8th International Workshop on Set-Oriented Numerics (SON)

List of abstracts

Speaker: Prof. Steve Brunton *(University of Washington)*

Title: *Discovery and Control of Nonlinear Dynamical Systems from Data*

Abstract: The ability to discover physical laws and governing equations from data is one of humankind's greatest intellectual achievements. A quantitative understanding of dynamic constraints and balances in nature has facilitated rapid development of knowledge and enabled advanced technology, including aircraft, combustion engines, satellites, and electrical power. There are many more critical data-driven problems, such as understanding cognition from neural recordings, inferring patterns in climate, determining stability of financial markets, predicting and suppressing the spread of disease, and controlling turbulence for greener transportation and energy. With abundant data and elusive laws, data-driven discovery of dynamics will continue to play an increasingly important role in these efforts.

This work develops a general framework to discover the governing equations underlying a dynamical system simply from data measurements, leveraging advances in sparsity-promoting techniques and machine learning. The resulting models are parsimonious, balancing model complexity with descriptive ability while avoiding overfitting. The only assumption about the structure of the model is that there are only a few important terms that govern the dynamics, so that the equations are sparse in the space of possible functions. This perspective, combining dynamical systems with machine learning and sparse sensing, is explored with the overarching goal of real-time closed-loop feedback control of complex systems. Connections to modern Koopman operator theory are also discussed.

Speaker: Prof. Christof Schütte *(Zuse Institute Berlin, FU Berlin)*

Title: *Transition manifolds of complex metastable systems: Theory and data-driven computation of effective dynamics*

Abstract: Joint work with Andreas Bittracher, Péter Koltai, Stefan Klus, Ralf Banisch, and Michael Dellnitz We consider complex stochastic dynamical systems showing metastable behavior but no local separation of fast and slow time scales as they appear in molecular dynamics. The talk raises the question of whether such systems exhibit a low-dimensional manifold supporting its effective dynamics. For answering this question, we aim at finding nonlinear coordinates, called reaction coordinates, such that the projection of the dynamics onto these coordinates preserves the dominant time scales of the dynamics. We show that, based on a specific reducibility property, the existence of such low-dimensional reaction is guaranteed. Based on this theoretical framework, we develop and test novel numerical algorithms for computing good reaction coordinates. The proposed algorithms are fully local and thus not prone to critical slow-down by the metastability of the dynamics. Hence, it is a promising method for data-based model reduction of complex dynamical systems such as in molecular dynamics.

Speaker: Prof. Frank Noé *(FU Berlin)*

Title: *Finding slow modes and accessing very long timescales in molecular dynamics*

Abstract: The sampling problem, i.e. the difficulty to sample rare events along the slow modes, is a key problem in molecular dynamics and many other microscopic dynamical systems. In thermal equilibrium, where the dynamics have a stationary state and are statistically reversible, we can derive a variational approach to approximate the eigenfunctions of the Koopman operator / transfer operator. Algorithmically, this can be achieved by computing covariance matrices from a set of basis functions and obtaining the optimal approximation of eigenfunctions from the eigenvectors of a generalized eigenvalue problem. This approach turns out to be identical to the more recently introduced Extended dynamic mode decomposition, and it has similarities the dynamic mode decomposition. We will show how the eigenfunction approximates can be used in order to approximate the essential dynamics in complex many-body systems and how this information can be exploited to enhance the sampling of rare events.

Speaker: Prof. Nathan Kutz *(University of Washington)*

Title: Data-driven discovery of governing equations and parametric reduced order models

Abstract: The emergence of data methods for the sciences in the last decade has been enabled by the plummeting costs of sensors, computational power, and data storage. Such vast quantities of data afford us new opportunities for data-driven discovery, which has been referred to as the 4th paradigm of scientific discovery. We demonstrate that we can use emerging, large-scale time-series data from modern sensors to directly construct, in an adaptive manner, governing equations, even nonlinear dynamics, that best model the system measured using modern regression techniques. Recent innovations also allow for handling multi-scale physics phenomenon and control protocols in an adaptive and robust way. The overall architecture is equation-free in that the dynamics and control protocols are discovered directly from data acquired from sensors. The theory developed is demonstrated on a number of canonical example problems from physics, biology and engineering.

Speaker: Prof. Yoshihiko Susuki *(Osaka University)*

Title: *Data-Driven Koopman Spectral Analysis in Power and Energy Systems*

Abstract: Koopman operator is an infinite-dimensional but linear operator defined for nonlinear dynamical systems. Spectral properties of the Koopman operator are naturally introduced and have been exploited for analysis and design of complex dynamics arising in science and technology. In particular, due to invent of the Koopman mode decomposition (KMD, or dynamic mode decomposition), the so-called data-driven approach to Koopman spectral analysis becomes promising. In this talk, I'll overview applied research on the data-driven Koopman spectral analysis to power and energy systems. Contents of the talk include (i) model-order reduction for precursor diagnostic of power grid swing instabilities, (ii) wave interpretation of the KMD for modeling of temperature-field evolution in a building, and (iii) characterization of local bifurcation for prediction of voltage collapse phenomena in a power grid. Recent studies will be also announced such as load modeling and inertia estimation.

Speaker: Prof. Alexandre Mauroy *(Université de Namur)*

Title: *Isochrons and isostables of dissipative systems*

Abstract: The spectral properties of the Koopman operator provide a powerful insight into the behaviors of dynamical systems. In particular, level sets of Koopman eigenfunctions are closely connected to key geometric properties of the underlying systems. This talk will present an overview of this interplay between spectral and geometric properties, with a focus on sets playing a central role in the case of dissipative systems: isochrons and isostables. In this context, it will be shown that the Koopman operator-theoretic approach provides a unified viewpoint, yielding novel computational methods that are efficient to deal with complex dynamics. Finally, we will explore recent connections to stability theory, optimal control, nonlinear normal mode analysis, and phase reduction in neuroscience.

Speaker: Prof. Umesh Vaidya *(Iowa State University)*

Title: *Data-Driven Approach for Inferring Causal Interactions and Topology Identification in Dynamical Systems.*

Abstract: We study the problem of identifying causal interaction among dynamical system components using noisy time-series data. A new measure based on information transfer between dynamical system states is proposed for inferring causal interaction between dynamical system components. We provide a data-driven approach for computing the information transfer in a dynamical system. In particular, an algorithm for robust data-driven approximation of transfer operator is proposed for computing the information transfer and hence determining causal interaction from time-series data. We show that the robust feature of the proposed algorithm is essential to explicitly account for the presence of noise in the time-series data thereby allowing us to predict the correct causal structure. We demonstrate the application of the developed methodology for network topology identification from noisy time- series data.

Speaker: Prof. Oliver Junge *(Technische Universität München)*

Title: *Variational approaches to the computation of invariant and coherent sets*

Speaker: Prof. Garry Froyland *(UNSW Sydney)*

Title: *FEM-based numerics for the dynamic Laplacian and optimal linear responses*

Speaker: Milan Korda *(UC Santa Barbara)*

Title: *Data-driven spectral analysis of the Koopman operator*

Abstract: Starting from measured data, we develop a method to compute the fine structure of the spectrum of the Koopman operator with rigorous convergence guarantees. The method is based on the observation that, in the measure-preserving ergodic setting, the moments of the spectral measure associated to a given observable are computable from a single trajectory of this observable. Having finitely many moments available, we use the classical Christoffel-Darboux kernel to separate the atomic and absolutely continuous parts of the spectrum, supported by convergence guarantees as the number of moments tends to infinity. In addition, we propose a technique to detect the singular continuous part of the spectrum as well as two methods to approximate the spectral measure with guaranteed convergence in the weak topology, irrespective of whether the singular continuous part is present or not. The proposed method is simple to implement and readily applicable to large-scale systems since the computational complexity is dominated by inverting an NxN Hermitian positive-definite Toeplitz matrix, where N is the number of moments, for which efficient and numerically stable algorithms exist; in particular, the complexity of the approach is independent of the dimension of the underlying state-space. We also show how to compute, from measured data, the spectral projection on a given segment of the unit circle, allowing us to obtain a finite-dimensional approximation of the operator that explicitly takes into account the point and continuous parts of the spectrum. Finally, we describe a relationship between the proposed method and the so-called Hankel Dynamic Mode Decomposition, providing new insights into the behavior of the eigenvalues of the Hankel DMD operator. A number of numerical examples illustrate the approach, including a study of the spectrum of the lid-driven two-dimensional cavity flow.

Speaker: Sebastian Peitz *(Universität Paderborn)*

Title: *A new framework for Koopman operator based open and closed loop control*

Abstract: With increasing complexity of modern applications, more and more advanced control techniques are required in order to steer or stabilize the system dynamics. In recent years, model predictive control has gained more and more importance, where the system dynamics are predicted using a (simplified) model and the optimal feedback is computed by open loop optimal control strategies. In order to achieve real time applicability, model simplification plays an important role. In many problems, this is achieved by linearization. Another approach is to introduce a reduced order model via Proper Orthogonal Decomposition (POD) and Galerkin Projection. More recently, reduced order models based on the Koopman operator have come to attention. The problem until now is that it is difficult to make statements about the quality of the solution based on this reduced model. Therefore, in this presentation, we will introduce a new method for open and closed loop control of dynamical systems based on the Koopman operator. In this approach, optimality of the solution can be guaranteed by formulating the control problem as a switching time problem and then utilizing recent convergence results for extended DMD towards the Koopman operator.

Speaker: Adrian Ziessler *(Universität Paderborn)*

Title: *The Computation of Invariant Manifolds for Partial Differential Equations by Set Oriented Numerics*

Abstract: In this talk we present a numerical framework for the computation of finite dimensional invariant manifolds for infinite dimensional dynamical systems. With this framework we extend classical set oriented numerical schemes (for the computation of invariant manifolds in finite dimensions) to the infinite dimensional context. The underlying idea is to utilize appropriate embedding techniques for the globalization of these manifolds in a certain finite dimensional space. Finally, we illustrate our approach by the approximation of invariant manifolds in the context of partial differential equations.

Speaker: Péter Koltai *(FU Berlin)*

Title: *From large deviations to transport semidistances: coherence analysis for finite Lagrangian data*

Abstract: In a quantitative, set-oriented approach to transport, finite time coherent sets play an important role. These are time-parametrized families of sets with unlikely transport to and from their surroundings under small random perturbations of the dynamics. Here we propose, as a measure of transport, (semi)distances that arise under vanishing perturbations in the sense of large deviations. Analogously, for given finite Lagrangian trajectory data we derive a discrete-time and space semidistance that comes from the ``best'' approximation of the randomly perturbed process conditioned on this limited information on the deterministic flow. It can be computed as shortest path in a graph with time-dependent weights. Furthermore, we argue that

coherent sets are regions of maximal farness in terms of transport, hence they occur as extremal regions on a spanning structure of the state space under this semidistance---in fact, under any distance measure arising from the physical notion of transport. Based on this notion we develop a tool to analyze the state space (or the finite trajectory data at hand) and identify coherent regions. We validate our approach on idealized prototypical examples and well-studied standard cases. This is joint work with Michiel Renger.

Speaker: Stefan Klus *(FU Berlin)*

Title*: Kernel-based approximation of transfer operators*

Abstract: Over the last years, several data-driven methods for the approximation of the eigenfunctions of the Perron–Frobenius and Koopman operator have been proposed. Examples of such methods are extended dynamic mode decomposition (EDMD) and the variational approach of conformation dynamics (VAC). These methods require solving eigenvalue problems whose size depends on the number of basis functions. Choosing a tensor-product of one-dimensional basis functions, the number of functions grows exponentially with the number of dimensions. Using the kernel trick, however, the eigenvalue problems can be reformulated in such a way that the size depends on the number of snapshots. We propose a kernel-based reformulation of EDMD for the Perron–Frobenius operator that resembles diffusion maps, but explicitly includes time information. We illustrate the efficiency of the algorithm on a set of well-known examples, namely a simple quadruple-well problem, the butane molecule, and the deca-alanine peptide.

Speaker: Amit Surana *(United Technologies Research Center)*

Title: *Koopman Operator Framework for Constrained State Estimation*

Abstract: We present a novel Koopman operator theoretic framework for nonlinear constrained state estimation (CSE) with non-convex state constraints. Exploiting linear representation induced by Koopman operator, we show that under certain conditions the CSE problem can be transformed into a higher dimensional but a convex problem. We present conditions under which the feasibility and optimality are preserved under this transformation. We numerically demonstrate the efficacy of the proposed approach and report superior performance compared to convexification based on successive linearization. The proposed framework could provide significant benefit in real time applications.

Speaker: Hassan Arbabi *(UC Santa Barbara)*

Title: *Computation of Koopman spectrum for high-dimensional systems*

Abstract: In this talk, we discuss the Hankel+DMD algorithm for computation of the Koopman spectrum in post-transient systems. The (Takens) delay-embedding of the data in the form of the Hankel matrix allows us to represent the dynamical system in the space of observables. In case of Koopman operator having discrete spectrum, applying DMD to such Hankel matrices recovers the Koopman eigenvalues and eigenfunctions. We discuss the application of this method through numerical examples and comment on its connection with Hankel-Alternative-View-of-Koopman (HAVOC) and Singular Spectrum Analysis (SSA).

Speaker: Alain Avila *(UC Santa Barbara)*

Title: *Application of Koopman Operator Theory to Highway Traffic Dynamics*

Abstract: The Koopman operator theory framework is a rapidly developing theory in dynamical systems that offers powerful methods for analyzing complex nonlinear systems. We demonstrate how the Koopman operator theory can offer a model and parameter free, data-driven approach to accurately analyzing and forecasting traffic dynamics. The effectiveness of this framework is demonstrated by an application to the Next Generation Simulation (NGSIM) data set collected by the US Federal Highway Administration and the Performance Measurement System (PeMS) data set collected by the California Department of Transportation. By obtaining a Koopman mode decomposition of the data sets, we are able to accurately reconstruct our observed dynamics, distinguish any growing or decaying modes, and obtain a hierarchy of coherent spatiotemporal patterns that are fundamental to the observed dynamics. Furthermore, it is demonstrated how the Koopman Mode Decomposition (KMD) can be utilized to accurately forecast traffic dynamics by obtaining a decomposition of a subset of the data, that is then used to predict a future subset of the data.