a statistical theory of semi-supervised learning which is needed in order to iteratively integrate information from fewer and fewer measurements of the protein-drug binding affinity, the more accurate these measurements become. We are an international and interdisciplinary research group and are looking for candiates that have a strong background in a quantitative discipline (Maths, Physics, Engineering), ideally have prior knowledge of machine learning and software development and are passionate about science.

BMS Research Training Area 8, Faculty: Frank Noé

AA2-8: Deep back flow for accurate solution of the electronic Schrödinger equation

Accurate and general solution of the electronic Schrödinger equation is one of the great challenges in computational materials science, since it provides straightforward access to many material properties. Among the numerous approximate methods, quantum Monte Carlo provides a platform for in-principle exact numerical solutions at favorable computational cost, but in practice is limited by the flexibility of the available wave function ansatzes. The cornerstone of this issue is a faithful representation of the so-called nodal surface, on which the antisymmetric electronic wave function changes sign. This project aims to establish a novel computational technique based on deep neural networks, called deep backflow, as a general solution to the nodal-surface representation problem. This will overcome the only existing fundamental limitation to the accuracy of quantum Monte Carlo calculations, opening the possibility of highly accurate electronic-structure calculations for much larger systems than previously possible.

BMS Research Training Area 8, Faculty: Jens Eisert, Frank Noé

AA3-9: Information Design for Bayesian Networks

This project studies a model for traffic networks where travel times are stochastic and depend on the total flow on the edge. A traffic service provider acts as a benevolent moderator who is able to observe the realization of the stochasticity in the edge costs and recommends routes to traffic participants. The project is concerned with characterizing and computing optimal route recommendations that minimize the overall travel time and satisfy the additional constraint that each traffic participant has an incentive to follow the route recommendation given by the moderator.

BMS Research Training Area 4, Faculty: Max Klimm

Berlin Mathematical School BMS

AA4-3: Equilibria for Energy Markets with Transport
Research in this project will concentrate on modeling, analytic, optimization and numerical aspects of generalized Nash equilibrium problems with partial differential equation constraints.
We are looking for candidates with knowledge of partial differential equations, continuous optimization and applied functional analysis as well as experience in the field of numerical and computer-aided implementation.

BMS Research Training Area 7, Faculty: Michael Hintermüller

AA4-7: Decision-making for Energy Network Dynamics
The move towards sustainable energy networks, with due consideration of the complexities arising from the integration of rather unsteady renewable resources, causes major operational challenges for network providers. Mathematical control theory provides a key technology for optimization-guided dispatching processes, but is facing the challenges of large-scale dynamics from physical models such as partial differential equations (PDEs) linked with discrete decision models such as 0-1 switching for connecting/disconnecting capacitors, generating units and transmission lines. These problems are to be solved fast and repeatedly while gathering data to adapt.

The research agenda of this project tackles fundamental questions concerning control and optimization in context of this application. It concerns mathematics at the interface and beyond the state-of-the-art in combinatorial optimization and control theory for partial differential equations (PDEs). The main goal is to establish novel stationarity concepts for broad classes of PDE-dynamic mixed-integer programs based on exact and approximative relaxation techniques for extended formulations of such optimization problems, their primal-dual optimality conditions and their numerical solutions using semismooth Newton methods and thresholding strategies. A strong focus is given to treat combinatorial restrictions modelling minimal up/down time, ramping or switching order constraints.

The applicability of the theoretical achievements will be showcased on electricity distribution networks by means of case studies.

BMS Research Training Area 6, Faculty: Falk Hante

AA4-8: Recovery of battery ageing dynamics with multiple timescales
Ageing is a major drawback of modern lithium ion batteries (LIB). The project aims at developing a data-driven methodology to recover the dynamics of battery ageing on the basis of a mathematical model in combination with numerical simulations and experimental data. The research plan covers three main aspects, (i) modeling of a porous battery cell with degradation effects, (ii) homogenization of the time periodic PDE system and (iii) determination of the parameter evolution as inverse problem with invertible neuronal networks.

We are looking for candidates with a strong background in applied mathematics, theoretical chemistry, physics or electrical engineering. Prior knowledge in continuum mechanics, thermodynamics, homogenization theory, software development, and machine learning is beneficial.

BMS Research Training Area 6, Research Training Area 7 or Research Training Area 8

Faculty: Martin Eigel, Martin Heida, Manuel Landstorfer

EF2-5: A Soft-Correspondence Approach to Shape Analysis
Despite many advances, frameworks for geometric morphometry still rely on point-to-point correspondences between shapes, either explicitly in form of homologous landmarks or implicitly in terms of diffeomorphisms of the ambient space. Point-to-point correspondences, however, have fundamental limitations that prohibit the analysis of shape collections with incomplete or topologically varying objects. This is a major problem for the analysis of empirically given sets of shapes, since these often contain topological variations ("real" ones as well as those caused by noise or reconstruction errors) or are incomplete (e.g. due to spatial limitations in tomographic reconstructions or due to destruction and decay). The goal of this project is to extend the scope of shape analysis methodology in order to overcome these limitations. To this end, we will generalize approaches defined in shape spaces based on explicit representations by adapting and refining the concept of soft correspondences. The methodological developments will be driven by applications from archaeology and biology.

BMS Research Training Area 5, Faculty: Christoph von Tycowicz

EF4-7: The impact of dormancy on the evolutionary, ecological and pathogenic properties of microbial populations
Dormancy is an ubiquitous trait in microbial communities. It describes the ability of an organism to switch into a metabolically inactive and protected state, for example in response to environmental stress. Having this ability has important implications for the evolutionary, ecological and pathogenic character of microbial systems. At the same time, dormancy leads to new mathematical objects with excitingly different properties such as the seed bank coalescent. In this project, we would like to better understand the patterns of genetic variability and species diversity resulting from dormancy as well as study invasion, fixation and coexistence regimes in microbial communities with dormancy. This will be done by deriving new individual based stochastic models and analysing their scaling limits with methods from mathematical population genetics (diffusions, duality, coalescent theory) and adaptive dynamics (branching processes, dynamical systems).

Any candidate should have a solid foundation in mathematical probability theory, in particular in stochastic processes. Knowledge of population genetics or adaptive dynamics is an additional advantage.

BMS Research Training Area 3, Faculty: Maite Wilke Berenguer, Jochen Blath

EF4-8: Concentration effects and collective variables in agent-based systems

Agent-based models (ABMs) are often high-dimensional and complex, making simulations costly and formal analysis hard. Low-dimensional model reduction is hence of great interest. The systems often showcase favorable properties, such that the complex overall behavior of the individual agents can be approximated by the stochastic evolution of a small number of macroscopic collective variables describing the effective dynamics of the system. Moreover, if the number of agents is large, one can observe a concentration of measure in the sense that the collective variables follow an almost deterministic and smooth evolution.

The goals of the project are to

- mathematically formalize and characterize the above reducibility properties;
- develop a computational machinery for finding collective variables and their effective evolution for complex systems;
- understand collective social behavior on an abstract and applied level.

You will work in an interdisciplinary environment in cooperation with scientists from Freie Universität Berlin and Potsdam Institute for Climate Impact Research (PIK). Advanced programming skills are required, ideally in Matlab, Python, Julia, C, C++, or similar languages.

BMS Research Training Area 3 or BMS Research Training Area 6,
Faculty: Jobst Heitzig, Péter Koltai, Stephanie Winkelmann

EF5-6: Evolution Models for Historical Networks

Studies of the material evidence of our past (foremost in the field of archaeology) deal with spatial distribution patterns that have been shaped by interactions along the links of trade or migration networks, which have (at best) been preserved partially. Mathematical models explaining the mechanisms behind network expansion then become fundamental for a detailed understanding of the archaeological and historical record.
This project aims at developing sequential models for the evolution of spatial networks. Compared to existing network evolution models, we intend to incorporate important features such as the formation of Steiner points and the suitability of terrain. The developed models will then be calibrated to historical data. Further, we will analyze fundamental properties of the formed networks, e.g., we will investigate whether hierarchical organization is a natural outcome of this process. Motivated by the study of the relationship between the political organization of a society and the structure of its network, we also aim at characterizing the inefficiency of the networks created by these models.

BMS Research Training Area 4, Faculty: Max Klimm, Guillaume Sagnol