6th International Workshop on Set-Oriented Numerics

Imperial College London, 28th September – 1st October 2015

Talk titles and abstracts

All talks will be given in Huxley Lecture Theater 130. Please note that the second floor is the ground floor of the Huxley building.

Ralf Banisch (FU Berlin)

Module Detection in Directed Transition Networks

Wednesday, 30 September 2015, 4.30pm–5.15pm

We present a new cycle-flow-based method for finding fuzzy partitions of weighted directed networks coming from time series data. We show that this method overcomes essential problems of most existing clustering approaches, which tend to ignore important directional information by considering only one-step, one-directional node connections. Our method introduces a novel measure of communication between nodes using multi-step, bidirectional transitions encoded by a cycle decomposition of the probability flow. Symmetric properties of this measure enable us to construct an undirected graph that captures the information flow of the original graph seen by the data and apply clustering methods designed for undirected graphs. Finally, we demonstrate our algorithm by analyzing earthquake time series data, which naturally induce (time-)directed networks.

Erik Bollt (Clarkson University)

Identifying the Coupling Structure in Complex Systems through the Optimal Causation Entropy Principle

Monday, 28 September 2015, 3.45pm–4.30pm

Inferring the coupling structure of complex systems from time series data in general by means of statistical and information-theoretic techniques is a challenging problem in applied science. The reliability of statistical inferences requires the construction of suitable information-theoretic measures that take into account both direct and indirect influences, manifest in the form of information flows, between the components within the system. In this work, we present an application of the optimal causation entropy (oCSE) principle to identify the coupling structure and jointly apply the aggregative discovery and progressive removal algorithms based on the oCSE principle to infer the coupling structure of the system from the measured data.

Fritz Colonius (Augsburg University)

Invariance entropy, quasi-stationary measures and control sets

Tuesday, 29 September 2015, 3.45pm–4.30pm

For control systems in discrete time, a notion of metric invariance entropy is constructed with respect to conditionally invariant (and, in particular, to quasi-stationary) measures. This entropy notion indicates the amount of information needed to keep the system within a given compact subset of the state space. It is shown that the metric invariance entropy is an invariant under appropriately defined conjugacies. Furthermore, the power rule holds and the topological notion of invariance entropy provides an upper bound. Finally, relations to subsets of complete approximate controllability (control sets) are indicated.

Andreas Denner (TU Munich)
Computing coherent sets using time-continuous diffusion
Tuesday, 29 September 2015, 2.45pm–3.15pm

In time dependent dynamics, it is often possible to divide phase space into sets which are seperated by transport barriers. Finding these sets helps to understand the global dynamical behavior of systems arising in, e.g. atmospheric flows, plasma physics and biological models. In this talk we present a new approach for the computation of coherent sets by incorporating time-continuous diffusion into the model. This leads to an advection-diffusion equation (the Fokker-Planck equation) whose solution we approximate using spectral collocation. The approach does not need any particle trajectories and is therefore suited for systems where these are hard to obtain, e.g. turbulent systems.

Rolf Findeisen (Magdeburg University)
Set-based methods for model validation and for verification of system properties
Thursday, 1 October 2015, 3.45pm–4.30pm

In many fields deriving a mathematical model represents the first step in improving the insight into a dynamical system. However, this is in general a nontrivial task, in particular if uncertainties have to be taken into account. In this talk we demonstrate how a polynomial model structure can be selected based on available uncertain measurement data and how to analyze system properties of such models. Uncertainties are considered here as unknown-but-bounded variables, i.e. variables that are allowed to take any value from a semi-algebraic set. Considered system properties include model validity, reachability and observability. The presented methods are based on reformulating the desired properties such that they can be checked with the help of polynomial feasibility problems that are subsequently relaxed into a semidefinite program. The employed methods are illustrated with several examples from different application areas.

Peter Giesl (University of Sussex)
Rigorous Computation of Lyapunov functions
Thursday, 1 October 2015, 2.00pm–2.45pm

Lyapunov functions are an important tool to determine the basin of attraction of equilibria in Dynamical Systems through their sublevel sets. Recently, several numerical construction methods for Lyapunov functions have been proposed, among them the RBF (Radial Basis Function) and CPA (Continuous Piecewise Affine) methods. While the first method, in its original form, does not include a verification that the constructed function is a valid Lyapunov function, the second method is rigorous, but computationally much more demanding.

In this talk, we propose a combination of these two methods, using their respective strengths: we use the RBF method to compute a Lyapunov function. Then we interpolate this function by a continuous piecewise affine (CPA) function. Checking a finite number of inequalities, we are able to verify that this interpolation is a Lyapunov function. Moreover, sublevel sets are arbitrarily close to the basin of attraction.

This is joint work with Sigurdur Hafstein (Reykjavik University, Iceland).

Mirko Hessel-von Molo (Paderborn University)
On the Computation of Attractors for Delay Differential Equations
Wednesday, 30 September 2015, 3.45am–4.30am

Abstract. In this talk we will introduce a numerical method which allows to approximate (low dimensional) invariant sets for infinite dimensional dynamical systems. We will particularly focus on the computation of attractors for delay differential equations. The numerical approach is inherently set oriented - that is, the invariant sets are computed by a sequence of nested, increasingly refined approximations -, and does not rely on long term simulations of the underlying system.

Oliver Junge (TU Munich)
Fast computation of coherent sets using radial basis functions
Wednesday, 30 September 2015, 2.00pm–2.45pm

Abstract: An expensive part of the transfer operator approach to detecting coherent sets is the construction of the operator itself. We present a numerical method based on radial basis function collocation and apply it to a recent transfer operator concept by Froyland based on a dynamic Laplace operator. The main advantage of our new approach is a substantial reduction in the number of Lagrangian trajectories that need to be computed. This is joint work with Gary Froyland.

Yannis Kevrekidis (Princeton University)
No equations, no variables: data, and the computational modeling of complex systems.
Monday, 28 September 2015, 1.30pm–2.30pm

I will first briefly review how matrix-free, and, in particular, timestepper-based matrix-free methods, can functionally link fine-scale simulators with coarse-grained, systems-level numerical tasks (like coarse stability and bifurcation computations) for complex dynamical models. I will discuss possible connections of these ideas with set-oriented numerical computations.

I will then outline what we are currently concerned about/working on in my group: the use of data-mining (the ”variable-free” component) in the overall computational process. Processing the results of brief bursts of multiscale simulations with tools like Diffusion Maps can sugggest good macro-scale observables (variables) in terms of which macroscopic equations can in principle be written/solved. Performing scientific computation in terms of these ’data-mining-based’ variables poses a number of interesting problems that I will outline and comment on.

Gabor Kiss (University of Szeged)
Periodic solutions of a delayed Van der Pol oscillator
Monday, 28 September 2015, 2.30pm–3.15pm

The Van der Pol oscillator has played an important role in modelling many real-world phenomena. We consider a delayed version of the equation, and report on the existence of periodic solutions which had been observed numerically some decades ago. Also, we describe our computational fixed-point theory, the method that we used to validate the existence of the period solutions in question. Joint work with Jean-Philippe Lessard, Laval University, Canada.

Stefan Klus (FU Berlin)
Tensor-based approximation of transfer operators
Thursday, 1 October 2015, 11.45am–12.30pm

The global behavior of dynamical systems can be studied by analyzing the eigenvalues and corresponding eigenfunctions of linear operators associated with the system. Two important operators which are frequently used to gain insight into the system's behavior are the Perron-Frobenius operator and the Koopman operator. Due to the curse of dimensionality, computing the eigenfunctions of high-dimensional systems is in general infeasible. We will propose a tensor-based reformulation of two numerical methods for computing finite-dimensional approximations of the aforementioned infinite- dimensional operators, namely Ulam's method and Extended Dynamic Mode Decomposition (EDMD). The aim of the tensor formulation is to approximate the eigenfunctions by low-rank tensors, potentially resulting in a significant reduction of the time and memory required to solve the resulting eigenvalue problems, provided that such a low-rank tensor decomposition exists.

Peter Koltai (FU Berlin)
Pseudogenerators for under-resolved molecular dynamics
Tuesday, 29 September 2015, 14.00pm–14.45pm

Many features of a molecule which are of physical interest (e.g. molecular conformations, reaction rates) are described in terms of its dynamics in configuration space. In this talk we consider the projection of molecular dynamics in phase space onto configuration space. Specifically, we study the situation that the phase space dynamics is governed by a stochastic Langevin equation. We review the classical result leading to the Smoluchowski equations as overdamped limit, and show that for small times a Smoluchowski equation, scaled non-linearly in time, governs the evolution of the configurational coordinate even for general damping. By using an adequate reduction technique, these considerations are then extended to one-dimensional reaction coordinates. We conclude by exploring connections with the Mori-Zwanzig formalism, and by discussing possible extensions to approximate the metastable behavior based on time-local information only.

Tony Lelièvre (ParisTec)
Metastable stochastic process and quasi stationary distribution
Wednesday, 30 September 2015, 9.30am–10.30am

We present a review of recent works on the mathematical analysis of algorithms which have been proposed by A.F. Voter and co-workers in the late nineties in order to efficiently generate long trajectories of metastable processes. The idea is to use the underlying jump process between metastable sets to accelerate the sampling of the original dynamics. These techniques have been successfully applied in many contexts, in particular in the field of materials science. The mathematical analysis we propose relies on the notion of quasi-stationary distribution

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Ian Mitchell (University of British Columbia)
Some algorithms and applications of numerical reachable sets and viability kernels
Wednesday, 30 September 2015, 11.00am–12.00pm

Reachable sets and viability kernels are powerful constructs for verifying the correct behaviour of dynamic systems, but numerical approximations remain challenging to compute. This talk will explore four algorithms for continuous state systems whose set representations are implicit surface functions, projection polygons, ellipsoids and support vectors respectively. These algorithms sample different points in the space of tradeoffs between generality of the allowed dynamics, robustness to uncertainty in the dynamics, accuracy and soundness of the approximation, scalability of the algorithm, and utility of the result. The algorithms will be illustrated with applications suitable for their particular strengths, including air traffic control, quadrotor stunt flying, integrated circuits, and automated anesthesia delivery.

Karin Mora (Paderborn University)
Multimode dynamics of a microbeam-string under parametric excitation with asymmetric electrodes
Thursday, 1 October 2015, 11.00am–11.45am

The dynamic motion of a parametrically excited microbeam-string affected by nonlinear damping is considered asymptotically and numerically. It is assumed that the geometrically nonlinear beam-string, subject only to modulated AC voltage, is closer to one of the electrodes, termed the asymmetric gap configuration. A consequence of these assumptions is a novel combined parametric and hard excitation in the derived continuum based model that incorporates both linear viscous and nonlinear viscoelastic damping terms. These assumptions influence the beam's performance near principal parametric and a three-to-one internal resonance. The conditions, under which these scenarios arise, are derived analytically from a reduced-order nonlinear model for the first three modes of the microbeam-string using the asymptotic multiple-scales method. The latter requires reconstitution of the slow-scale evolution equations to deduce an approximate spatio-temporal solution. The response analysis reveals a bifurcation structure that includes coexisting solutions and numerically obtained loss of orbital stability.

This is joint work with Oded Gottlieb (Technion, Israel).

Kathrin Padberg-Gehle (TU Dresden)
Cluster-based extraction of finite-time coherent sets from sparse and incomplete trajectory data
Tuesday, 29 September 2015, 4.30pm–5.15pm

Coherent features in time-dependent dynamical systems are difficult to identify. Most identification algorithms require knowledge of the dynamical system or high-resolution trajectory information, which in applications may not be available. We present a fast and simple method that is based on spatio-temporal clustering of trajectory data. It provides a rough and rapid coherent structure analysis and is particularly aimed at situations where the available information is poor: there are few trajectories, the available trajectories do not span the full time duration under consideration, and there are missing observations within trajectories. This is joint work with Gary Froyland (UNSW Australia).

Sebastian Peitz (Paderborn University)
Multiobjective Optimal Control Methods for Fluid Flow Using Reduced Order Modeling
Wednesday, 30 September 2015, 2.45pm–3.15pm

In a wide range of applications it is desirable to optimally control a dynamical system with respect to concurrent, potentially competing goals. This gives rise to a multiobjective optimal control problem where, instead of computing a single optimal solution, the set of optimal compromises is sought. When the problem under consideration is described by a partial differential equation (PDE), as is the case for fluid flow, the computational costs quickly become infeasible. Reduced order modeling is a very popular method to reduce the computational costs, especially in a multi query context such as optimization. In this presentation, we show how to combine reduced order modeling and multiobjective optimal control techniques in order to efficiently solve multiobjective optimal control problems constrained by PDEs. We consider a global, derivative free optimization method as well as a local, gradient based approach for which the optimality system is derived. The methods are illustrated using the example of the two-dimensional incompressible flow around a cylinder.

Katja Polotzek (TU Dresden)
Set-oriented approximation of the rotation set of torus homeomorphisms
Tuesday, 29 September 2015, 5.15pm–5.45pm

The rotation theory of mappings $f : \mathbb{T}^m \longrightarrow \mathbb{T}^m$ on the m-dimensional torus $\mathbb{T}^m := \mathbb{R}^m/\mathbb{Z}^m$ focusses on limits of sequences of the form

$$\left(\frac{F^{n_i}(x_i) - x_i}{n_i}\right)_{i\in\mathbb{N}}$$

with respect to a lift $F : \mathbb{R}^m \longrightarrow \mathbb{R}^m$ of f and with $x_i \in \mathbb{R}^m, n_i \in \mathbb{N}, i \in \mathbb{N}$ and $n_i \to \infty$ as $i \to \infty$. The set of all accumulation points of these sequences is called the *rotation set* $\rho(F)$ of F. In the two-dimensional case, for homeomorphisms homotopic to the identity this set is known to be compact and convex [2] and, generically, it appears polygonial [3].

As its rotation set provides strong information about the system's behavior but, in general, is not given analytically, one is interested in a numerical approximation of this set. In the talk, a direct approach [1] to this task is presented in order to illustrate the limits of the pointwise detection of rotation sets. We formulate a set-oriented algorithm and obtain good numerical representations of the rotation sets for several example maps.

References: [1] P.-A. Guiheneuf, How roundoff errors help to compute the rotation set of torus homeomorphisms, eprint arXiv:1406.2254 (06/2014) [2] M. Misiurewicz and K. Ziemian, Rotation sets for maps of tori, J. London Math. Soc. (2) 40 (1989), no. 3, 490–506. [3] A. Passeggi, Rational polygons as rotation sets of generic homeomorphisms of the two torus, J. London Math. Soc., jdt040 (2013).

Naratip Santitissadeekorn (University of Surrey)
Sequential Data Assimilation for the urban crime model
Thursday, 1 October 2015, 9.30am–10.30am

In this work we explore some of the various issues that may occur in attempting to fit a dynamical systems (either agent- or continuum-based) model of urban crime to data on just the attack times and locations. We show how one may carry out a regression analysis for the model described by [M.B. Short, M.R. DOrsogna, V.B. Pasour, G.E. Tita, P. Je rey Brantingham, A.L. Bertozzi, and L.B. Chayes, Math. Mod. Meth. Appl. Sci. 2008] by using simulated attack data from the agent-based model. It is discussed how one can incorporate the attack data into the partial differential equations for the expected attractiveness to burgle and the criminal density to predict crime rates between attacks. We also develop a Poisson-Kalman filtering scheme for tracking the parameter switching in the urban crime model.

Christof Schütte (FU Berlin)
Set-Oriented Numerics and Molecular Design
Tuesday, 29 September 2015, 11.00am–12.00pm

Molecular dynamics and related computational methods enable the description of biological systems with all-atom detail. However, these approaches are limited regarding simulation times and system sizes. A systematic way to bridge the micro-macro scale range between molecular dynamics and experiments is to apply coarse-graining (CG) techniques. We will discuss Markov State Modelling (MSM), a set-oriented CG technique that has attracted a lot of attention in physical chemistry, biophysics, and computational biology in recent years.

Mathematically, MSM is based on discretization of transfer operators. However, the standard approach via a box discretization (Ulams method) often is infeasible because of the curse of dimension.

In this talk, we will first introduce some new ideas regarding discretization of the transfer operator in high dimensions, then we will discuss the question of how to apply it to designing molecules with prescribed biological function.

All of this will be illustrated by telling the story of the design process of a pain relief drug without concealing the potential pitfalls and obstacles.

Eric Vanden-Eijnden (Courant Institute)
Markov State Models
Tuesday, 29 September 2015, 9.30am–10.30am

Markov State Models have emerged has a popular way to interpret and analyze time-series data generated e.g. in the context of molecular dynamics simulations. The basic idea of these models is to represent the dynamics of the system as memoryless jumps between predefined sets in the systems state space, i.e. as a Markov jump process (MJP). Performing this mapping typically involves two nontrivial questions: first how to define these sets and second how to learn the rate matrix of MJP once the sets have been identified? Both these questions will be discussed in there talk, with emphasis put on the problem of model specification error.

Matthias Wagner (TU Dresden)
A GPU-accelerated library for set-oriented methods
Thursday, 1 October 2015, 2.45pm–3.15pm

The software package GAIO [2] is a powerful implementation of set-oriented algorithms for the numerical analysis of dynamical systems. Starting from an initial hyperrectangle ('box'), the basic subdivision algorithm uses bisection and selection of boxes to obtain finer and finer coverings of the structures of interest such as attractors and almost-invariant sets. On this basis quantities like invariant measures, Lyapunov exponents, or fractal dimensions can be approximated. GAIO is implemented by means of a dynamic binary tree. Due to this dimension-independent scheme, the data structure wastes much less memory than a naive coordinate-vector-based storage. Set-oriented algorithms are in general highly parallelisable. At the same time, the development of graphics cards (GPUs), with thousands of processing units, increased dramatically in recent years, so that increasingly complex scientific applications can be handled. We thus introduce a possible GPU software package based on the ideas of GAIO. Graphic cards usually provide faster but smaller memory than the 'normal' RAM. We present an efficient storage scheme that only stores the leaves of the binary tree in vectors. This does not only lead to coalesced memory but also to at least eight times less memory consumption. To facilitate the implementation the recently developed GPU-accelerated library Thrust [1] was used. This library provides vector containers for CPU and GPU memory, algorithms for reducing, searching, sorting etc., and so-called 'fancy' iterators. We will present a brief overview of these powerful tools and also possible applications.

References: [1] Nathan Bell and Jared Hoberock. Thrust: A 2 6. GPU Computing Gems Jade Edition, page 359, 2011. [2] Michael Dellnitz, Gary Froyland, and Oliver Junge. The algorithms behind GAIO - Set oriented numerical methods for dynamical systems. In Ergodic theory, analysis, and efficient simulation of dynamical systems, pages 145–174. Springer, 2001.

Fabian Wirth (Passau University)

Numerical Methods for Stability of Large-Scale Systems

Monday, 28 September 2015, 4.30pm–5.15pm

In the stability analysis of large-scale interconnected systems stability criteria for large-scale interconnections can be formulated using so-called small-gain conditions which are formulated in terms of a monotone operator. These conditions can be used to give explicit constructions of Lyapunov functions. The key obstacle lies in the determination of a decay point of the gain operator. That is, a point whose image under the monotone operator is strictly smaller than the point itself. The set of such decay points plays a crucial role in checking, in a semi-global fashion, the local input-to-state stability of an interconnected system, and in the numerical construction of a LISS Lyapunov function. We provide a homotopy algorithm that computes a decay point of a monotone operator. For this purpose we use a fixed point algorithm and provide a function whose fixed points correspond to decay points of the monotone operator.