DY 6: Machine Learning in Dynamics and Statistical Physics I

Time: Monday 9:30–13:00 Location: HÜL/S186

DY 6.1 Mon 9:30 HÜL/S186

Reservoir Computing with Hydrodynamically Coupled Active Colloidal Oscillators — •Veit-Lorenz Heuthe[1], Lukas Seemann[1], Samuel Tovey[2], and Clemens Bechinger[1,3] — [1]Universität Konstanz, Konstanz, Germany — [2]Universität Stuttgart, Stuttgart, Germany — [3]Centre for the Advanced Study of Collective Behavior, Konstanz, Germany

Reservoir computing is a newly emerging framework that exploites the dynamical response of complex physical systems to external perturbations. The high-dimensional, non-linear dynamics of active matter systems with hydrodynamic interactions offsers great potential for highly tunable physical reservoirs. Here, we present a physical reservoir that exploits the hydrodynamic interactions between several hundred colloidal oscillators for chaotic timeseries forecasting. We demonstrate that the inherent memory in this system facilitates detection of hidden anomalies in non-Markovian time-signals. Our results highlight the potential of active matter for locating subtle, non-disruptive signatures in e.g. financial stock markets, physiological measurements or seismic and climate data. Achieving such computing functinalities in physical systems could enable the development of intelligent hardware for edge-computing.

DY 6.2 Mon 9:45 HÜL/S186

From Phase-Space Fluctuations to Predictive Power: Entropy Production as a Metric for Swarm Reservoir Computing — •Patrick Egenlauf[1,2] 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

In reservoir computing, a time-varying input is projected onto a high-dimensional state space, allowing a simple linear readout to retrieve task-relevant features. Physical substrates such as active-matter swarms promise efficient, low-energy computation, but a quantitative selection criterion, that reliably indicates a good reservoir, is missing. We simulated an interacting swarm subjected to an external driver and evaluated two entropy measures: system entropy, quantifying phase-space density fluctuations, and environment entropy, representing heat dissipation. For each parameter set of the swarm interactions, we computed the relative differences for the system and environment entropy between undriven and driven cases and measured the driver work performed on the system. Both relative differences display robust linear correlations with forecast accuracy, while the driver work matches the performance curve almost perfectly, indicating that driver-induced entropy production dominates the reservoir's information-processing capacity. Consequently, entropy production offers a quantitative metric for tuning swarm-based reservoirs toward optimal performance.

DY 6.3 Mon 10:00 HÜL/S186

Performing inference with physical response: Reservoir computing with active matter substrates — Mario U. Gaimann[1] and •Miriam Klopotek[1,2] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]WIN-Kolleg of the Young Academy, Heidelberg Academy of Sciences and Humanities, Heidelberg, Germany

We explore questions of real-time inference and forecasting of chaotic signals, re-interpreting them in terms of nonequilibrium physical response, by studying a model of information processing with an active matter substrate used in the reservoir computing (RC) paradigm. The system becomes robustly optimal for computing in a particular dynamical regime due to its intrinsic ability to relax efficiently, which, under driving, unlocks maximal dynamical diversity and susceptibility to chaotic input signals; the mechanisms include self-healing, multi-step dynamical response, and adaptive morphological reorganization [1,2]. Shifting the system's response away from direct-agent toward collective variables is key, as evidenced by cross-correlative functions in dynamics [2]. These ideas shed light on self-optimizing inference in bio-inspired or material computing that flexibly exploits dynamics across diverse collective scales.

[1] M. U. Gaimann and M. Klopotek, `arXiv:2505.05420` (2025).
[2] M. U. Gaimann and M. Klopotek, `arXiv:2509.01799` (2025).

DY 6.4 Mon 10:15 HÜL/S186

Learning single and multiple chaotic systems with minimal reservoir computers — •Francesco Martinuzzi and Holger Kantz — Max Planck Institute for the Physics of Complex Systems

Chaotic dynamics are present in a multitude of natural and engineered systems. Recently, chaos has been modeled using machine learning (ML) methods thanks to their ability to infer underlying governing equations without directly accessing them. Among ML models, echo state networks (ESNs) have been widely investigated because of their simple construction and efficient training. However, ESNs typically rely on randomly initialized reservoirs whose stochastic connectivity makes them difficult to interpret and tune. To what extent are random and complex reservoir topologies actually necessary for learning chaotic dynamics with ESNs? We show that deterministic constructions of the reservoir matrix outperform random initializations for the reconstruction of chaotic attractors. By testing ten distinct deterministic topologies against random reservoirs on over 90 different attractors, our results demonstrate consistently better performance for deterministic reservoirs. Furthermore, we show how the same deterministic reservoir topologies can be leveraged to learn multiple chaotic systems with a single reservoir computer, thereby showcasing multifunctionality.

DY 6.5 Mon 10:30 HÜL/S186

Understanding task performance of time-multiplexed optical reservoir computing via polynomial expansion — •Elias Koch[1], Julien Javaloyes[2], Svetlana V. Gurevich[1,3], and Lina Jaurigue[4] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str.9 48149 Münster, Germany — [2]Departament de Física and IAC3, Universitat de les Illes Balears, Campus UIB 07122 Mallorca, Spain — [3]Center for Data Science and Complexity (CDSC), University of Münster, Corrensstrasse 2, Münster, 48149, Germany — [4]Institute of Physics, Technische Universität Ilmenau , 98693 Ilmenau, Germany

We study the dynamics of a reservoir computer, realized as a linear optical microcavity with a time-multiplexed injection stream. In the first step, the output is processed with different nonlinearities, allowing to analyze the resulting polynomials and to what extend they can approximate different tasks. To that end, we compare two different discrete tasks, both derived from the Lorenz system through integration with a Runge-Kutta (4) scheme, but sampled to different stepsizes. There, we identify the respective underlying polynomial map and discuss the occuring terms. We compare these results with the impact of employing nonlinear nodes by introducing a Kerr nonlinearity in the optical microcavity.

DY 6.6 Mon 10:45 HÜL/S186

Physical Reservoir Computing with Ferroelectric Oxides for Time-series Classification Tasks — •Atreya Majumdar[1], Yan Meng Chong[2], Dennis Meier[1,2,3], 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 — [3]Research Center Future Energy Materials and Systems, Research Alliance Ruhr, Bochum, Germany.

Physical reservoir computing leverages the intrinsic complexity, nonlinearity, and fading memory of material systems to process temporal data for solving time-series pattern recognition tasks. Magnetic and ferroelectric materials have recently emerged as promising reservoir computers, offering dynamics well suited for processing time-dependent signals [1]. Here, we demonstrate that the photocurrent dynamics of the ferroelectric semiconductor ErMnO3 can be harnessed as an effective physical reservoir for real-time time-series classification. Moreover, the relaxation time of the photocurrent can be controllably tuned, providing flexibility to capture different temporal features and thereby enhancing performance. Altogether, the results highlight the potential of ferroelectric oxides as scalable, energy-efficient platforms for real-time physical reservoir computing.

[1] K. Everschor-Sitte, et al., Topological magnetic and ferroelectric

systems for reservoir computing. Nat. Rev. Phys. 6, 455 (2024).

15 min. break

DY 6.7 Mon 11:15 HÜL/S186

Checking the superiority of multi-model mean forecasts by reservoir computing — Daniel Estevez Moya[1,3], Erick A. Madrigal Solis[1,2], Ernesto Estevez Rams[3], and •Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Techology, Dresden, Germany — [3]Facultad de Física, Universidad de La Habana, Cuba

In weather prediction and climate forecasts it has been observed that taking the arithmetic mean forecast of an ensemble of different models is often superior to most of the individual models. We use Reservoir Computing to generate easily a large ensemble of models and study their performance on deterministic toy models. While each individually trained reservoir comes with its own model error which is a systematic error, we verify that the arithmetic mean of these forecasts is closer to the truth than most of the individual forecasts. We present a detailed dynamical explanation for this observation.

DY 6.8 Mon 11:30 HÜL/S186

Controlling dynamical systems into unseen target states using machine learning — Daniel Köglmayr[1,2], Alexander Haluszczynski[3], and •Christoph Räth[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt (DLR) — [2]Ludwig-Maximilians-Universität (LMU) — [3]Allianz Global Investors (AGI)

Controlling nonlinear dynamical systems is a central task in many different areas of science and engineering. Combining previous work on controlling chaotic systems to arbitrary states [1] and extrapolating the system behavior into unseen parameter regions [2] using machine learning, we present here a novel, model-free, and data-driven methodology for controlling complex dynamical systems into previously unseen target states, including those with significantly different and complex dynamics. Leveraging a parameter-aware realization of next-generation reservoir computing (NGRC), our approach accurately predicts system behavior in unobserved parameter regimes, enabling control over transitions to arbitrary target states utilizing a new prediction evaluation and selection scheme [3]. By extending the applicability of machine learning-based control mechanisms to previously inaccessible target dynamics, this methodology opens the door to transformative new applications while maintaining exceptional efficiency. Our results highlight reservoir computing as a powerful alternative to traditional methods for dynamic system control.

[1] A. Haluszczynski & C. Räth, Sci Rep 11, 12991 (2021), [2] D. Köglmayr & C. Räth, Sci Rep 14, 507 (2024), [3] D. Köglmayr, A. Haluszczynski & C. Räth, submitted (https://arxiv.org/abs/2412.10251)

DY 6.9 Mon 11:45 HÜL/S186

Noise-Balanced Sparse Grid Surrogates for Multiscale Coupling of Monte Carlo and Continuum Models — •Tobias Hülser and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

Incorporating a high-fidelity microscopic Monte Carlo model into multiscale simulations can easily become intractable, implying the necessity of surrogate models in many practical applications. Unfortunately, if the microscopic model depends on many macro-variables this can become quite challenging due to the 'curse of dimensionality'. Furthermore, the sampling noise in the underlying Monte Carlo data can lead to uncontrolled errors corrupting the surrogate even though it would be highly accurate in the case of noise-free data. To address these points, we have developed a novel sparse grids interpolation approach which balances interpolation and noise induced errors complemented by a multilevel on-the-fly construction during the multi-scale simulation. Besides its efficiency, an appealing feature is the ease of use of the approach with a single hyperparameter controlling the whole surrogate construction - from which data needs to be created (and how accurately) to the surrogate's accuracy with guaranteed convergence. We demonstrate the approach on examples from heterogenous catalysis, incorporating microscopic kinetic Monte Carlo models into convection-diffusion type reactor scale simulations.

DY 6.10 Mon 12:00 HÜL/S186

Learning Time Trajectories of a Stochastic Dynamical System with a Slowly Varying Parameter — •Changho Kim[1], Zihan Xu[1], Andrew Nonaka[2], and Yuanran Zhu[2] — [1]University of California, Merced, California, USA — [2]Lawrence Berkeley National Laboratory, Berkeley, California, USA

The statistics-informed neural network (SINN) is a reliable machine learning approach for learning and reproducing stochastic trajectories based on the statistical properties of sample trajectory data, particularly for stationary, Gaussian-like, multidimensional stochastic processes. However, to enable practical applications–such as surrogate modeling for the development of hybrid simulation methods–SINN must be extended to learn quasi-stationary dynamics driven by a slowly varying parameter. We enhance the SINN framework by incorporating this parameter as an additional input and by introducing loss functions to capture its influence, as well as proposing a new neural network structure that takes both white noise sequences and time trajectories of the slowly varying parameter as inputs. Additionally, we propose an alternative method for estimating a conditional probability density function to address computational constraints. We validate our approach through two benchmark problems: the dissociative adsorption problem and Langevin dynamics in an oscillating double-well potential.

DY 6.11 Mon 12:15 HÜL/S186

Learning spatiotemporal patterns from mean-field data — •Edmilson Roque dos Santos[1] and Tiago Pereira[2] — [1]MPI-PKS,Germany — [2]University of São Paulo, Brazil

Networks of coupled dynamical systems are fundamental models across the sciences, from physics to neuroscience. Despite their success, the governing equations of such systems are often unknown, limiting our ability to predict and control their dynamics. A major current effort is to learn these governing equations directly from data. However, existing approaches typically require access to the time series of all node states, which is rarely available outside controlled experiments. In most realistic scenarios, only aggregate or mean-field data, such as linear combinations of node states, can be measured. In this case, learning the governing equations from mean-field data inevitably becomes a secondary goal, since one must first learn the network trajectory that generated the observed measurements. This task is inherently challenging because distinct network states can yield identical macroscopic observations. Here, we address the problem of learning the network trajectory from random mean-field measurements. We show that accurate reconstruction becomes possible when the network exhibits structured spatiotemporal patterns, such as traveling waves. By representing these patterns sparsely in the Fourier domain, we leverage compressive sensing theory to formulate a convex optimization problem that robustly reconstructs the network trajectory. We illustrate our findings using a unidirectional ring of coupled Stuart-Landau oscillators.

DY 6.12 Mon 12:30 HÜL/S186

Discovering Mechanisms and Governing Laws with Sparse Regression — •Gianmarco Ducci, Maryke Kouyate, Juan Manuel Lombardi, Artem Samtsevych, Karsten Reuter, and Christoph Scheurer — FHI Berlin

Interpretable data-driven methods have proven viable for deriving complex vector fields directly from experimental data. Their inherent differential formulation, however, make them vulnerable to noise, which can compromise the sparsity of the inferred models. In order to promote sparsity, a weak formulation can be employed. Then, finding the optimal set of basis functions is a necessary prerequisite, yet a challenging task to determine in advance.

We present the release version of the Data-Driven Model Optimizer `ddmo`, a symbolic regression tool which provides fine-grained control over the admissible space of candidate terms. Its core contribution lies in the systematic optimization of the library of functions, implemented through two complementary engines: a standard SINDy-based differential formulation and a weak-form variant. Its modular structure further enables the optimization of test functions within the weak formulation. An overview of the software capabilities is provided, alongside with a case study illustrating the reconstruction of effective kinetics from experimental reactor data.

DY 6.13 Mon 12:45 HÜL/S186

POD-Subspace Reconstruction of Convective Reversal Dynamics from Limited Sensor Data — •Tim Kroll and Oliver Kamps — CDSC ,University of Münster

We introduce a data-driven modelling framework that leverages a hybrid LSTM-neural-network architecture to capture convection reversals from limited time-series measurements.. The method operates entirely in POD space, enabling efficient and accurate reconstruction of complex dynamical systems from limited observations by modelling non-orthogonal modes as a superposition of POD modes. The corresponding dynamics are modelled by an LSTM, incorporating knowledge about the history of the timeseries. We demonstrate its effectiveness on convection processes, showing that measurements from a single sensor - of either temperature T or velocity V - are sufficient to recover the full spatiotemporal dynamics, consisting of temperature, velocity or a combination of both, within the reduced representation. Furthermore this approach has potential to be applied in different scientific fields detached from convection or fluid dynamics.