DY 17: Machine Learning in Dynamics and Statistical Physics I

Time: Tuesday 10:00–12:45 Location: ZEU 160

DY 17.1 Tue 10:00 ZEU 160

On-the-fly adaptive sparse grids for coupling high-fidelity and coarse-grained models — •Tobias Hülser, Sina Dortaj, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin, Germany

Most simulations of continuum models require the repetitive evaluation of some non-linear functions. If the latter are only given by the outcome of some high-fidelity simulation, these evaluations can easily become the computational bottleneck of the coupled simulation. To overcome this limitation, computationally efficient machine-learning models have become popular as surrogates of the high-fidelity model in the continuum scale simulation. However, if the input dimension of these models is high, the training of the surrogate often requires infeasible numbers of simulations, the so-called curse of dimensionality. We present an on-the-fly adaptive sparse grids approach, which lifts these limitations. This exploits that, on the one hand, sparse grids are only mildly affected by the curse of dimensionality and allow for an adaptive, local error based training set design. On the other hand, we utilize that, during a continuum simulation, only a small low-dimensional subset of the high-dimensional input space of the high-fidelity model is visited. We therefore construct the surrogate on the fly during the continuum simulation, only generating the high-fidelity data which is needed to interpolate this subset.

We demonstrate the approach on exemplary physical-chemical models from the field of heterogeneous catalysis. We find that our approach can significantly reduce the number of high-fidelity evaluations compared to the direct coupling.

DY 17.2 Tue 10:15 ZEU 160

Reservoir Computing using Active Matter Model Systems: A Physics Viewpoint — •Mario U. Gaimann and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Spatio-temporal prediction of chaotic systems is a challenging problem that is relevant for many fields (weather, finance, energy, and other dynamic systems). Recurrent neural networks and specifically neuron-based reservoir computing were previously used to approach this problem [1,2]. However, these learning systems are typically treated as black boxes, and do not incorporate reasoning or analysis in terms of physical laws and dynamics. Here we study the non-equilibrium dynamics of simple active matter models serving as reservoir computing substrates [3]. This allows us to determine and interpret the state of our reservoir and relate the learning problem to other generic phenomena in statistical physics. With this knowledge we aim to understand optimal conditions for learning in relation to critical states and physical constraints.

[1] Tanaka, G. *et al.* (2019), *Neural Networks* **115**, 100-123.
[2] Nakajima, K. and Fischer, I. (2021). *Reservoir Computing.* Springer Singapore.
[3] Lymburn, T. *et al.* (2021), *Chaos* **31(3)**, 033121.

DY 17.3 Tue 10:30 ZEU 160

Machine Learning Percolation: Does it understand the physics? — •Djénabou Bayo[1,2], Andreas Honecker[2], and Rudolf A. Römer[1] — [1]Departement of Physics, University of Warwick, Coventry, CV47AL, United Kingdom — [2]Laboratoire de Physique Théorique et Modélisation (LPTM) (CNRS UMR8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France

The percolation model is one of the simplest models in statistical physics displaying a phase transition at a critical site occupation probability p_c. The hallmark of the percolation transition is the emergence of a spanning cluster of connected neighboring sites across the lattice. Machine learning (ML) approaches to percolation have shown that the non-spanning ($p < p_c$) and the spanning ($p > p_c$) phases can be identified reasonably well with supervised deep learning (DL) strategies for classification based on convolutional neural networks (CNNs). Surprisingly, the role of the spanning cluster seems to be less prominent in such DL methods. Here, we show that CNNs, when trained with the site occupation probabilities p as labels, can classify not only the two phases $p < p_c$ and $p > p_c$, but also according to the many individual p's. Nevertheless, the same CNNs struggle when trying to predict the emergence of the spanning cluster. Indeed, when we train with correlation lengths or the existence of the spanning cluster, the results suggest that the CNNs seem to rely mostly on the p's as a proxy measure. This suggests that the essential physics of the spanning cluster is not actually what determines the DL results.

DY 17.4 Tue 10:45 ZEU 160

Bayesian deep learning for error estimation in the analysis of anomalous diffusion — •Henrik Seckler[1] and Ralf Metzler[1,2] — [1]Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany. — [2]Asia Pacific Centre for Theoretical Physics, Pohang 37673, Republic of Korea

Modern single-particle-tracking techniques produce extensive time-series of diffusive motion in a wide variety of systems, from single-molecule motion in living-cells to movement ecology. The quest is to decipher the physical mechanisms encoded in the data and thus to better understand the probed systems. We here augment recently proposed machine-learning techniques for decoding anomalous-diffusion data to include an uncertainty estimate in addition to the predicted output. To avoid the Black-Box-Problem a Bayesian-Deep-Learning technique named Stochastic-Weight-Averaging-Gaussian is used to train models for both the classification of the diffusion model and the regression of the anomalous diffusion exponent of single-particle-trajectories. Evaluating their performance, we find that these models can achieve a well-calibrated error estimate while maintaining high prediction accuracies. In the analysis of the output uncertainty predictions we relate these to properties of the underlying diffusion models, thus providing insights into the learning process of the machine and the relevance of the output.

DY 17.5 Tue 11:00 ZEU 160

A machine learned classical density functional for orientational correlations in the Kern-Frenkel model for patchy particles — •Alessandro Simon[1,2] and Martin Oettel[1] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Models of patchy particles in a generic form (hard spheres decorated with a fixed number of attraction sites), posses an interesting phase behaviour, despite their apparent simplicity. This includes gel-formation and a vanishing fluid density at the gas-liquid coexistance, as the number of attractive patches and temperature is decreased. Using simulations of a symmetric four-patch model, we examine the orientational order of the particles and the effects of their tetrahedral symmetry on the expansion of density profiles and pair correlations in rotational invariants. Building on an existing classical density functional model which is formulated on the basis of Wertheim's theory for associating liquids and does not resolve orientational correlations [Stopper et al. J. Chem. Phys. 149, 224503 (2018)], we construct an improved density functional using machine learning and show that it yields the correct orientation distribution in slit-like geometries.

15 min. break

DY 17.6 Tue 11:30 ZEU 160

Classification of Gel Networks using Graph Convolutional Neural Networks — •Matthias Gimperlein and Michael Schmiedeberg — FAU Erlangen-Nürnberg, Erlangen, Germany

The structural properties of gel networks are important for the mechanical properties of the corresponding gels. We analyze gel networks and their structure using a machine learning approach based on graph convolutional networks (GCN) employing only the local neighborhood of particles as input information.

Using these we define a GCN-Autoencoder to reconstruct adjacency matrices of networks and quantitatively analyze in which properties the prediction of the network differs from the original input. This includes analysis on the abstract graph level as well as on the real physical network level.

Furthermore we use GCNs to classify gel networks depending i.e. on the loopsizes which are present in the network. Our goals include getting robust classification of strongly or weakly connected gel networks, predictions of minimal connecting structures and an insight how - according to an artificial intelligence - gel networks look like.

DY 17.7 Tue 11:45 ZEU 160

A 3-layer injection-locked multimode semiconductor laser neural network — •Elizabeth Robertson[1,3], Romain Lance[2], Anas Skalli[2], Xavier Porte[2], Janik Wolters[1,3], and Daniel Brunner[2] — [1]Deutsches Zentrum für Luft-und Raumfahrt, 12489 Berlin, Germany — [2]Institut FEMTO-ST, Université Bourgogne Franche-Comté, CNRS UMR6174, Besançon, France — [3]Technische Universität Berlin, Institut für Optik und Atomare Physik, 10623 Berlin, Germany

Optical hardware implementations of artificial neural networks (ANNs) have become a hot topic of research due to the inherent parallelism, potentially high speed and energy efficiency of optics [1]. Semiconductor laser networks are of specific interest as they are highly non-linear systems, which can be modulated at high throughput [2]. Previous work using spatial modes as nodes of an ANN, illustrated the use of multimode large area VSCELs for neural network computing in a fully parallel substrate, without pre- or post-processing [3,4]. We further expand this concept to a three-layer network consisting of mutually coupled multimode VSCELs, injection locked to a DFB laser. Here, information is fed into the network by modulating the injection laser, and boolean output weights are implemented using a digital micromirror device. We present an outline of the system, investigate its locking behavior and non-linear response. [1] Huang C. et al., Advances in Physics: X 7, 1 (2022) [2] Skalli A. et al., Opt. Mater. Express 12, 2395-2414 (2022) [3] Porte X. et al., J. Phys. Photonics 3 024017 (2021) [4] Skalli A. et al., Opt. Mater. Express 12, 2793-2804 (2022)

DY 17.8 Tue 12:00 ZEU 160

Efficiently compressed time series approximations — •Paul Wilhelm[1] and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute of Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Germany — [2]Lakeside Labs, Klagenfurt, Austria

Time series emerge from a broad range of applications, for instance as stock market pricing, electrocardiographic recordings or trajectories in chaotic dynamical systems. Long time series require an approximation scheme for compressing and storing, analyzing or predicting them.

How can we construct efficient approximations? Continuous, piecewise linear functions with variable knots that mark the end points of each segment are easy to handle and often used. However, fitting the knots is highly nonlinear and only feasible with a lucky initial guess. Here we propose a novel method that exploits repeating motifs in the data and thereby avoids fitting each knot independently, significantly accelerating the construction of the approximation.

Starting from the beginning of a time series, the method iteratively integrates subsequent data points. For each extension, it tries to reuse parts of the already existing function to approximate the yet uncovered data points. If successful, each motif is approximated only once and reused multiple times. As a result, the knots of the function are interdependent and can thus be represented in compact form. In contrast to deep neural networks that also find a piecewise linear approximation, our approach offers a efficient and explainable method and thereby a novel perspective onto why and how deep neural networks may work.

DY 17.9 Tue 12:15 ZEU 160

Active Learning Strategies for Molecular Dynamics with Machine-learned Potentials — •Shubham Sharma[1] and Mariana Rossi[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Machine-learning potentials (MLPs) have allowed the efficient modelling of complex atomistic systems with ab-initio accuracy. Normally, the construction of sufficiently large and diverse reference datasets, using first-principles calculations, is a bottleneck for training. Therefore, several active-learning strategies have been proposed, which aim to make the training more efficient, especially when used together with molecular-dynamics techniques [1]. In this work, we explore building protocols for training sets of high-dimensional neural-network potentials (HDNNPs), targeting specifically weakly-bound condensed-phase systems. For that, we show how we can use and augment the committee-model framework within the i-PI code [2]. We show results for acene-based molecular crystals and discuss the advantages and limitations of different learning strategies to treat different crystal polymorphs, at various thermodynamic conditions. [1] C. Schran et. at., J. Chem. Phys. **153**, 104105 (2020). [2] V. Kapil et. al., Comput. Phys. Commun. **236**, 214 (2019).

DY 17.10 Tue 12:30 ZEU 160

Machine learning-based prediction of dynamical clustering in excited granular media — •Sai Preetham Sata, Dmitry Puzyrev, and Ralf Stannarius — Institute of Physics and MARS, Otto von Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Granular gases excited by external force tend to undergo gas-like to cluster transitions when the filling fraction of particles reaches sufficient value. In order to understand the clustering dynamics, experiments were performed in microgravity [1,2]. A numerical simulation model based on DEM is available. By varying geometrical and material parameters, a phase diagram is obtained. Cumulative distribution functions of the density profiles and uniform distribution profiles are obtained and the maximum distance between these curves is compared to the Kolmogorov-Smirnov (KS) test threshold to detect gas-cluster transitions. We aim to predict the formation of dynamical clusters with the use of machine learning techniques as an alternative to DEM simulations, requiring much less computational effort. We confirm the reliability of the predictions for relatively well-studied spherical beads, with the perspective of analysis of clustering of more complicated particle shapes.

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References: [1] S. Aumaître, et al. Review of Scientific Instruments 89, 075103 (2018) [2] M. Noirhomme et al. EPL 123, 14003 (2018) [3] Puzyrev, D., Fischer, D., Harth, K. et al., Sci Rep 11, 10621 (2021).