The integration of stiff systems of ODEs using multistep methods

Elisabete Alberdi Celaya
Department of Applied Mathematics, EUIT de Minas y Obras Públicas, UPV/EHU, Spain
elisabete.alberdi@ehu.es

The second order Ordinary Differential Equation (ODE) system obtained after semidiscretizing the wave-type Partial Differential Equation (PDE) with the Finite Element Method (FEM), shows strong numerical stiffness. Although it can be integrated using Matlab ode-solvers, the function `ode15s` offered by Matlab for solving stiff ODE systems does not result very efficient as its resolution requires the use of numerical methods with good stability properties and controlled numerical dissipation in the high-frequency range. This has lead us to study the Backward Differentiation Formulae (BDF) in which this ode-solver is based on and to work in two directions:

• The study and application of methods which use superfuture points and which result unconditionally stable up to order 4.

• The review of direct methods for second order ODEs used in computational mechanics, in particular the Newmark parametric family in which the second order accurate and unconditionally stable HHT-α is based. This method offers high frequency dissipation for some values of the parameter α. In this sense, we have constructed a modification of the 2-order BDF method (the BDF2 method), which we have called BDF-α. This new method is second-order accurate and with a smaller local truncation error than the BDF2, it is unconditionally stable for some values of α and it permits a parametric control of the numerical dissipation.

In collaboration with J. J. Anza Aguirrezabala, Department of Applied Mathematics, ETS de Ingeniería de Bilbao, Universidad del País Vasco UPV/EHU, Spain.

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From delay differential equations to ordinary differential equations

Dimitri Breda
Department of Mathematics and Computer Science, University of Udine, Italy
dimitri.breda@uniud.it

Delay differential equations generate dynamical systems on a infinite-dimensional state space. Numerical methods developed to either approximate solutions or detect stability of equilibria and cycles represent, soon or later, a form of reduction to finite dimension, read ordinary differential equations. We are interested in analyzing the dynamical implications of this discretization when pseudospectral methods are applied to nonlinear problems, focusing on the step from infinite to finite rather than on its later use.

Rigorous computation of a bifurcation diagram for a reaction diffusion system

Maxime Breden
ENS-Cachan, France
maxime.breden@ens-cachan.fr

In this talk, I'll present the study of a 3-component reaction diffusion system, coming from biology, and its behaviour depending on the diffusion parameter. More precisely, there is a homogeneous steady state for this system, which become unstable for some values of this diffusion parameter. This Turing instability leads to the appearance of new non-homogeneous steady states, and the goal is to describe their evolution with respect to the diffusion coefficient.
Rigorous computation is a very efficient method to tackle this kind of problems: the numerical computations are easy to obtain and then we manage to make them rigorous. I'll detail how this can be done to prove the existence and compute the bifurcation diagram for the steady states of our system.

The Belly Phase: Geometric Mixing, Peristalsis, and the Geometric Phase of the Stomach

Julyan H. E. Cartwright
Instituto Andaluz de Ciencias de la Tierra (IACT), CSIC−Universidad de Granada,Spain,
julyan.cartwright@csic.es

How may fluid be mixed at low Reynolds number? Such mixing is normally performed with a stirrer, a rotating device within the container that produces a complex, chaotic flow. Alternatively, in the absence of a stirrer, rotation of the container walls themselves can perform the mixing, as occurs in a cement mixer. At the lowest Reynolds numbers, under what is known as creeping flow conditions, fluid inertia is negligible, fluid flow is reversible, and an inversion of the movement of the stirrer or the walls leads — up to perturbations owing to particle diffusion — to unmixing, as Taylor and Heller demonstrated. This would seem to preclude the use of reciprocating motion to stir fluid at low Reynolds numbers; it would appear to lead to perpetual cycles of mixing and unmixing. Consider a biological case of cavity flow: the stomach. In the stomach food and drink are mixed to form a homogeneous fluid termed chyme, which is then digested by the intestines. Gastric mixing is produced by what is called peristalsis: by the stomach walls moving in a rhythmic fashion. In mathematical terms, the shape of the stomach walls undergoes a closed cycle in the space of shapes during each peristalsis cycle. Obviously only shape cycles that do not require a cumulative net displacement between any two sections of the stomach can be considered. How then is this peristaltic movement of the stomach walls able to produce mixing, especially in animals in which the stomach dimensions are such that fluid inertia of the stomach contents is negligible? The solution to this conundrum involves a geometric phase induced by a cyclic variation of the boundary shape. A geometric phase is an example of anholonomy: the failure of system variables to return to their original values after a closed circuit in the parameters. We propose what we term geometric mixing: the use of the geometric phase introduced by the deformable boundaries of a container as a tool for fluid mixing at low Reynolds number. To exemplify how this process leads to efficient mixing, we use the well-known two-dimensional mixer based on the journal bearing flow but subject to a much-less-studied rotation protocol that satisfies the geometrical constraints required by the stomach example. We lastly show that peristaltic mixing and digestion may operate thanks to a geometric phase in the stomach.

Computing tangent bundle for hyperbolic periodic orbits of system of ODEs

Roberto Castelli
Basque Center for Applied Mathematics, Bilbao, Spain
rcastelli@bcamath.org

The stability of a T-periodic orbit of a dynamical system is encoded in the spectral properties of the so-called Monodromy matrix. Such matrix is defined as the solution at time T of the non-autonomous linear differential equations with periodic coefficients arising by linearizing the dynamical system around the periodic orbit. In general, the solution of such linear differential equation can not be analytically computed.
In this talk, taking advantage from the theory of Floquet, a new rigorous numerical method to compute fundamental matrix solutions of non-autonomous linear differential equations with periodic coefficients is introduced. As an application, the method is used to rigorously compute the Monodromy matrix and the stable and unstable bundles of periodic orbits. Examples are given in the context of the Lorenz equations, Arneodo system and a reduced PDE (Kuramoto Sivashinsky).

Log-rolling and kayaking: periodic dynamics of a nematic liquid crystal in a shear flow

David Chillingworth
Mathematical Sciences, University of Southampton, Highfield, Southampton, U.K.
D.R.Chillingworth@soton.ac.uk

Dynamics of a nematic liquid crystal in a steady shear flow can be modelled by a system of ODEs on the 5-dimensional space of 3 x 3 symmetric traceless real matrices. We use methods of geometry and symmetry to describe several distinct modes of periodic behaviour, and to obtain precise criteria for the existence of the more unusual and (probably) numerically observed 'kayaking' regime.

Powered invariant manifold transfers between libration point orbits in the Sun-Earth-Moon system

Elena Fantino
Institut d'Estudis Espacials de Catalunya (IEEC, Barcelona)
elena.fantino@upc.edu

Over the past three decades, ballistic and impulsive trajectories between libration point orbits (LPOs) in the Sun-Earth-Moon system have been investigated to a large extent. It is known that exploiting the invariant manifolds of LPOs of two different circular restricted three-body problems (CR3BPs) (i.e., the Sun-Earth and the Earth-Moon systems) can lead to significant propellant savings in specific transfers, such as from a low Earth orbit to the Moon's vicinity. We present an investigation that compares the use of impulsive maneuvers with low-thrust trajectory arcs to connect LPOs using invariant manifold dynamics.

A Mathematical Model of the Genetic Code, the Origin of Protein Coding, and the Ribosome as a Dynamical Molecular Machine

Diego L. González
CNR-IMM, University of Bologna, Italy
gonzalez@bo.imm.cnr.it

A paradigm shift is needed in order to interpret the huge quantity of complex experimental data arriving mainly from genetics and molecular biology. Mathematical modelling, as the history of physics demonstrate, is the main way for coping with such a situation. Mathematical models serve as a reference conceptual framework for interpreting experimental data and allow to suggest new experiments. In a dialectic manner, comparison between theory and experiments allows the optimization of existing models or their replacement with more accurate ones when optimization is not more possible. In this contribution we present a mathematical model of the nuclear genetic code that describes completely its degeneracy distribution. Moreover, it allows the uncovering of many symmetry properties of the code that are related with the structure of genetic information. In such a way the statistical study of actual coding sequences becomes feasible from a new theoretical point of view. The model can be extended to include the vertebrate mitochondrial genetic code (tesserae model) allowing new insight on the difficult problem of the origin of protein synthesis and the biological mechanisms which are devoted to ensure the quality of genetic coding and decoding (mutation robustness and error detection/correction, circular and comma-free coding for frame maintenance, etc.). The possibility that error correction should be implemented by taking profit of the dynamics of the synthesis apparatus is also briefly explored.

Linear stability of relative equilibria in n-body-type problems

Riccardo Jadanza
Politecnico di Torino, Italy
riccardo.jadanza@polito.it

We address the question of linear and spectral stability of relative equilibria for two important classes of singular potentials: the α-homogeneous one, where $\alpha \in (0, 2)$, which includes the gravitational case ($\alpha = 1$), and the logarithmic one.
Our main results are two sufficient conditions to detect linear instability. Namely, we first prove that if the Morse index of a central configuration with even nullity is odd, then the associated relative equilibrium is spectrally (hence linearly) unstable. Furthermore, in the α-homogeneous case we establish an inequality (written in terms of the central configuration only) which, when satisfied, implies the spectral (hence linear) instability of the associated relative equilibrium. The proof of the first result is based on some refined formulae for computing a celebrated topological invariant known in literature as the spectral flow, which we utilise here for paths of Hermitian operators.

In collaboration with Vivina L. Barutello and Alessandro Portaluri.

Transition state geometry near higher-rank saddles in phase space

Jesús Palacián
Public University of Navarre, Pamplona, Spain
palacian@unavarra.es

We present a detailed analysis of invariant phase space structures near higher-rank saddles of Hamiltonian systems. Using the theory of pseudo-hyperbolic invariant surfaces, we show the existence of codimension-one normally hyperbolic invariant manifolds that govern transport near the higher-rank saddle points. Such saddles occur in a number of problems in celestial mechanics, chemical reactions, and atomic physics. As an example, we consider the problem of double ionization of helium in an external electric field, a basis of many modern ionization experiments. In this example, we illustrate our main results on the geometry and transport properties near a rank-two saddle.

In collaboration with George Haller, Charles Jaffé, Turgay Uzer and Patricia Yanguas.

Study on Controlled Radical Polymerization

Simone Rusconi
Basque Center for Applied Mathematics, Bilbao, Spain
srusconi@bcamath.org

Controlled radical polymerization (CRP) is a process to form polymers by successive monomers additions. This growing process is mainly made by three events: propagation, if the next monomer is linearly added to the chain, backbiting, when the free radical changes its position and a new branch will start growing perpendicular to the previous one, and termination, if the chain stops to grow.
We have proposed a model describing the CRP process and offered two different approaches for solving it: Partial Differential Equations solutions (PDE) and stochastic simulation algorithm based on Monte Carlo estimations (MC).
In this presentation, the model and the two approaches are summarized and their benefits as well as drawbacks are discussed. The future developments with the focus on the real applications are outlined.

This work is performed under the supervision of Elena Akhmatskaya (BCAM) and Dmitri Sokolovski (UPV/EHU).

Control of pattern formation by time-delay feedback with global and local contributions

Michael Stich
School of Engineering and Applied Science, Aston University
m.stich@aston.ac.uk:

We consider the suppression of spatiotemporal chaos in the complex Ginzburg-Landau equation by a combined global and local time-delay feedback. Feedback terms are implemented as a control scheme, i.e., they are proportional to the difference between the time-delayed state of the system and its current state. Feedback is efficient in suppressing spatiotemporal chaos and gives rise to a wide range of patterns, among which we study in detail (a) uniform oscillations, (b) standing waves, and (c) the stationary state. By changing the ratio between local and global terms, we can control the stabilization of different solutions. We show analytical results (such as stability analysis) and numerical simulations.

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A semi-classical take on quantum control

Holger Teismann
Acadia University, Nova Scotia, Canada
holgertn@gmail.com

After a brief introduction into quantum control, we review some of the important mathematical results about the possibilities and limitations of controlling quantum systems.
We then review some semi-classical techniques of quantum theory, such as WKB approximation, quantum trajectories, fluid-dynamical and phase-space formulations, and discuss their potential implication for the quantum-control problem..
Specifically, we suggest that finite-dimensional approximations to the full quantum dynamics a la Ehrenfest can provide insight into the control process and/or exhibit obstacles to controllability. (This last part of the talk is work in progress and somewhat speculative.)

Rigorous continuation in a nutshell.

Matthieu Vanicat
ENS-Cachan, France
matthieu.vanicat@gmail.com

Rigorous computation can be used in dynamical systems to prove existence and local uniqueness of solution for a class of nonlinear problems: steady states for PDE's, periodic solutions for delay equations,... In this talk I will try to give a general outline of this rigorous continuation technique. A first step is to rewrite the problem as $f(x)=0$ and compute a numerical solution. Then we construct explicitly a Newton-like operator in the neighbourhood of the numerical approximated solution. This operator is built such that x is a fixed point of this operator if and only if $f(x)=0$. The proof of existence and local uniqueness lies on the uniform contraction principle. An effective way to check the hypotheses of this theorem is to construct radii polynomials which will control the truncation error of the numerical approximation and show that this radii polynomials are simultaneously negative on an interval. This check is done rigorously using interval arithmetic.

Fractal properties of generalized Bessel functions

Domagoj Vlah
Faculty of Electrical Engineering and Computing, Unska 3, 10000 Zagreb, Croatia.
domagoj.vlah@fer.hr

The fractal oscillatority of solutions $x = x(t)$ of ordinary differential equations at $t = \infty$ is measured by *oscillatory* and *phase dimensions* defined through the box dimension. Oscillatory and phase dimensions are defined as box dimensions of the graph of $X(\tau) = x(1/\tau)$ near $\tau = 0$ and trajectory $(x, \dot{x})$ in $\mathbb{R}^2$, respectively, assuming that $(x, \dot{x})$ is a spiral converging to the origin. The box dimension of a plane curve measures the accumulation of a curve near a point, which is in particular interesting for non-rectifiable curves. The oscillatory dimension of solutions of Bessel equation has been determined by Pašić and Tanaka (2011). Here, we compute the phase dimension of solutions of a class of ordinary differential equations, including Bessel equation. These solutions we call generalized Bessel functions. The phase dimension of Bessel functions is computed to be equal to 4/3.

We relate these results to the result from Ž□ubrinić and Ž□upanović (2008) about the box dimension of spiral trajectories of planar vector fields, depending on the asymptotic behavior of iterates of the Poincaré map. They applied it to the Hopf bifurcation and Liénard systems. Also, they obtained all possible values of box dimensions of spiral trajectories around a weak focus, associated with polynomial vector fields.

Computation of the phase dimension of generalized Bessel functions use asymptotic expansions of Bessel functions. Due to a very large number of terms, we have to employ methods of computer algebra.