SOE 13: Data Analytics of Complex Dynamical Systems (joint session DY/SOE)

Time: Thursday 9:30–12:00 Location: MOL 213

SOE 13.1 Thu 9:30 MOL 213

Reverse-engineering method for XPCS studies of non-equilibrium dynamics — •Anastasia Ragulskaya[1], Vladimir Starostin[1], Nafisa Begam[1], Anita Girelli[1], Hendrik Rahmann[2], Mario Reiser[2], Fabian Westermeier[3], Michael Sprung[3], Fajun Zhang[1], Christian Gutt[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]DESY, Germany

X-ray photon correlation spectroscopy (XPCS) is a powerful tool for the investigation of dynamics covering broad time and length scales [1]. For non-equilibrium states, the resulting time-dependent dynamic behavior can be described using the two-time correlation function (TTC), which often contains more interesting features than only the component along the diagonal, and cannot be easily interpreted via classical simulation methods. Here, a reverse-engineering (RE) approach is proposed based on particle-based simulations [1]. This approach is applied to XPCS measurements on a protein solution undergoing liquid-liquid phase separation. We demonstrate that the rich features of experimental TTCs can be well connected with the key control parameters including size distribution, concentration, viscosity, and mobility of domains. The dynamic information obtained from this RE analysis goes beyond existing theory. The RE approach established in this work is applicable to other processes such as film growth, domain coarsening, or phase transformations.

[1] A. Ragulskaya et. al., IUCrJ 9 (2022), 439.

SOE 13.2 Thu 9:45 MOL 213

Sensitivity of principal components to changes in the presence of non-stationarity — •Henrik Bette and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Deutschland

Non-stationarity affects the sensitivity of change detection in correlated systems described by sets of measurable variables. We study this by projecting onto different principal components. Non-stationarity is modeled as multiple normal states that exist in the system even before a change occurs. The studied changes occur in mean values, standard deviations or correlations of the variables. Monte Carlo simulations are performed to test the sensitivity for change detection with and without knowledge about the non-stationarity for different system dimensions and numbers of normal states. A comparison clearly shows that the knowledge about the non-stationarity of the system greatly improves change detection sensitivity for all principal components. This improvement is largest for those components that already provide the greatest possibility for change detection in the stationary case.

SOE 13.3 Thu 10:00 MOL 213

Inferring partial differential equations from molecular dynamics simulations — •Oliver Mai, Tim Kroll, Uwe Thiele, and Oliver Kamps — Institute of Theoretical Physics and Center for Nonlinear Science, University of Münster

Although integral to scientific or engineering applications, deriving partial differential equations (PDEs) solely from experimental data proves quite challenging and in most cases relies on physical principles in addition to qualitative behaviour of the system. In the last decade various efforts based on empirical data have been put forth to supplement first-principle derivations in theoretical sciences. That is in place of or in addition to typical conservation laws or phenomenological observations, time series data has been used to yield analytic expressions to describe the spatio-temporal evolution of a given dynamical system. While there have been various improvements in the sparsity and interpretability of the results, we provide another approach to optimization using the predictive power of the estimation when integrating it. Additionally aggregated small scale behaviour in macro- or mesoscopic experiments may exhibit unknown governing laws and as such a way for comparing data more directly to models derived in statistical physics may prove critical in furthering our understanding. To this end we study the application of system identification methods on molecular dynamics (MD) simulations.

SOE 13.4 Thu 10:15 MOL 213

Reproducibility of analysis workflows in biomedical physics — •Alexander Schlemmer[1,4], Inga Kottlarz[1,2], Baltasar Rüchardt[1,3,4], Ulrich Parlitz[1,2,4], and Stefan Luther[1,2,3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany — [3]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany — [4]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Germany

Sustainable and well-documented data analysis workflows are essential for effectiveness and reproducibility in data-intensive research. In our terminology, documentation includes method and algorithm descriptions as well as human- and machine-readable representations of parameters, initial conditions and data, versions and dependencies and a well-defined software execution environment.

In practice, many software frameworks for reproducibility fail to achieve a widespread adoption. Using examples from data analysis in cardiac research, we illustrate typical challenges and show, how simple guidelines - when implemented in a pragmatic way - can already lead to a high degree of documentation and reproducibility. Furthermore, we discuss the employment of containers and semantic data management which simplify reproducibility, findability and interoperability.

SOE 13.5 Thu 10:30 MOL 213

Bayesian approach to anticipate critical transitions in complex systems — •Martin Hessler[1,2] and Oliver Kamps[2] — [1]Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Center for Nonlinear Science, Westfälische Wilhelms-Universität Münster, 48149 Münster

Complex systems in nature, technology and society can undergo sudden transitions between system states with very different behaviour. In order to avoid undesired consequences of these tipping events, statistical measures have been proposed as leading indicators. They can give a hint of an ongoing bifurcation-induced (B-tipping) destabilization process. However, we present an alternative approach that is open-source available and more robust under numerous aspects. It assumes the dynamical system to be described by a Langevin equation. Starting from this stochastic description, we combine MCMC sampling, rolling window methods and Bayesian reasoning to derive the drift slope as an alternative early warning sign including credibility bands which make it easier to distinguish significant leading indicator trends prior to B-tipping. Furthermore, our approach provides information about an increasing noise level in a multi-stable system. This is an important information related to the Kramers escape rate of a noise-induced tipping (N-tipping) event. We show some results and discuss the method's potential to be applied in N-tipping scenarios and under more complex conditions like correlated non-Markovian or multiplicative noise. Finally, possible limitations and tasks of future research are mentioned.

15 min. break

Invited Talk SOE 13.6 Thu 11:00 MOL 213

Power law error growth rates – a dynamical mechanism for a strictly finite prediction horizon in weather forecasts — Hynek Bednar[1,2], Jonathan Brisch[1], Burak Budanur[1], and •Holger Kantz[1] — [1]Max Planck Insstiute for the Physics of Complex Systems, Dresden, Germany — [2]Dept. of Atmospheric Physics, Charles University, Prague, Czech Republic

While conventional chaotic systems have a finite positive Lyapunov exponent, physical arguments and observations suggest that the maximal Lyapunov exponent of the model equations of the atmosphere is the larger the smaller are the resolved spatial scales. Specifically, a power law divergence of the scale dependent error growth rate would translate into a strictly finite prediction horizon, since due to the divergence, additional accuracy of initial conditions is not translated into longer prediction times. We present conceptual toy models with such behavior, we show its presence in a more realistic spatially extended system with advective transport, and we present numerical results from turbulence simulations where the largest Lyapunov exponent scales as an inverse power of spatial resolution. The idea of a power law scale dependence of error growth rates and of a finite prediction horizon is also supported by re-analysis of numerical error growth experiments performed with an operational weather model. Altogether, this sug-

gests that the prediction horizon of numerical weather prediction is strictly finite.

SOE 13.7 Thu 11:30 MOL 213

Wave Digital Optimization of a Modified Compact Models of 1T-1R Random Resistive Access Memory Cells — •Bakr Al Beattie[1], Max Uhlmann[2], Gerhard Kahmen[2], and Karlheinz Ochs[1] — [1]Ruhr-Universität Bochum, Lehrstuhl für digitale Kommunikationssysteme, Bochum, Deutschland — [2]Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Deutschland

Random Resistive Access Memory (RRAM) cells are popular memristive devices that are commonly used in neuromorphic applications. In this context, RRAM cells are usually utilized to embed synaptic plasticity, a property that is exhibited by biological synapses, into analog-based artificial neural networks. However, since RRAM-based technology has yet to reach a state of maturity, circuit designers are usually forced to make use of compact models to avoid dealing with device-to-device variabilities. The Stanford PKU model is a well-established compact model that has been developed to capture the dynamics of 1T-1R RRAM cells. In this contribution, we present a modified compact model, based on the Stanford PKU model, that takes more properties of real RRAM cells into account, such as the RESET voltage shift in multilevel devices. To demonstrate the capabilities of our model, we exploit the wave digital concept to apply a live parameter optimization, which fits the model parameters to a technologically reproducible device from the Leibniz Institute for High Performance Microelectronics (IHP).

SOE 13.8 Thu 11:45 MOL 213

Discovering Causality and Coupling in high dimensional nonlinear dynamical systems — •Tim Kroll[1,2] and Oliver Kamps[2] — [1]Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Center for Nonlinear Science, Westfälische Wilhelms-Universität Münster, 48149 Münster

In this talk we present a method to infer causal relationships between observables from data of systems where the underlying dynamics are not known a priori. The method is based on the hypothesis that the system of interest can in principle be described by a set of coupled nonlinear ordinary differential equations. Following the work of Prusseit and Lehnertz in 2008 we can then determine the couplings between observables by integrating out all other observables. Since the estimation of the underlying dynamical system invokes the efficient representation in terms of polynomials the method can be applied also to hight dimensional systems. We demonstrate the capabilities of the method by inferring the network structure of coupled Rössler-Attractors.