ID 01 Logics for dynamical systems and practical theorem proving tools

MATH PI: André Platzer, Alexander von Humboldt Professor on Logic of Autonomous Dynamical Systems, Institute of Information Security and Dependability (KASTEL), Institute for Reliability of Autonomous Dynamical Systems (VADS) of the Karlsruhe Institute of Technology (KIT)

SEE PI: *tbd*

Department(s): Informatics, Mathematics

Type of position: 100% FTE, TV-L E13 (GFA)

The group of **André Platzer**, the **Alexander von Humboldt Professor** for Logic of Autonomous Dynamical Systems, in the Department of Informatics at KIT, Karlsruhe, is recruiting a PhD Student or Doctoral Researcher. Exceptionally qualified applicants for postdoc positions may be considered as well. Our research develops logics for dynamical systems and practical theorem proving tools, such as KeYmaera, for analyzing and correctly building cyber-physical systems, and provably safe AI techniques. Our techniques are used to analyze the safety of autonomous cars, airplanes and collision avoidance protocols in aerospace applications, robotics, and train control. Your exciting mathematical research can have a direct impact on making the world a better place.

The successful candidate is able to quickly get into new research areas and will be responsible for actively engaging in novel research questions, publishing and communicating research results, advising junior students, assisting in research grants, implementation of research results in formal methods or theorem proving tools, and demonstrating their applicability in cyber-physical systems applications.

Group: The Alexander von Humboldt Professorship, Germany's most highly endowed international research award, is endowed with up to five million euros. With this award, the Alexander von Humboldt Foundation honors internationally leading researchers of all disciplines.

Key requirements for successful applications:

- Excellent M.Sc. degree in computer science, mathematics or related subjects.
- Strong demonstrable commitment to research.
- Strong background in logic, theorem proving, formal methods, or programming language theory.
- Strong background in mathematics, physics, or engineering, especially ordinary differential equations.
- Proficiency in English, excellent speaking and writing skills.
- Experience in software development projects is a plus.

ID 02 Deep Boltzmann - Structure-preserving deep neural networks to accelerate the solution of the Boltzmann equation

MATH PI: Prof. Dr. Martin Frank, Steinbuch Centre for Computing (SCC), Computational Science and Mathematical Methods

SEE PI: *tbd*

Department(s): Mathematics, *tbd*

Type of position: 75% FTE, E13 TV-L (UA)

The goal of this project is to use deep neural networks as building blocks in a numerical method to solve the Boltzmann equation. This is a particularly challenging problem since the equation is a high-dimensional integro-differential equation, which at the same time possesses an intricate structure that a numerical method needs to preserve. Thus, artificial neural networks might be beneficial, but cannot be used out-of-the-box.

We follow two main strategies to develop structure-preserving neural network-enhanced numerical methods for the Boltzmann equation. First, we target the moment approach, where a structure-preserving neural network will be employed to model the minimal entropy closure of the moment system. By enforcing convexity of the neural network, one can show, that the intrinsic structure of the moment system, such as hyperbolicity, entropy dissipation and positivity is preserved. Second, we develop a neural network approach to solve the Boltzmann equation directly at discrete particle velocity level. Here, a neural network is employed to model the difference between the full non-linear collision operator of the Boltzmann equation and the BGK model, which preserves the entropy dissipation principle. Furthermore, we will develop strategies to generate training data which fully sample the input space of the respective neural networks to ensure proper functioning models.

This project is part of the DFG Priority Program "Theoretical Foundations of Deep Learning".

Special requirements:

- Programming skills, especially knowledge of current deep learning frameworks
- Basic knowledge of partial differential equation theory and numerics

ID 03 Optimization and acceleration of aerosol dynamics and chemistry sub-processes in weather and climate models

MATH PI: Prof. Dr. Martin Frank, Dr.-Ing. Uğur Çayoğlu, Steinbuch Centre for Computing (SCC), Computational Science and Mathematical Methods

SEE PI: Prof. Dr. Corinna Hoose, Prof. Dr. Peter Braesicke, Institute of Meteorology and Climate Research, Department Troposphere Research (IMK-TRO)

Department(s): Mathematics/Computer Science, Physics

Type of position: 75% FTE, E13 TV-L (UA). *Please note: This position is subject to funding approval.*

Aerosols and chemically reactive gases affect weather and climate by scattering, absorbing and re-emitting radiation and interacting with clouds, and are therefore also called short-lived climate forcers. In contrast to long-lived greenhouse gases, they exhibit a strong geographical variability in emission, atmospheric abundance and their trends. Due to the high resolution and complexity of the models, these calculations are often very demanding on computing resources. This is especially true when the model is to be used for both short-term (weather) and long-term (climate) predictions.

In this project, to reduce computational costs, ML methods are regarded as an appealing alternative to simulate complex nonlinear systems. In recent years, ML has been extensively used in atmospheric modelling. We will follow two complementary approaches to accelerate the aerosol and chemistry treatment to allow simulations fast enough for flexible scientific and near-operational seasonal/decadal simulations of atmospheric composition. The different acceleration strategies will be modular, such that they can be employed individually or in combination.

Tasks include:

- Analysis of ML approaches
- Acceleration of aerosol dynamics with ML
- Integration of ML model into ICON
- Automation and model isolation

Special requirements:

- We are looking for a Doctoral Researcher (PhD student) with a background in either computer sciences or meteorology/atmospheric sciences.
- Solid knowledge of Machine Learning theory.
- Experience with Machine Learning frameworks.
- Interest in atmospheric sciences and interdisciplinary research.
- Very good knowledge of English is required.
- Previous experience with numerical models and programming in Python is an asset.

The dissertation that can be written during this project can either be in the field of Meteorology or Computer Sciences.

ID 04 Exploring the Potential of machine learning methods for improving operational hydrological forecasting and prediction (EPOforHydro)

MATH PI: TT-Prof. Dr. Sebastian Krumscheid, Institute for Applied and Numerical Mathematics and Steinbuch Centre for Computing (SCC)

SEE PI: PD Dr.-Ing. Uwe Ehret, Institute of Water and River Basin Management

Department(s): Civil Engineering, Geo and Environmental Sciences, Mathematics

Type of position: 75% FTE, E13 TV-L (UA). *Please note: ~~This position is subject to funding approval.~~ Update: Funding for this position has been approved.*

Methods from Machine Learning (ML) are currently revolutionizing (not only) hydrological modeling. In close cooperation with the Landesanstalt für Umwelt Baden-Württemberg (LUBW), it is the goal of this proposal to i) systematically explore how ML methods can improve operational hydrological forecasting, especially for floods, along the entire forecasting chain and to ii) further develop existing ML methods. We expect that the project outcomes will help to substantially improve and accelerate operational hydrological forecasting practice in Baden-Württemberg.

Special requirements:

- Solid knowledge of machine learning theory and probability theory.
- Knowledge of current deep learning frameworks (e.g., PyTorch) and programming skills (e.g., Python).
- Preferably background in hydrology and hydrological modeling

ID 05 Multilevel Methods for Quality Assessment of Injection Molding under Uncertainty

MATH PI: TT-Prof. Dr. Sebastian Krumscheid, Institute for Applied and Numerical Mathematics and Steinbuch Centre for Computing (SCC)

SEE PI: Dr.-Ing. Florian Wittemann, Prof. Dr.-Ing. Luise Kärger, Institute of Vehicle System Technology (FAST) – Lightweight Design Division (LB)

Department(s): Mechanical Engineering, Mathematics

Type of position: 75% FTE, E13 TV-L (GFA/UA). *Please note: ~~This position is subject to funding approval.~~ Update: Funding for this position has been approved.*

In today's polymer part production, injection molding is one of the most critical manufacturing

processes used in various engineering tasks. However, due to natural fluctuations in material properties and process controls, the injection molding process is affected by uncertainties. In fact, uncertainties affecting the manufacturing process can significantly affect a part's quality. Therefore, it is indispensable to assess the quality of injection molding processes under uncertainties, particularly for safety-critical applications.

The objectives of this project are twofold. Firstly, we will develop advanced uncertainty quantification techniques for an efficient assessment of the effects of uncertainties in computational models. Specifically, we will investigate and analyze novel hierarchical (e.g., multi-level) sampling strategies for approximating so-called risk measures that provide a more refined uncertainty analysis than expected values alone. Secondly, the new methodological developments will be particularized and tailored for application in injection molding under uncertainties. A focus will be on process simulations to quantify the scatter of part properties due to uncertainties in material state and process conditions and their effects on the part's robustness.

Special requirements:

- Solid knowledge of numerical analysis as well as probability theory and statistics. Experience with uncertainty quantification techniques is advantageous.
- Python programming skills.
- Interest in fluid mechanics and manufacturing process simulation.

ID 06 Theoretical and Empirical Analysis of Matheuristics

MATH PI: Dr. John Alasdair Warwicker, Institute of Operations Research (IOR)

SEE PI: Dr.-Ing. Marion Baumann, Institute for Material Handling and Logistics (IFL)

Department(s): Economics and Management, Mechanical Engineering

Type of position: 75% FTE, TV-L E13 (UB)

Matheuristics (MAs) concern the interoperation of Mathematical Programming (MP) and Metaheuristics (MH), in which one of the techniques is used to design or enhance existing models from the other. For example, consider mixed-integer programs, whose solution methods often take advantage of solving a series of auxiliary linear programs (LPs). Heuristic solvers can be used to solve such LPs.

A number of empirical analyses have attempted to understand the performance of MAs, including for real-world applications, such as routing problems. Vehicle routing problems concern deciding the optimal set of routes to be taken by a fleet of vehicles in order to deliver items to a set of customers at different locations. Typically, these problems involve deciding on the clustering of customers to vehicles, and the routes of the vehicles.

However, a rigorous and foundational theoretical understanding of MAs is lacking, which would allow us to provide guarantees about their computational complexity and, alongside rigorous empirical analyses, would allow a far greater understanding of the scope of MAs.

The goal of this project is to present performance guarantees and insights on problem classes where MAs are effective, through a series of theoretical analyses. This will lead to further insights into how to apply and design MAs for real-world problems, including routing.

Special requirements:

Introductory knowledge of Mathematical Programming or Metaheuristics approaches.

Knowledge of at least one programming language (desirable).