DY 14: Machine Learning in Dynamics and Statistical Physics II

Time: Monday 15:00–18:30 Location: HÜL/S186

DY 14.1 Mon 15:00 HÜL/S186

Machine-learned classical density functional theory in higher dimensions with convolutional layers — Felix Glitsch, Jens Weimar, and •Martin Oettel — Institut für Angewandte Physik, Universität Tübingen

Through minimization of a grand free energy functional in classical density functional theory (cDFT), inhomogeneous systems in equilibrium can be efficiently computed. For that, the functional of the excess (over ideal gas) free energy is required which is known explicitly only in a few cases. Recent advancements use machine learning for constructing this functional from simulation data, mostly for systems with one-dimensional, planar inhomogeneities. We propose a machine learning model for application in two dimensions [1] akin to density functionals in weighted density forms, as, e.g., in fundamental measure theory. We implement the model with fast convolutional layers only and apply it to a system of hard disks in fully 2D inhomogeneous situations. The model is trained on a combination of smooth and steplike external potentials in the fluid phase. Pair correlation functions from test particle geometry show very satisfactory agreement with simulations although these types of external potentials have not been included in the training. The method should be fully applicable to 3D problems.

[1] F. Glitsch, J. Weimar and M. Oettel, Phys. Rev. E 111, 055305 (2025)

DY 14.2 Mon 15:15 HÜL/S186

Scalable Boltzmann Generators for equilibrium sampling of large-scale materials — •Maximilian Schebek[1], Frank Noé[1,2,3,4], and Jutta Rogal[1,5] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin, 14195 Berlin — [3]Microsoft Research AI for Science, 10178 Berlin — [4]Department of Chemistry, Rice University, Houston, Texas 77005, USA — [5]Initiative for Computational Catalysis, Flatiron Institute, New York, New York 10010, USA

Generating equilibrium ensembles is essential for modeling molecules and materials, yet traditional simulators like molecular dynamics suffer from limited sampling efficiency. Boltzmann Generators introduced the concept of one-shot deep learning for equilibrium sampling, but scalability to large systems has remained a major challenge. Here, we overcome this scaling limitation with a new Boltzmann Generator architecture that can model large materials systems. Our approach combines augmented coupling flows with graph neural networks to exploit local environments, enabling energy-based training and rapid inference. Compared to previous designs, it trains faster, uses fewer resources, and achieves superior sampling efficiency. Crucially, it transfers to much larger system sizes, allowing efficient sampling of materials with simulation cells exceeding a thousand atoms. We demonstrate its capabilities on Lennard-Jones crystals, mW water ice phases, and the silicon phase diagram, producing accurate equilibrium ensembles and free energies across scales where finite-size effects vanish.

DY 14.3 Mon 15:30 HÜL/S186

Autoencoder Learning Dynamics on MCMC Ising Dataset — •Max Weinmann[1,2,3] and Miriam Klopotek[1,3] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D, Stuttgart, Germany — [3]Heidelberger Akademie der Wissenschaften, WIN-Kolleg, Heidelberg, Germany.

While consistent and abstract descriptions of learning dynamics in neural networks remain rare, they have become omnipresent and are used in many branches of science. As a result, predicting dynamics under diverse choices of ML model parameters can fail catastrophically and it remains difficult to mitigate these failures. Reliable control requires a deep understanding of the relevant mechanisms and conditions for learning particular kinds of datasets. Our study focuses on autoencoder architectures that perform well if they encode the dataset into a compressed representation that reflects core physical concepts of the data it is trained on, succeeding at a self-learned inverse model to decode this representation to reconstruct the original input (of physical origin). Some physical concepts are learned in a particular order, which depend on theoretical complexity of the representation and that of the ML architecture. We measure generalization ability against hard theoretical baselines and investigate the information geometry, stability, and physical interpretability of latent space over training time.

DY 14.4 Mon 15:45 HÜL/S186

Learning order: can neural networks discover phase transitions without symmetry functions? — •Carina Karner — Institute for Theoretical Physics, TU Wien, Vienna, Austria

Phase transitions in soft matter systems from crystallization to gelation arise from collective particle rearrangements that are challenging to capture in full microscopic detail. Conventional approaches rely on order parameters or symmetry functions to characterize emerging structures, but such descriptors may overlook crucial features in the often complex organisation of biolgical materials or synthetic superstructures. Here we investigate whether machine learning can uncover these hidden features directly from raw particle configurations. Using autoencoders trained on simulated trajectories of serveral soft matter systems, we show that the latent space encodes clear signatures of structural transitions without the need for handcrafted inputs. Our results suggest that neural networks can serve as unbiased tools to detect and interpret phase behavior in complex soft matter systems, revealing patterns that elude traditional symmetry-based analysis.

DY 14.5 Mon 16:00 HÜL/S186

Microscopy on Autopilot: Self-Supervised Transformers for Feature Detection and Control — •Damián Baláž, Gianmarco Ducci, Christoph Scheurer, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

The evaluation of microscopy experiments often relies on manual inspection or supervised machine learning. The former is inefficient, whereas the latter requires extensive labeling and may introduce human bias. Self-supervised learning, by contrast, learns from raw image data, capturing intrinsic visual patterns without the need for manual annotation. This improves generalization and objectivity, making it ideal for complex and dynamic microscopy data. Motivated by these advantages, we use a pre-trained self-supervised machine learning model (DINO), based on vision transformer architecture. This constitutes our central tool for feature detection and temporal analysis in microscopy experiments.

We demonstrate the versatility of our approach for two microscopy experiments: i) observing graphene flake growth on liquid copper ii) tracking crack formation in a cobalt oxide catalyst. In both cases, the model enables label-free, qualitative monitoring by identifying related structures based on similarity in the learned feature space. Beyond using it for analysis, we show how the same feature space representations can be used to predict experimental dynamics to autonomously steer processes toward desired targets via planning in feature space. Our findings highlight the potential of self-supervised vision models for real-time analysis and control in microscopy-based experiments.

DY 14.6 Mon 16:15 HÜL/S186

Learning microstructure in active matter — •Writu Dasgupta, Suvendu Mandal, Aritra Mukhopadhyay, and Benno Liebchen — Technische Universität Darmstadt, Darmstadt, Germany

Understanding the full parameter dependence of microscopic structure in active matter remains a central challenge, particularly for strong activity and high density, where simulations become increasingly expensive. Here, we present a data-driven approach that learns radial and angular correlations in terms of the pair-correlation function $g(r,\theta)$ of passive and active Brownian particles. Our predictions are in close quantitative agreement with Brownian dynamics simulations, even for parameter values that the neural networks had not previously encountered during training. Our predictions are subsequently distilled into compact, closed-form expressions using symbolic regression, providing an interpretable description of the underlying structure. Our approach offers a unified and computationally efficient route to understanding non-equilibrium correlations.

DY 14.7 Mon 16:30 HÜL/S186

Physical embodiment enabled learning for autonomous navigation of active particles in complex flow fields — •Diptabrata Paul[1], Nikola Milosevic[2], Nico Scherf[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft

Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Max Planck Institute for Human Cognitive and Brain Sciences, 04103 Leipzig, Germany

Autonomous navigation at the microscale is a major challenge in active matter due to strong environmental noise and hydrodynamic disturbances. While living systems rely on sophisticated sensing and feedback to regulate functions from sub-cellular processes to chemotactic navigation strategies, artificial microswimmers lack such adaptive mechanisms and therefore struggle to respond effectively to stationary or dynamic perturbations. In this work, we introduce an actor-critic reinforcement learning (RL) framework and demonstrate that physical embodiment alone enables adaptive navigation without explicit environment sensing. Training of the active particle agent in strong and spatially varying flow fields leads to emergence of robust strategies that counteract hidden hydrodynamic perturbations excluded from the agent's observation space. This reveals that embodied dynamics encode sufficient information for effective decision-making, enabling RL to exploit morphology-environment coupling as an implicit sensing channel. Our approach bridges the gap between simple stimulus response schemes and higher-level adaptive behavior and establishes a foundation for online learning, and microscale robotics.

15 min. break

DY 14.8 Mon 17:00 HÜL/S186

Machine Learning for Electric-Field Driven Nuclear Dynamics in Solids and Liquids — •Elia Stocco[1], Christian Carbogno[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Fritz Haber Institute of the MPS, Berlin, Germany

Simulating the interaction of electric fields with matter is fundamental to study dielectric properties and their interplay with structural and vibrational degrees of freedom. Therefore, it is desirable to obtain a general method that is able to deal with static and time-dependent fields, that is scalable to large complex systems, and that retains ab initio accuracy. We describe a machine-learning molecular dynamics method within the electric dipole approximation that describes the coupling of insulating materials to diverse electric fields, spanning liquids, solids, and confined systems [1]. In particular, we also take into account the influence of the electric field on the lattice degrees of freedom. We train equivariant MACE models [2], using density-functional theory data to learn the potential energy and dipole surfaces, including the multivalued nature of the polarization in periodic systems. The external forces on various degrees of freedom are obtained through automatic differentiation. We present calculations of the dielectric permittivity of water, the temperature and light-driven ferroelectric-paraelectric phase transition of $LiNbO_3$, and simulations of piezoelectric systems. [1] Stocco, E., Carbogno, C. Rossi, M., Npj Comput. Mater. 11, 304 (2025). [2] Batatia, I., et al., Adv. Neural Inf. Proc. Sys. 35, 11423 (2022).

DY 14.9 Mon 17:15 HÜL/S186

Machine-learned Potentials for Vibrational Properties of Acene-based Molecular Crystals — •Shubham Sharma, Burak Gurlek, Paolo Lazzaroni, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Machine-learning potentials (MLPs) have enabled efficient modelling of complex atomistic systems with ab-initio accuracy. A major challenge, however, is the construction of sufficiently large and diverse reference datasets using first-principles calculations. To mitigate this, several active-learning strategies have been proposed to improve training efficiency, especially when combined with molecular-dynamics sampling. In this work, we develop protocols for building training sets of MACE potentials [1], targeting an accurate description of the vibrational properties of weakly-bound condensed-phase systems [2]. We assess the performance of MACE against the VASP-ML framework [3], highlighting differences in predictive accuracy for energies, forces, and vibrational properties. We also propagate committee-based uncertainties to estimate errors in dynamical quantities coming from imperfect force predictions. Finally, we demonstrate the generalisation capability of the acene-based potential by applying it to host-guest systems, enabling the identification of distinct vibrational modes within the complex dynamical spectra. [1] I. Batatia et. al., Nat Mach Intell 7, 56-67 (2025); [2] B. Gurlek, S. Sharma et. al., npj Comput Mater 11, 318 (2025); [3] R. Jinnouchi et. al., PRB 100, 014105 (2019).

DY 14.10 Mon 17:30 HÜL/S186

Spin-phonon systems in the age of modern atomistic simulations — •Ilija Srpak[1,2], Michael J. Willatt[2], Stuart C. Althorpe[1], and Ali Alavi[1,2] — [1]Yusuf Hamied Department of Chemistry, University of Cambrige, Cambridge, United Kingdom — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Spin-phonon systems are molecules or crystals containing open-shell atoms whose spin-spin interaction is significantly affected by lattice displacements, sometimes leading to spin-Peierls phase transition. They typically inherit some of the most challenging aspects of statistical physics where many configurations across the phase space may contribute to its properties, and of "strongly-correlated" physics where mean-field methods such as density functional theory and self-consistent field approaches break down.

Over the years a plethora of Monte Carlo based techniques was developed to tackle this problem with some success, but not without (sometimes significant) limitations. Approaching this problem from atomistic simulations background, we developed a path integral molecular dynamics framework which doesn't require any Monte Carlo during the simulation runtime to sample the phase space, it can take arbitrary system parametrizations or even ab-initio description and simulate the system at an arbitrary temperature as well as include nuclear quantum effect. Using neural networks we have developed this framework further. We achieved a speed up of 2-3 orders of magnitude and are able to treat higher dimensional systems.

DY 14.11 Mon 17:45 HÜL/S186

Self-Consistent Benchmarking of Machine Learning Force Fields via Energy-Landscape Exploration — •Anand Sharma[1,2], Igor Poltavskyi[1], and Alexandre Tkatchenko[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Indian Institute of Science Education and Research Pune, India

The rapid growth of Machine Learning Force Field (MLFF) models has prompted the development of diverse benchmarks to assess their accuracy and transferability. Most existing approaches rely on predefined test datasets, introducing biases and limiting fair comparison between models.

We introduce a general, system- and model-agnostic benchmarking framework that evaluates MLFFs through self-generated datasets. For each model, molecular structures are obtained by sampling random initial configurations of atoms and relaxing them using the model's predicted forces. The resulting datasets are analyzed through (i) comparison with the model's original training data, (ii) validation against ab-initio reference calculations, and (iii) cross-model dataset comparison. Applied to the SO3LR [1] and MACE-MP-0 [2] models, our framework identifies gaps in their training set coverage and enables unbiased evaluation of models' predictive capabilities. Overall, our approach provides a consistent, extensible foundation for comparing and improving next-generation broadly applicable MLFFs.

[1] A. Kabylda, et. al, J. Am. Chem. Soc. 147, 33723 (2025).
[2] I. Batatia, et. al, J. Chem. Phys. 163, 184110 (2025).

DY 14.12 Mon 18:00 HÜL/S186

Solving Classical and Quantum spin glasses with Deep Boltzman Quantum States — Luca Leone[1], •Arka Dutta[1], Markus Heyl[1], Enrico Prati[2], and Pietro Torta[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany. — [2]Department of Physics, University of Milan, Milan, Italy.

Variational neural network models achieved remarkable success in preparing the ground state of quantum many-body systems. However, addressing classical and quantum spin glasses remains challenging, as exponential growth of deep local energy minima due to disorder and energy frustration hinder conventional Monte Carlo methods. To bridge this gap, we introduce Deep Boltzmann Quantum States, a class of neural quantum states inspired by deep Boltzmann machines, trained by devising Neural Quantum Annealing, an algorithm incorporating the principles of quantum annealing. It solves large-scale classical and quantum spin glasses, matching the exact solution or the best available estimate for several instances of Ising spin-glass models with infinite-range interactions and hundreds of spins.

DY 14.13 Mon 18:15 HÜL/S186

Optimization and Representability of time-dependent Neural Quantum States: a study of the 1D critical quantum Ising model — •Wladislaw Krinitsin[1,2], Mohammad Abedi[1,2],

Jonas Rigo[2], and Markus Schmitt[1,2] — [1]PGI-8, Forschungszentrum Jülich, Jülich, Germany — [2]Faculty for Informatics and Data Science, Regensburg University, Germany

In recent years, neural quantum states have emerged as a competitive and powerful numerical approach for many body systems. While they provide a flexible and scalable ansatz, able to represent any state as suggested by the function-approximation theorem, their practical limitations are still opaque, in particular regarding representability and optimization. In this work we investigate these questions within the framework of variational Monte Carlo on the example of the time evolution of the critical transverse-field Ising model in one dimension. Even for moderate system sizes, the departure from the exact solution occurs very early in the dynamics, allowing us to systematically analyze the representability of the state at each time step as well as the impact of different sampling strategies.