DY 39: Machine Learning in Dynamics and Statistical Physics II

Time: Thursday 15:00–16:30 Location: H47

DY 39.1 Thu 15:00 H47

Fast and energy-efficient reservoir computing using a resonant-tunneling diode — •Osamah Sufyan[1], Antonio Hurtado[2], and Kathy Lüdge[1] — [1]Technische Universität Ilmenau, Institut für Physik, Weimarer Straße 25, 98693 Ilmenau, Germany — [2]University of Strathclyde, Institute of Photonics, Glasgow, United Kingdom

Resonant-tunneling diodes (RTDs) have garnered significant attention as platforms for neuromorphic computing, owing to their fast operation and intricate nonlinear dynamics. Among the most hardware-friendly and energy-efficient paradigms in this domain is reservoir computing (RC), where the nonlinear dynamics of a physical system are leveraged to perform complex computational tasks.

In this work, we explore the use of a single RTD as a reservoir, employing time-multiplexing techniques for chaotic time-series prediction achieving similar performance to previous RC approaches [1]. Our findings highlight the relationship between the RTD's distinct dynamical regimes and the reservoir's performance in predicting future values of the Mackey-Glass and Lorenz system time series. Additionally, we investigate the RTD as an excitable system, demonstrating its potential for spiking neural network applications. We examine various data encoding and decoding strategies for spike-based operations, further underscoring the versatility of RTDs in neuromorphic computing.

[1] L. Jaurigue and K. Lüdge, *Neuromorph. Comput. Eng.*, **4**, 014001 (2024).

DY 39.2 Thu 15:15 H47

Tailored minimal reservoir computing: Connecting nonlinearities in the input data with nonlinearities in the reservoir — Davide Prosperino[1], Haochun Ma[1], Vincent Gross[2], and •Christoph Räth[3,2] — [1]Allianz Global Investors (AGI) — [2]Ludwig-Maximilians-Universität (LMU) — [3]Deutsches Zentrum für Luft- und Raumfahrt (DLR)

The traditional setup of reservoir computing (RC) for predicting time series uses random matrices to define the underlying network and the input layer. Here, we show that a few modifications, which eliminate randomness and minimize computational resources and data requirements, lead to significant and robust improvements in short- and long-term predictive performance. We introduce block-diagonal reservoirs, which implies that a reservoir can be composed of multiple smaller reservoirs. Further, the non-linear activation function at the nodes can be dispensed with if the non-linear step in the analysis chain is shifted to the output layer. The input weights are determined according to well-defined rules. Any random initialization has thus been eliminated. By varying the remaining four hyperparameters, it is now possible to systematically investigate the transition from a linear, disjunct mapping of the input data to the output data to a combined nonlinear one. It is further demonstrated that there is a connection between the nonlinearities in the input data and the nonlinearities in the reservoir such that the best prediction results are obtained when both nonlinearities match. It becomes thus possible to define an optimally tailored setup for minimal RC for data sets with given nonlinearities.

DY 39.3 Thu 15:30 H47

Physical Reservoir Computing with Ferroelectric Oxides — •Atreya Majumdar[1], Yan Meng Chong[2], Dennis Meier[2], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Physical reservoir computing has shown remarkable potential in magnetic systems by utilizing their complex, non-linear, and history-dependent intrinsic dynamics for machine learning tasks [1]. More recently, ferroelectric materials - the electrical analogs of magnetic systems - have garnered attention. These materials not only meet all the essential criteria for reservoir computing but also bring unique advantages [2]. Here, we introduce the ferroelectric semiconductor ErMnO3 as a novel physical reservoir. By utilizing the material's non-linear and history-dependent photocurrent response, we demonstrate its capability to recognize varying input light pulse intensities. This study highlights the potential of ferroelectric materials in physical reservoir computing, paving the way for energy-efficient and scalable computing architectures.

[1] O. Lee, et al., Perspective on unconventional computing using magnetic skyrmions. Appl. Phys. Lett. 122, 260501 (2023).

[2] K. Everschor-Sitte, A. Majumdar, et al., Topological magnetic and ferroelectric systems for reservoir computing. Nat. Rev. Phys. 6, 455 (2024).

DY 39.4 Thu 15:45 H47

Describing heat transport in crystalline polymers in real and reciprocal space — Lukas Reicht[1], Lukas Legenstein[1], Sandro Wieser[2], and •Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]TU Wien, Austria

Heat transport modelling either relies on describing the propagation of phonons employing the Boltzmann transport equation or on simulating the real-space dynamics of atoms using (non)-equilibrium molecular dynamics techniques. Due to the structural complexity of crystalline polymers both approaches call for a highly accurate but at the same time numerically extremely efficient strategy for describing interatomic interactions. This is achieved via machine-learned potentials, where we combine an efficient active-learning strategy with moment-tensor potentials.[1,2] Additionally, real-space and reciprocal space approaches make fundamentally different approximations regarding anharmonicities and phonon occupations. Here, we show that for polymers of intermediate complexity, like crystalline polythiophene, real- and reciprocal space approaches yield consistent values of the thermal conductivities at least when using an accurate machine-learned potential. Interestingly, for the seemingly much simpler crystalline polyethylene such an agreement is only obtained when higher-order phonon scattering is considered. This can be traced back to a selection rule arising from the comparably simple phonon band structure of polyethylene. [1] npj Comput Mater 10, 18 (2024); [2] Molecules 29, 3724 (2024)

DY 39.5 Thu 16:00 H47

Reinforcement learning for autonomous navigation of active particles in complex flow fields — •Diptabrata Paul and Frank Cichos — Peter Debye Institute for Soft Matter Physics, Universität Leipzig, 04103 Leipzig, Germany

Sensing and feedback on environmental stimuli are integral to regulating diverse functions in living systems, ranging from sub-cellular processes to evolution of navigation strategies such as chemotaxis and phototaxis. Unlike living systems, noisy artificial microswimmers have limited ability to adapt to various stationary and dynamic environmental perturbations to yield optimized behaviour for a given task. Consequently, reacting to such environmental cues becomes indispensable for achieving effective navigation and control in complex and noisy settings. In this context, we explore incorporation of machine learning algorithm for autonomous decision making for navigation of an active microswimmer within noisy environments. While naive navigation policies yield inefficient and ineffective solutions under changing conditions, employing actor-critic reinforcement learning (RL) framework trained in experiments leads us to quasi-optimal policies that are capable of navigating, even in presence of complex flow fields. Our study exhibits that a model trained under noisy conditions successfully learns effective navigation policies and are robust with respect to environmental perturbations such as hydrodynamic flow fields as well as varying initial conditions. This work paves the way for development of online RL for modelling adaptive behaviour and navigation of active microswimmers in complex fluidic scenarios.

DY 39.6 Thu 16:15 H47

Predictability Analysis of Discrete Time-Series Data with a Hamiltonian-Based Filter-Projection Approach — •Henrik Kiefer and Roland Netz — Freie Universität Berlin, Fachbereich Physik, Berlin, Deutschland

The generalized Langevin equation (GLE), derived by projection from a general many-body Hamiltonian, exactly describes the dynamics of an arbitrary coarse-grained variable in a complex environment. However, analysis and prediction of real-world data with the GLE is hampered by slow transient or seasonal data components and time-

discretization effects. Machine-learning (ML) techniques work but are computer-resource demanding and difficult to interpret. We show that by convolution filtering, time-series data decompose into fast, transient and seasonal components that each obey Hamiltonian dynamics and, thus, can be separately analyzed by projection techniques. We introduce methods to extract all GLE parameters from highly discretized time-series data and to forecast future data including the environmental stochasticity. For daily-resolved weather data, our analysis reveals non-Markovian memory that decays over a few days. Our prediction accuracy is comparable to ML long short-term memory (LSTM) methods at a reduced computational cost compared to LSTM. For financial data, memory is very short-ranged and the dynamics effectively is Markovian, in agreement with the efficient-market hypothesis; consequently, models simpler than the GLE are sufficient. Our GLE framework is an efficient and interpretable method for the analysis and prediction of complex time-series data.