FOCM 2014 - Workshop A1
Computational Dynamics

A1 - December 11, 14:30 – 14:55

A parametrized Newton-Kantorovich method for rigorously computing (un)stable manifolds: non-resonant and resonant spectra

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In this talk we present numerical techniques for the rigorous computation of parametrizations for (un)stable manifolds to hyperbolic fixed points of analytic vector fields via the so called parametrization method. We facilitate our analysis by interpreting the infinite sequence of homological equations derived from the invariance equation fulfilled by the parametrization as an equivalent zero finding problem on the space of geometrically decaying sequences. Using this viewpoint an approach to compute rigorous error bounds on approximate parametrizations is presented. It is based on solving an equivalent parametrized fixed point problem on a ball around a numerical approximation using the contraction principle. In particular our analysis is successful even if internal non-resonance conditions crucial to previous methods fail to hold. We finish the talk by showing example implementations.

Joint work with Jan Bouwe van den Berg (VU University Amsterdam, Netherlands) and Jason Mireles-James (Florida Atlantic University, USA).

A1 - December 11, 15:00 – 15:25

Computing global invariant manifolds of dynamical systems

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Global bifurcations of dynamical systems are characterised by the re-arrangement of the higher dimensional stable and unstable manifolds of invariant objects under parameter variation. This may result in drastic changes of the dynamics, including transitions to chaotic regimes, transforming or creating basins of attraction and, ultimately, reorganising the overall structure of the phase space. The aim of this talk is to discuss how the study of global invariant manifolds by analytical and computational methods allows one to obtain deeper insight into the nature of global bifurcations.

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Coexistence of chaos and hyperchaos

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Chaotic attractors can have a very nonuniform internal structure. Even on the plane the well known Newhouse phenomenon guarantees that small sinks of very high periods may be embedded in large chaotic zones. For higher dimensional systems one can expect coexistence of chaotic and hyperchaotic dynamics, i.e. topological horseshoes with more than one positive Lyapunov exponents.

Consider the classical 4D Rossler system

$$\dot{x} = -y - w, \quad \dot{y} = x + ay + z, \quad \dot{z} = dz + cw, \quad \dot{w} = xw + b$$

with the parameter values $a = 0.27857$, $b = 3$, $c = -0.3$, $d = 0.05$. Let

$$\Pi = \{(x, 0, z, w) \in \mathbb{R}^3, \dot{y} = x + z < 0\}$$

be the Poincare section and let $P : \Pi \to \Pi$ be the associated Poincare map.

We prove that

1) there is an explicitly given trapping region $B \subset \Pi$ for P, i.e. $P(B) \subset B$,

2) the maximal invariant set $A = \text{inv}(P, B)$ contains three invariant sets, say H_1, H_2, H_3, on which the dynamics is Σ_2 chaotic, i.e. it is semiconjugated to the Bernoulli shift on two symbols,

3) H_1 is a chaotic set with two positive Lyapunov exponents,

4) H_2 and H_3 are chaotic sets with one positive Lyapunov exponent,

5) there is a countable infinity of heteroclinic connections linking H_1 with H_2, H_2 with H_3 and H_1 with H_3,

6) there is countable infinity of periodic orbits and heteroclinic/homoclinic orbits inside each horseshoe.

Joint work with Roberto Barrio (Universidad de Zaragoza, Spain) and Sergio Serrano (Universidad de Zaragoza, Spain).

A1 - December 11, 16:00 – 16:25

Computer-assisted analysis of Craik's 3D dynamical system

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The following system of equations is studied:

$$\dot{x} = ayz + bz + cy, \dot{y} = dzx + ex + fy, \dot{z} = gxy + hy + kx,$$

where $x(t), y(t)$, and $z(t)$ are real-valued functions, $\dot{x}, \dot{y}$, and $\dot{z}$ are their derivatives with respect to the independent variable t, and the coefficients a to k are real constants. This system arises several contexts in mechanics and fluid mechanics. Especially, Craik has shown that the equations of the form describe a class of exact solutions of the full incompressible Navier-Stokes equations.

Most of solution orbits for the system are unbounded. We can, however, observe characteristic behaviour. A typical solution orbit draws a helical curve, which changes amplitude in a vicinity of the origin. Some solutions change only the amplitude, while some solutions change not only the amplitude but also the axis along which they go to infinity as $t \to \infty$. Craik and Okamoto have found a four-leaf structure and a periodic orbit, which play an important role in controlling the solution orbits. We prove the existence of such a periodic orbit by a method of numerical verification.

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Coexistence of hexagons and rolls

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In this talk we introduce a rigorous computational method for finding heteroclinic solutions of a system of two second order differential equations. These solutions correspond to standing waves between rolls and hexagonal patterns of a two-dimensional pattern formation PDE model. After reformulating the problem as a projected boundary value problem (BVP) with boundaries in the stable/unstable manifolds, we compute the local manifolds using the Parameterization Method and solve the BVP using Chebyshev series and the radii polynomial approach. Our results settle a conjecture by Doelman et al. about the coexistence of hexagons and rolls.

Joint work with Jan Bouwe van den Berg (VU Amsterdam), Andréa Deschênes (Laval) and Jason Mireles James (Rutgers).

A1 - December 11, 17:30 – 17:55

Golden mean Siegel disks: renormalization hyperbolicity and applications

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We discuss two different renormalization techniques for golden mean Siegel disks, cylinder renormalization and renormalization for commuting pairs, and describe our recent computer-assisted proof of the renormalization hyperbolicity for almost commuting pairs.

This proof closes the issue of the golden mean universality in Siegel disks, and also leads to existence of golden mean Siegel cylinders in $\mathbb{C}^2$ for a class of two-dimensional perturbations of the golden mean quadratic polynomial.

Joint work with Michael Yampolsky (University of Toronto, Canada).

A1 - December 11, 18:00 – 18:25

Topological Data Analysis on Amorphous Structures

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Description of amorphous structures has been a long standing problem. What is lacking there is an appropriate language to describe geometric structures including short-range order (SRO) and medium-range order (MRO). In this talk, we present computational topological methods based on persistent homology and apply them into atomic arrangements of silica (SiO2) and granular systems. The results elucidate the following new geometric features in amorphous structures: (i) clear identification of amorphous states in silica by using persistence diagrams, (ii) hierarchical relationships between SRO and MRO in silica, (iii) presence of specific packing states (FCC, HCP, BCC, etc) in three dimensional granular packing experiments and transitions among them.

A1 - December 12, 14:35 – 15:25

Developing a computationally efficient algebraic/combinatorial framework for nonlinear dynamics

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Typical descriptions of the behavior of nonlinear dynamical systems focus on invariant sets. This leads to an amazingly rich mathematical theory, both in terms of the variety of invariants and the variety of bifurcations between different invariant sets. This richness leads to problems in the context of multiscale applications where one does not have exact models, i.e. the nonlinearities are not known from first principles, or equivalently parameters are unknown or at best poorly known, and in settings in which only crude measurements of the system can be made.

With this in mind I will describe our efforts to develop a computationally efficient, but mathematically rigorous framework for extracting combinatorial/algebraic topological descriptions of the global dynamical structures of multi-parameter nonlinear systems.

A1 - December 12, 15:30 – 15:55

Detecting Morse decompositions of the global attractor of regulatory networks by time series data

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Complex network structure frequently appear in biological systems such as gene regulatory networks, circadian rhythm models, signal transduction circuits, etc. As a mathematical formulation of such biological complex network systems, Fiedler, Mochizuki and their collaborators (JDDE 2013) recently defined a class of ODEs associated with a finite digraph called a regulatory network, and proved that its dynamics on the global attractor can in principle be faithfully monitored by information from a (potentially much) fewer number of nodes called the feedback vertex set of the graph.

In this talk, I will use their theory to give a method for detecting a more detailed information on the dynamics of regulatorynetworks, namely the Morse decomposition of its global attractor. The main idea is to take time series data from the feedback vertex set of a regulatory network, and construct a combinatorial multi-valued map, to which we apply the so-called Conley-Morse Database method.

As a test example, we study Mirsky's mathematical model for mammalian circadian rhythm which can be represented as aregulatory network with 21 nodes, and show that numerically generated time series data from its feedback vertex set consisting of 7 nodes correctly detect a Morse decomposition in the global attractor, including 1 stable periodic orbit, 2 unstable periodic orbits, and 1 unstable fixed point.

Joint work with B. Fiedler (Free University of Berlin, Germany), H. Kokubu (Kyoto University, Japan), G. Kurosawa (RIKEN, Japan), and A. Mochizuki (RIKEN, Japan).

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Switching networks database as a platform for parameter search in gene regulatory networks

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Experimental data on gene regulation and protein interaction is often very qualitative, with the only information available about pairwise interactions is the presence of either up- or down- regulation. Since majority of the parameters for any model in such a situation are not constrained by data, it is important to understand how different choices of parameters affect the dynamics and, therefore, the predictions of such a model. Continuous time Boolean networks, or switching networks, represent an attractive platform for qualitative studies of gene regulation, since the dynamics at fixed parameters is relatively easily to compute. However, it is quite difficult to analytically understand how changes of parameters affect dynamics. On the other hand, the Database for Dynamics is an numerical approach to study global dynamics over a parameter space. The results obtained by this method provably capture the dynamics a predetermined spatial scale. We combine these two approaches to present a method to study switching networks over parameter spaces. We apply our method to experimental data for cell cycle dynamics.

Joint work with Bree Cummins (Montana State University, USA), Bridget Fan (Montana State University, USA), Konstantin Mischaikow (Rutgers University, USA), Arnaud Goullet (Rutgers University, USA), Shaun Harker (Rutgers University, USA).

A1 - December 12, 17:00 – 17:25

An application of the persistence paradigm to the computation of the Conley index

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A new idea for determining the Conley index will be introduced, using an approximate isolating neighborhood and an approximation of a map. The approach is based on the persistence paradigm applied to a sequence of candidates for index pairs, whose relative homology is linked by homomorphisms corresponding to inclusions. A construction will be proposed in which the exit set is defined depending on the percentage of the image that falls outside of the neighborhood. A few sample applications of this method to discrete-time dynamical systems and to flows will be shown. These applications are based on combinatorial sets and outer approximations of maps with respect to a cubical grid in the Euclidean space.

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Analyzing the dynamics of pattern formation in the space of persistence diagrams

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Persistence diagrams are a relatively new topological tool for describing and quantifying complicated patterns in a simple but meaningful way. We will demonstrate this technique on patterns appearing in Rayleigh-Benard convection. This procedure allows us to transform experimental or numerical data from experiment or simulation into a point cloud in the space of persistence diagrams. There are a variety of metrics that can be imposed on the space of persistence diagrams. By choosing different metrics one can interrogate the pattern locally or globally, which provides deeper insight into the dynamics of the process of pattern formation. Because the quantification is being done in the space of persistence diagrams this technique allows us to compare directly numerical simulations with experimental data.

Joint work with Konstantin Miscahikow (Rutgers, USA), Rachel Levanger (Rutgers, USA), Shaun Harker (Rutgers, USA)., Michael Schatz (Georgia Tech, USA), Jeffrey Tithof (Georgia Tech, USA), Balachandra Suri (Georgia Tech, USA), Mark Paul (Virginia Tech, USA) and Mu Xu (Virginia Tech, USA).

A1 - December 13, 14:35 – 15:25

The Dynamics of Nucleation

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The Cahn-Hilliard equation is one of the fundamental models to describe phase separation dynamics in metal alloys. In this talk, I will focus on applying traditional dynamical tools, such as bifurcation theory and computational topology in order to gain a better understanding of the droplet formation during nucleation for the stochastic Cahn-Hilliard equation. I will consider different types of noise and different types of boundary conditions.

A1 - December 13, 15:30 – 15:55

Rigorous Continuation of Solutions of PDEs

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We present a rigorous numerical method to compute solutions of infinite dimensional nonlinear problems. The method combines classical predictor corrector algorithms, analytic estimates and the uniform contraction principle to prove existence of smooth branches of solutions of nonlinear PDEs. The method is applied to compute equilibria and time periodic orbits for PDEs defined on two- and three-dimensional spatial domains.

A1 - December 13, 16:00 – 16:25

Existence of globally attracting solutions of the viscous Burgers equation on the line with periodic boundary conditions and nonautonomous forcing

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We prove the existence of globally attracting solutions of the viscous Burgers equation with periodic boundary conditions on the line for some particular choices of viscosity and non-autonomous forcing

$u_t + u \cdot u_x - \nu u_{xx} = f(t,x)$.

The attracting solution is periodic if the forcing is periodic. The convergence towards attracting solution is exponential. The proof is computer assisted. The method is general and can be applied to other similar partial differential equations including the Navier-Stokes equations.

The technique we use is not restricted to some particular type of equation nor to the dimension one, as we are not using any maximum principles, nor unconstructive functional analysis techniques. We need some kind of 'energy' decay as a global property of our dissipative PDEs and then if the system exhibits an attracting orbit, then we should in principle be able to prove it independent of the dimensionality of of the system. At the present state our technique strongly relies on the existence of good coordinates, the Fourier modes in the considered example. We hope that the further development of the rigorous numerics for dissipative PDEs based on other function bases, e.g. for example the finite elements, should allow to treat also different domains and boundary conditions in near future.

[1] J. Cyranka, P. Zgliczyński, Existence of globally attracting solutions for one-dimensional viscous Burgers equation with nonautonomous forcing - a computer assisted proof, in revision, arXiv:1403.7170.

[2]J. Cyranka, P. Zgliczyński: The effect of fast movement in dissipative PDEs with the forcing term, preliminary preprint, arXiv:1407.1712.

Joint work with Piotr Zgliczyński (Jagiellonian University, Poland).

A1 - December 13, 17:00 – 17:25

Persistent homology of self-maps

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When a topological space is known only from sampling, persistence provides a useful tool to study its homological properties. In many applications one can sample not only the space, but also a map acting on the space. The understanding of the topological features of the map is often of interest, in particular in the analysis of time series dynamics but also in the dynamics of a map or differential equation given explicitely when the rigorous study is computationally too expensive and only numerical experiments are available. The aim of the talk is to present an extension of persistent homology to the case of a continuous self-map together with the associated algorithm and numerical examples based on the implementation of the algorithm.

Joint work with Ulrich Bauer (IST, Austria), Herbert Edelsbrunner (IST, Austria) and Grzegorz Jablonski (Jagiellonian University, Poland).

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Discrete and classical vector field dynamics

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The Forman's discrete Morse theory is an analogy of the classical Morse theory with, so far, only informal ties. Our goal is to establish a formal tie on the level of induced dynamics. Following the Forman's 1998 paper on "Combinatorial vector fields and dynamical systems", we start with a possibly non-gradient combinatorial vector field. We construct a flow-like upper semi-continuous acyclic-valued mapping whose dynamics is equivalent to the dynamics of the Forman's discrete vector field, in the sense that isolated invariant sets and index pairs are in one-to-one correspondence. The passage to an equivalent continuous single-valued vector field is completed using the graph approximation. This is a joint work with M. Mrozek and Th. Wanner. In my talk, I focus on the construction and properties of the linking multivalued mapping and refer to the Mrozek's talk at the B2 workshop for the extension of the Conley index theory in the combinatorial setting.

Joint work with Marian Mrozek (Jagiellonian University, Krakow, Poland), and Thomas Wanner (George Mason University, Fairfax, USA).
