DY 28: Poster: Machine Learning, Data Science

Time: Wednesday 15:00–18:00 Location: P4

DY 28.1 Wed 15:00 P4

Thermal Neural Quantum States — •Atiye Abedinnia and Annabelle Bohrdt — Institute of theoretical physics, University of Regensburg

Finite-temperature effects play an important role in the design and optimization of quantum devices, as decoherence and noise often originate from thermal fluctuations. At finite temperatures, quantum systems are described by a statistical ensemble of states rather than a single pure state. Simulating such thermal states requires constructing the thermal density matrix, which suffers from significant computational challenges due to the exponential growth of the Hilbert space with system size. So far, purification methods(thermofield) in the context of MPS and Minimally Entangled Typical Thermal States (METTS) approach have been developed in the context of tensor networks. In this work, we propose using neural quantum states (NQS), leveraging the expressivity and scalability of transformer-based architectures to address the challenges of thermal equilibrium density matrix representation.

DY 28.2 Wed 15:00 P4

Neural Networks for Phase Recognition on Lattice Systems — •Shashank Kallappara and Martin Weigel — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

The Ising model undergoes a phase transition in dimensions d > 1, with its magnetisation as the order parameter. Fully connected neural networks have been shown to learn the translational invariance of the Ising model when learning its phases. This requires only a single hidden layer; analytic solutions for the same exist for highly compact networks that are constructed to obey the translational invariance automatically. Here, we show this learning of the invariance in single-layer networks of different widths and compare the networks performance in classifying the phases. We also consider a highly compact network to study the gradient descent dynamics during training over its loss landscape; we suggest a few changes to this that greatly improve its performance while preserving interpretability. Another problem we consider is percolation on a square two-dimensional lattice. Here, we leverage convolutional neural networks to detect the phase transition by training on different properties of the systems and evaluate its effectiveness.

DY 28.3 Wed 15:00 P4

optimization of the algorithm of operation of a series-parallel combined power plant — •Malika Allakulyyeva — Moscow, Russia

Over the past 15 years, work on the creation of a combined power plant (CEP) of a car has become an independent direction of modern electromechanics, characterized by its scientific problems, the specifics of performing applied research, and the expanding field of practical use of developments. This article presents the results of experimental studies of series-parallel power plants on the educational laboratory stand of the CO3221-6X model *Cars with power plants and electric vehicles* and proposes an alternative algorithm for the operation of a combined power plant.

DY 28.4 Wed 15:00 P4

Stability of Machine-Learned Interatomic Potentials in Molecular Dynamics Simulations for Complex Organic Crystals — •Martin Tritthart, Florian Linder, Lukas Legenstein, Florian Unterkofler, Martin Klotz, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, NAWI Graz, AUSTRIA

Understanding thermal conductivity and mechanical stability is crucial for several applications of organic semiconductors (OSCs) and metal-organic frameworks (MOFs). Molecular dynamics (MD) simulations are commonly used to deduce these properties, and in recent years, machine Learned interatomic potentials (MLIPs) have been employed to enhance accuracy compared to classical force fields. MLIPs are orders of magnitude faster than ab initio methods and can achieve close to DFT accuracy. Their accuracy,however, heavily depends on the quality of the training data. Incorrect predictions of forces and energies for atomic configurations outside the training dataset can accumulate in the MD trajectory, potentially even leading to disintegration of the (molecular) building blocks. This, however, limits long-time simulations, which are necessary to investigate thermal transport properties. To mitigate these issues and to realize a robust MLIP, reliable uncertainty estimates are needed especially for atomic configurations outside the region of the phase space sampled during training. Structures characterized by high uncertainties can then be calculated by ab initio methods and incorporated into the training dataset. This approach is tested in my contribution for prototypical MOF and OSC materials.

DY 28.5 Wed 15:00 P4

Estimating parameters for a simple tipping model from complex Earth system model output — •Jonathan Krönke[1,2], Jonathan F. Donges[1], Johan Rockström[1], Nils Bochow[3], and Nico Wunderling[1,2] — [1]Earth Resilience Science Unit, Potsdam-Insitute for Climate Impact Research, Potsdam, Germany — [2]Center for Critical Computational Studies, Goethe University Frankfurt, Frankfurt am Main, Germany — [3]Department of Mathematics and Statistics, UiT - The Arctic University of Norway, Tromsø, Norway

The existence of large-scale tipping points - thresholds where small changes can trigger drastic, often irreversible shifts in the climate system - has been a major concern of climate science in the past two decades. The ability to evaluate tipping risks using computationally manageable models is crucial to assess the resilience of the climate system and also to identify safe global warming trajectories for tipping elements. Here, we present an approach to estimate parameters of a simple tipping model based on complex Earth system model output. We validate our results by reproducing simulations that have not been used in the training process and apply the model to major earth system tipping elements such as the Greenland Ice Sheet. A simple model that captures essential behaviour of complex earth system models provides an important step towards a tipping point emulator for extensive tipping risk analyses.

DY 28.6 Wed 15:00 P4

Advanced Framework for State of Health Estimation Using Equivalent Circuit Models and Machine Learning — •Limei Jin[1,2], Franz Bereck[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]IET-1, Forschungszentrum Jülich

Traditional Electrochemical Impedance Spectroscopy (EIS) techniques for characterizing a battery's behavior face several limitations, including time-consuming data collection, assumptions of system linearity, and difficulties in accurately assessing State of Charge (SoC) and State of Health (SoH). To address these challenges, we developed a robust framework for estimating SoH within a low-dimensional latent space using an autoencoder applied to raw time-domain battery data. This methodology combines synthetic training data from equivalent circuit models with machine learning techniques, specifically utilizing Chebyshev-based parameter space expansion to vary models on the SoC and SoH scale. Thereby, our framework effectively captures dynamic aging patterns while ensuring efficient data generation with minimal experimental input. Additionally, we introduced a stochastic pulse load profile to the models, which overcomes limitations of conventional frequency-based EIS measurements to better reflect real-world battery usage. This approach was initially validated on coin cell batteries in the lab, requiring only three standard spectroscopy experiments to train the framework. It will be extended to larger batteries, such as LFP batteries commonly used in automotive applications, offering scalable solutions for real-time monitoring and enhanced longevity.

DY 28.7 Wed 15:00 P4

Parameter estimation and Bayesian comparison of Langevin models describing cell motility — •Yusuke Kato[1,2], Jan Albrecht[1], Hiroshi Kori[2], Robert Grossmann[1], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Department of Complexity Science and Engineering, Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan

In nature, motile bacteria and eukaryotic cells exhibit spontaneous movement. This cell motility plays an essential role in both maintaining homeostasis (such as the migration of immune cells to a wound site) and the pathogenesis of certain diseases (like the aggregation of cancer cells to other organs in metastasis). Various SDE-based Langevin

models have been proposed to describe cell motility.

In this study, we adopt a Bayesian approach using the likelihood approximation technique introduced in Ref. [arxiv:2411.08692] to estimate parameters of tentative first- and second-order models. In order to compare the different models, we develop a framework that ranks them using Bayesian model comparison. We test and benchmark the approach using synthetic data and subsequently apply it to time-series data of ameboid cells in order to find the best model for their ameboid motility.