Special Session 10: Computational and Nonautonomous Dynamics

Michael Dellnitz, University of Paderborn, Germany
Oliver Junge, Technische Universitaet Muenchen, Germany
Stefan Siegmund, Technische Universitaet Dresden, Germany

Computational techniques for dynamical and control systems have grown to powerful tools beyond mere simulation. In this session, state of the art computational methods, as well as theoretical foundations, for the analysis and synthesis of such (non-)autonomous systems are presented, with a focus on real world applications. One of our primary goals is to detect new links between dynamical systems resp. systems theory and such diverse fields as graph theory, numerics, mechanics, optimization, statistics, and topology.

A computer assisted enclosure for invariant manifolds

Gianni Arioli
Politecnico di Milano, Italy
gianni.arioli@polimi.it
Davide Ambrosi, Hans Koch

We describe a new technique to compute a very tight enclosure for the stable and unstable manifolds at a stationary point of an autonomous, finite dimensional dynamical system. We apply the technique to prove the existence of a traveling wave for a PDE modeling the propagation of electric signals in biological tissues, and provide a very accurate rigorous estimate of the wave speed.

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Macro-state models for protein modeling

Eric Darve
Stanford, USA
darve@stanford.edu

We present and discuss various numerical algorithms to calculate slow reaction rates in protein modeling. These rates typically correspond to conformational changes in protein such as folding or binding. These rates are associated with rare transition events from one metastable state to another metastable state. Such rare events, by definition, are difficult to observe through direct simulation and therefore getting accurate statistical information and kinetics is challenging. We will discuss methods that attempt to enhance the sampling and improve the accuracy using macro-states, which form a partition of the conformational space of the protein. By computing statistics of transition between these macro-states, in appropriate ways, one can reconstruct the kinetic information of interest.

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Multiscaling and coarse-graining for coagulation processes in high dimension

Lee Deville
University of Illinois, USA
rdeville@illinois.edu
Matt West, Nicole Riemer

We consider particle processes where the state-space has high dimension and pairwise events dominate the dynamics. (A concrete example of this is computing the time evolution of the multi-dimensional size distribution of interacting aerosol particles in a regime where coagulations dominate the cost of the computation.) We will discuss several methods of speeding up such particle methods when multiscaling is applicable and show that this applies to several concrete problems in atmospheric sciences.

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Rotation number and QR based techniques for exponential dichotomy: numerical comparisons

Cinzia Elia
University of Bari, Italy
elia@math.gatech.edu
Roberta Fabbri

We propose numerical techniques based on the continuous Iwasawa decomposition to compute the rotation number for Hamiltonian linear systems of dimension greater or equal than 2. The rotation number allows us to infer whether a given system has exponential dichotomy or not. We employ these techniques to study the Schroedinger operator and the Schroedinger equation in 2 dimensions. Comparisons with QR based techniques for exponential dichotomy allow us to recover new information on the spectrum of the Schroedinger operator. The talk focuses on the numerical aspects while theoretical results will be addressed in Roberta Fabbri's talk.

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Rotation number and exponential dichotomy for linear Hamiltonian systems: theoretical and numerical aspects

Roberta Fabbri
Universita' di Firenze, Italy
roberta.fabbri@unifi.it
Cinzia Elia

The talk considers the properties of the rotation number for a family of linear nonautonomous Hamiltonian systems and its relation with the exponential dichotomy concept. In particular, we relate the rotation number to the presence of an exponential dichotomy for some Hamiltonian systems perturbed according to an Atkinson-type condition. Using the continuous Iwasawa decomposition of a symplectic matrix, we compute the rotation number of a linear Hamiltonian system and we employ these techniques to study the quasi-periodic Schroedinger operator in one dimension and the 2-dimensional Schroedinger equation. We refer to the talk of Cinzia Elia for the introduction and analysis of the numerical techniques considered.

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Finite-time transport analysis for nonautonomous deterministic and stochastically perturbed systems

Gary Froyland
University of New South Wales, Australia
g.froyland@unsw.edu.au

We discuss finite-time transport for both deterministic dynamical systems and those subjected to stochastic perturbations. We will elucidate a new theory for characterising Lagrangian coherent sets in both deterministic and stochastic settings. The constructions are based around singular vectors of evolution operators (Perron-Frobenius operators). We also discuss how small random perturbations influence the maximal level of coherence.

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Accelerating molecular dynamics: some ideas from robust and risk-sensitive control

Carsten Hartmann
Institut für Mathematik, Freie Universität Berlin, Germany
chartman@mi.fu-berlin.de
Christof Schütte and Stefanie Winkelmann

In the talk I will present some recent developments in robust control of bilinear systems that appear relevant in the context of nonequilibrium molecular dynamics and quantum control. A particular focus is on low-rank approximation techniques that make the calculation of an optimal control numerically feasible.

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Computing invariant sets with Newton-type iterations: towards a covering approach

Mirko Hessel-von molo
University of Paderborn, Germany
mirkoh@math.upb.de
Michael Dellnitz, Ioannis G. Kevrekidis

The approximation of invariant sets is an important task in the numerical treatment of dynamical systems. Recent work approaches this problem by transferring it into a Banach space setting, using the formalism of directed sets, and employing Newton-type iterations for its solution. This approach is limited in the class of sets that can be approximated: only convex sets are feasible. We will present steps towards overcoming this limitation with a covering approach that represents invariant sets as (subsets of) unions of convex sets.

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Characterization of pullback attractors

José A. Langa
Seville University, Spain
langa@us.es
A.N. de Carvalho, J.C. Robinson

In this talk we present some recent results on the characterization of attractors for non-autonomous dynamical systems. We will pay attention in the upper and lower semicontinuity of attractors and on Morse decomposition of these families, which describes the internal dyanamics on these sets. All our work is made in an infinite dimensional framework, so that specially well suited to apply to PDEs. Some open problems and future further reseach will be also presented.

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Lazy global feedbacks for quantized nonlinear event systems

Oliver Junge
Technische Universitaet Muenchen, Germany
oj@tum.de
Stefan Jerg

We consider nonlinear event systems with quantized state information and design a globally stabilizing controller from which only the minimal required number of control value changes along the feedback trajectory to a given initial condition is transmitted to the plant. In addition, we present a non-optimal heuristic approach which might reduce the number of control value changes and requires a lower computational effort. The constructions are illustrated by two numerical examples.

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Invariant manifolds in finite-time dynamics

Daniel Karrasch
TU Dresden, Germany
Daniel.Karrasch@tu-dresden.de

We present and discuss finite-time invariant manifolds from two perspectives. The first perspective is via finite-time hyperbolic trajectories and their (inherently non-unique) finite-time stable and unstable manifolds. We show an intrinsic (i.e. without infinite-time extensions) approach to the proof of a finite-time Local Stable Manifold Theorem and present a complete local description of the geometry close to hyperbolic trajectories. The second perspective is from ensemble dynamics, as often applied in the modelling of geophysical flows, for instance. We generalize a variational approach to hyperbolic Lagrangian Coherent Structures (LCS), recently proposed by Haller [Physica D, 2011], towards LCS of higher codimension and, second, to filtrations of embedded LCS.

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Global stability design for non-linear dynamical systems

Péter Koltai
Technische Universität München, Germany
koltai@ma.tum.de
Alexander Volf

Given a stable non-linear system, one would like to compute its stability region. Often, the system depends on parameters, which should be tuned in order to shape this region according to one's needs. More generally, one would like to optimize the global stable behavior of the system; e.g. reducing transient motions.

In this talk I introduce a fairly general framework for doing this by approximating the dynamics by a finite dimensional stochastic process (closely related to the upwind scheme). Translating the desired objectives in the terms of this process enables the simple application of many optimization algorithms. In particular, no trajectory simulation is needed during the computation. The main advantage of the method lies in the resulting numerical efficiency and the general applicability for a wide range of different objectives.

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Simple heteroclinic orbit examples in the plane

Stephen Lucas
James Madison University, USA
lucassk@jmu.edu
James S Sochacki

There is much known about heteroclinic orbits in the plane and their properties. However, there are still open questions, and phase portraits highlighting unique features are still being sought. We present two classes of ODEs for the plane. The first one is a quadratic polynomial system that has a closed form solution, where every point is on a heteroclinic orbit with the same limit points. We demonstrate that this system has sensitive dependence on initial conditions and allows spiraling from one equilibrium to another. The second class of ODEs allows for an infinite number of heteroclinic limit points along arbitrary curves in the plane. We highlight an interesting quadratic polynomial that has its heteroclinic limit points defined by a single line in the plane.

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Mesohyperbolicity and other ergodic theory concepts in nonautonomous dynamical systems

Igor Mezic
UCSB, USA
mezic@engineering.ucsb.edu

We discuss the concept of mesohyperbolicity for studying properties of non-autonomous dynamical systems. The idea was introduced in the context of two-dimensional, divergence free flows. We extend the analysis to higher-dimensional systems and provide connections with other concepts such as that of ergodic partition. We present some applications, including the study of oil and gas evolution on the subsurface and subsurface during the Deepwater Horizon oil spill in the Gulf of Mexico.

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On the development and analysis of variational integrators for multirate dynamical systems

Sina Ober-Bloebaum
University of Paderborn, Germany
sinaob@math.upb.de
Sigrid Leyendecker

The use of discrete variational principles results in symplectic and momentum preserving variational integrators that exhibit excellent long-time behavior. In this talk variational integrators are developed for the integration of systems with dynamics on different time scales, for which the slow part of the system

is integrated with a relatively large step size while the fast part is integrated with a small time step to save function evaluations and decrease integration time. Based on a derivation in closed form via a discrete variational principle on a time grid consisting of macro and micro time nodes such a multirate variational integrator can be constructed. The structure preserving properties as well as the convergence behavior of the multirate integrator are analyzed and its performance is demonstrated by numerical examples.

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Set-oriented numerical analysis of time-dependent transport

Kathrin Padberg-Gehle
Technische Universitaet Dresden, Germany
kathrin.padberg@tu-dresden.de
Gary Froyland

The numerical analysis of transport processes is central for understanding the macroscopic behavior of classical dynamical systems as well as time-dependent systems such as fluid flows. We review different theoretical concepts and their numerical implementation into a set-oriented framework. We demonstrate that the geometric approach based on invariant manifolds and Lagrangian coherent structures and the probabilistic concept which relies on transfer operators give consistent results. Finally, potential combinations of these techniques are discussed.

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Rigorous connecting orbits from numerics

Ken Palmer
Providence University, Taiwan
palmer@math.ntu.edu.tw
Brian A. Coomes, Huseyin Kocak

A rigorous numerical method for establishing the existence of an orbit connecting two hyperbolic equilibria of a parametrized autonomous system of ordinary differential equations is presented. Given a suitable approximate connecting orbit and assuming that a certain associated linear operator is invertible, the existence of a true connecting orbit near the approximate orbit and for a nearby parameter value is proved. It turns out that inversion of the operator is equivalent to the solution of a boundary value problem for a nonautonomous inhomogeneous linear difference equation. A numerical procedure is given to verify the invertibility of the operator and obtain a rigorous upper bound for the norm of its inverse. Using this method, the existence of various kinds of homoclinic orbits including saddle-focus homoclinic orbits which imply the presence of chaos is demonstrated on examples including the Lorenz system.

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The dynamics of non-autonomous Lotka-Volterra ODEs

James Robinson
University of Warwick, England
j.c.robinson@warwick.ac.uk
Jose Langa, Antonio Suarez

Lotka-Volterra equations, coupled systems of ODEs modelling two competing species, are a canonical example in the qualitative theory of low-dimensional dynamical systems. In this talk I will show how ideas from the theory of pullback attractors for non-autonomous dynamical systems can be used to analyse the same simple models when some of the parameters are allowed to depend on time. Although the problem and the anlaysis is relatively simple, it provides a good demonstration of many of the techniques that can be used in more complicated problems, including order-preserving properties, the existence of maximal elements of the attractor, and perturbation results for invariant manifolds.

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Designing scalable algorithms for complex networks

Tuhin Sahai
United Technologies Research Center, USA
tuhin.sahai@gmail.com
Andrzej Banaszuk, Amit Surana, Alberto Speranzon

Complex networks such as building systems, UAV swarms and communication networks are of paramount importance to modern day applications and particularly challenging from an analysis perspective.

For scalable analysis of large networks, our approach uses a novel decentralized clustering approach, based on propagating waves in the graph. The algorithm recovers the solution obtained from spectral clustering without the need for expensive eigenvalue/vector computations. We prove that, by propagating waves through the graph, a local fast Fourier transform yields the local component of every eigenvector of the Laplacian matrix, thus providing clustering information. For large graphs, the proposed algorithm is orders of magnitude faster than random walk based approaches.

We then use the above decentralized partitioning approach to develop polynomial chaos based methods for uncertainty quantification in large networks. Polynomial chaos is used extensively for propagating uncertainty through smooth dynamical systems. Though useful for systems of small to moderate dimension, the curse of dimensionality restricts the applicability of these methods to high dimensional dynamical systems. We construct iterative schemes (intrusive and non-intrusive), for scalable uncertainty quantification in complex networks

that utilize "weak" interactions between clusters to quickly compute the approximate output distributions in large networks with bounded error. We will demonstrate these techniques on models of energy efficient buildings.

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Towards automatic computation of the Conley index over a base

Jacek Szybowski
AGH University of Science and Technology, Krakow, Poland
szybowsk@agh.edu.pl
Pawel Pilarczyk, Kinga Stolot

We introduce an algorithmic method for the computation of the Conley index over the phase space for discrete-time semidynamical systems. This is a considerable step forward towards the computation of the Conley index over a base, and—to the best of our knowledge—the first algorithmized approach to this problem. In this talk, we recall the definition of the homological version of the index, we introduce an algorithm for the construction of appropriate index pairs using uniform cubical grids, and we show some examples in which we prove the lack of continuation between some dynamical systems, not distinguishable using the regular Conley index approach. This is joint work with P. Pilarczyk and K. Stolot.

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Sacker-Sell spectrum and Lyapunov spectrum for random dynamical systems

Guangwa Wang
Jiangsu Normal University, Peoples Rep of China
wanggw7653@163.com
Yongluo Cao

The significance and importance of Sacker-Sell spectrum and Lyapunov spectrum for dynamical systems is well-known. This talk is mainly concerned with the two kinds of spectra for random dynamical systems (RDS). More precisely, in the first part, we will establish the Sacker-Sell Spectral Decomposition Theorem in some different frameworks of RDS: finite dimensional case, infinite dimensional case with compactness and infinite dimensional case with some kind of weak compactness, respectively. In the second part, taking the ideas from Mane and Thieullen, we will obtain the Multiplicative Ergodic Theorem about Lyapunov exponents for a very general infinite dimensional RDS. Moreover, in the third part, the relations between Sacker-Sell spectrum and Lyapunov spectrum in three different frameworks of RDS will be discussed.

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Multiscale time evolution for Markov jump particle systems

Matthew West
University of Illinois at Urbana-Champaign, USA
mwest@illinois.edu

We present a new time evolution scheme for efficiently generating realizations of Markov jump processes for particle systems, which can efficiently simulate highly multiscale particle distributions and event rates. Multiscale particle distributions are represented as weighted point samples, and time evolution occurs using a binned tau-leaping scheme with approximate rate sampling. A convergence proof as well as applications to aerosol particle simulation are given.

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