SOE 6: Data Analytics for Complex Systems (joint session DY/SOE)

Time: Monday 15:00–17:45 Location: H18

SOE 6.1 Mon 15:00 H18

Estimating covariant Lyapunov vectors from data — •Nahal Sharafi, Christoph Martin und Sarah Hallerberg — Hamburg University of Applied Sciences, Hamburg, Germany

Covariant Lyapunov vectors characterize the directions along which perturbations in dynamical systems grow. They have also been studied as predictors of critical transitions and extreme events. For many applications, it is necessary to estimate these vectors from data since model equations are unknown for many interesting phenomena. We propose a novel approach for estimating covariant Lyapunov vectors based on data records without knowing the underlying equations of the system. In contrast to previous approaches, our approach can be applied to high-dimensional datasets. We demonstrate that this purely data-driven approach can accurately estimate covariant Lyapunpov vectors from data records generated by low and high-dimensional dynamical systems. Additionally we test for the robustness against noise in a low-dimensional dynamical system.

SOE 6.2 Mon 15:15 H18

Extending the limits of Electrochemical Impedance Spectroscopy with Machine Learning and Digital Twins — •Limei Jin[1,2], Franz P. Bereck[2], Christian H. Bartsch[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]IEK-9, Forschungszentrum Jülich, Jülich, Germany

Electrochemical impedance spectroscopy (EIS) is widely used to characterize electrochemical energy conversion systems. The traditional analysis with equivalent circuit models (ECM) has recently been augmented by a transform based distribution of relaxation times (DRT) analysis which allows one to reduce the ambiguity in the construction of ECMs and thus overfitting. Yet, DRT, just like most traditional analyses, is firmly based in the linear response regime as well as based on frequency sweeps on a logarithmic scale. The latter makes these approaches time-consuming, the first limits their scope severely. To develop novel experimental spectroscopic excitation schemes that address these limitations, a model space of sufficiently realistic systems is required that substitutes for time-consuming measurements in terms of a digital twin. We present a joint experimental and theoretical approach for the construction of such a target space for the case of battery cell performance and ageing behaviour.

SOE 6.3 Mon 15:30 H18

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 as variance, autocorrelation, skewness and kurtosis have been proposed as leading indicators based on time series analysis. Under favourable conditions they can give a hint of an ongoing bifurcation-induced destabilization process. However, they suffer from their loose connection to complex system dynamics, sensitivity to noise and sometimes misleading trends. Therefore, we want to present an alternative approach assuming the dynamical system being 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. The Bayesian approach enables us to define credibility bands which make it easier to distinguish random fluctuations from real trends that imply a less resilient system. Our investigations suggest that the estimation procedure is rather robust even under strong noise. Besides, the noise level of the system is computed to get insights into the probability of a noise induced transition. We want to present some of the results and discuss possible limitations and tasks of future research.

SOE 6.4 Mon 15:45 H18

Stochastic Interpolation of Sparsely Sampled Time Series by a Superstatistical Random Process and its Synthesis in Fourier and Wavelet Space — •Jeremiah Lübke[1], Jan Friedrich[2], and Rainer Grauer[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany — [2]ForWind, Institute of Physics, University of Oldenburg, Küpkersweg 70, 26129 Oldenburg, Germany

A novel method is presented for stochastic interpolation of a sparsely sampled time signal based on a superstatistical random process generated from a Gaussian scale mixture. In comparison to other stochastic interpolation methods such as kriging, this method possesses strong non-Gaussian properties and is thus applicable to a broad range of real-world time series. A precise sampling algorithm is provided in terms of a mixing procedure that consists of generating a field $u(\xi, t)$, where each component $u_\xi(t)$ is synthesized with identical underlying noise but covariance $C_\xi(t, s)$ parameterized by a log-normally distributed parameter ξ. Due to the Gaussianity of each component $u_\xi(t)$, standard sampling algorithms and methods to constrain the process on the sparse measurement points can be exploited. The scale mixture $u(t)$ is then obtained by assigning each point in time t a $\xi(t)$ and therefore a specific value from $u(\xi, t)$, where $\log \xi(t)$ is itself a realization of a Gaussian process with a correlation time large compared to the correlation time of $u(\xi, t)$. Finally, a wavelet-based hierarchical representation of the interpolating paths is introduced, which is shown to provide an adequate method to locally interpolate large datasets.

SOE 6.5 Mon 16:00 H18

Global sensitivity analysis of Monte Carlo models using Cramer-von Mises distance — •Sina Dortaj[1,2] and Sebastian Matera[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Mathematics, Freie Universität Berlin, Arnimallee 6, 14195 Berlin, Germany

Typically, the parameters entering a physical simulation model carry some kind of uncertainty, e.g. due to the intrinsic approximations in a higher fidelity theory from which they have been obtained. Global sensitivity analysis (GSA) targets quantifying which parameters uncertainties impact the accuracy of the simulation results, e.g. to identify which parameters need to be determined more accurately.

We present a GSA approach on basis of the Cramers-von Mises distance. Unlike prevalent approaches it combines the following properties: i) it is equally suited for deterministic as well as stochastic model outputs, ii) it is free of gradients, and iii) it can be estimated from any suitable numerical quadrature (NQ) without further numerical tricks. Using Quasi-Monte Carlo for NQ and prototypical first-principles kinetic Monte Carlo models (kMC), we examine the performance of the approach. We find that the approach typically converges in a modest number of NQ points. Furthermore, it is robust against even extreme relative noise. All these properties make the method particularly suited for expensive (kinetic) Monte Carlo models, because we can reduce the number of simulations as well as the target variance of each of these.

15 min. break

SOE 6.6 Mon 16:30 H18

Reproducible and transparent research software pipelines using semantic research data management and common workflow language — •Alexander Schlemmer[1,2,5], Inga Kottlarz[1,3], Baltasar Rüchardt[1,5], Ulrich Parlitz[1,3,5], and Stefan Luther[1,4,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]IndiScale GmbH, Göttingen — [3]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen — [5]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen

Sustainable and well-documented scientific software is essential for effectiveness and reproducibility in data-intensive research. In practice, incompletely documented software hinders in many cases replicability, reproducibility and method comparison. 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. We present an approach combining semantic data management with CaosDB and processing pipelines with Common Workflow Language (CWL), showing use cases from dynamical systems research. The CWL-based environment provides a transparent

description of the process and includes metadata that can be searched within CaosDB. Input-/output-data and parameters can be directly linked to algorithms and software snapshots. The employment of containers simplifies reproducibility and interoperability.

SOE 6.7 Mon 16:45 H18

MDSuite: A post-processing engine for particle simulations — •Fabian Zills[1], Samuel Tovey[1], Francisco Torres-Herrador[2], Christoph Lohrmann[1], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany — [2]von Karman Institute for Fluid Dynamics, Rhode-St-Genese, Belgium

Particle-based simulations are experiencing a rapid growth wherein system sizes in the hundreds of thousands or even millions are becoming commonplace. With this growth in system size comes the additional challenge of post-processing the simulation data.

In this talk, we introduce the Python package MDSuite. MDSuite is designed for the post-processing of particle-based simulation in an efficient manner and on modern hardware. Built on top of TensorFlow, MDSuite calculators are fully parallelised, gpu-enabled, and, due to the use of modern data pipe-lining methods, completely memory safe. Furthermore, the use of HDF5 and SQL database structures enables effective tracking of calcualtion parameters as well as a compressed trajectory storage medium. We present MDSuite as a standalone package for the storage, analysis, and comparison of large-scale simulation studies.

SOE 6.8 Mon 17:00 H18

Distinguishing noise from high-dimensional chaos — •Inga Kottlarz[1,2] and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany

The ordinal pattern-based Complexity-Entropy Plane is a popular tool in nonlinear dynamics for distinguishing noise from chaos. While successful attempts to do so have been documented for low-dimensional maps and continuous-time systems, high-dimensional systems have been somewhat neglected so far. To address the question in which way time series from highdimensional chaotic attractors can be characterized by their location in the Complexity-Entropy Plane we analyze data from the high-dimensional continuous-time Lorenz-96 system, the discrete generalized Hénon map and the Mackey-Glass equation as a delay system and discuss the crucial role of the lag and the pattern length or the ordinal pattern, and the length of the available time series.

SOE 6.9 Mon 17:15 H18

The impact of the UEFA European Football Championship on the spread of COVID-19 — •Jonas Dehning[1], Sebastian B. Mohr[1], Sebastian Contreras[1], Philipp Dönges[1], Emil Iftekhar[1], Oliver Schulz[2], Philip Bechtle[3], and Viola Priesemann[1,4] — [1]MPI for Dynamics and Self-Organization, 37077 Göttingen — [2]MPI for Physics, 80805 München — [3]Physikalisches Institut, University of Bonn — [4]Institute for the Dynamics of Complex Systems, University of Göttingen

Large-scale international events like the UEFA Euro 2020 football championship offer a unique opportunity to quantify the impact of match-related social gatherings on COVID-19, as the number of matches played by participating countries resembles a randomized trial. Moreover, soccer-related activities have a marked gender-imbalance that we can exploit for inference. In our work, we build a differentiable Bayesian SEIR-like model. Its parameters are inferred with Hamiltonian Monte-Carlo using the PyMC3 package. Our model simulates COVID-19 spread in each country using a discrete renewal process and gender-resolved case numbers. On average, 3.2% (95% CI: [1.3%, 5.2%]) of new cases in the 12 analyzed countries can be associated with the match-related social gatherings throughout our analysis period. Individually, England, the Czech Republic and Scotland showed a significant effect. Besides these insights on the spread of COVID-19 during large-scale events, our approach is an example of how modern Bayesian tools can be leveraged to gain insights on a complex dynamic process.

SOE 6.10 Mon 17:30 H18

Recurrence-based analysis of instantaneous fractal characteristics of geomagnetic variability — •Reik V. Donner[1,2], Tommaso Alberti[3], and Davide Faranda[4] — [1]Hochschule Magdeburg-Stendal, Magdeburg, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]National Institute for Astrophysics, Rome, Italy — [4]LSCE, Université Paris-Saclay, Gif-sur-Yvette, France

We employ two complementary approaches based on the concept of recurrences in phase space to quantify the local (instantaneous) and global fractal dimensions of the temporal variations of a suite of low (SYM-H, ASY-H) and high latitude (AE, AL, AU) geomagnetic indices and discuss similarities and dissimilarities of the obtained patterns for one year of observations during a solar activity maximum. Subsequently, we introduce bivariate extensions of both approaches, and demonstrate their capability of tracing different levels of interdependency between low and high latitude geomagnetic variability during periods of magnetospheric quiescence and along with perturbations associated with geomagnetic storms and magnetospheric substorms, respectively. Our results open new perspectives on the nonlinear dynamics and intermittent mutual entanglement of different parts of the geospace electromagnetic environment, including the equatorial and westward auroral electrojets, in dependence of the overall state of the geospace system affected by temporary variations of the solar wind forcing.