Helsinki University of Technology Institute of Mathematics Reports
Espoo 2009 C020

WORKSHOP ON NUMERICS IN DYNAMICAL SYSTEMS
TKK, APRIL 23–25, 2009
ABSTRACTS

Timo Eirola, Olavi Nevanlinna, Santtu Ruotsalainen (eds.)

TEKNILLINEN KORKEAKOULU
TEKNISKA HÖGSKOLAN
HELSINKI UNIVERSITY OF TECHNOLOGY
TECHNISCHE UNIVERSITÄT HELSINKI
UNIVERSITE DE TECHNOLOGIE D'HELSINKI

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Faculty of Information and Natural Sciences

Department of Mathematics and Systems Analysis

Timo Eirola, Olavi Nevanlinna, Santtu Ruotsalainen (eds.): *Workshop on Numerics in Dynamical Systems 2009 - Abstracts*; Helsinki University of Technology Institute of Mathematics Reports C020 (2009).

Abstract: *This report contains the program, list of participants, and abstracts for the invited presentations of the international conference Workshop on Numerics in Dynamical Systems 2009, held at the Helsinki University of Technology, April 23–25, 2009, as a part of Special Year in Numerics 2008–2009.*

AMS subject classifications: 65-06

Keywords: numerical analysis, dynamical systems, conference abstracts

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http://dyn.math.tkk.fi/numericsyear/numdyn/

ISBN 978-951-22-9868-6 (print)
ISBN 978-951-22-9869-3 (PDF)
ISSN 0784-6460 (print)
ISSN 1797-5875 (PDF)

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Contents

Special Year in Numerics

The Finnish Mathematical Society has chosen Numerical Analysis as the theme for its visitor program for the period 2008–2009. The main events of Special Year in Numerics are meetings and short courses organized between May 2008 and June 2009. These are connected to the 100th anniversary celebration of Helsinki University of Technology in 2008.

Acknowledgements

Special Year in Numerics is sponsored by the Academy of Finland, the Väisälä Fund of the Finnish Academy of Science and Letters, as well as the Finnish Cultural Foundation.

1 General Information

Directions

Helsinki University of Technology (TKK) is located in Otaniemi, Espoo. It is a five minutes walk from Hotel Radisson SAS Espoo to the main building of TKK (number 1 on the map of Otaniemi). The talks will be held in the lecture hall E which is located on the ground floor of the main building of TKK. The registration desk is located outside the lecture hall E.

Lunches

There is the restaurant Alvari (Thursday and Friday lunches) on the ground floor of the main building near the lecture hall E. The opening hours are 8.00–18.00. Tables are reserved for lunch. There is also the restaurant Dipoli (number 19 on the map of Otaniemi) which is located in the campus. Tables are reserved at Dipoli for Saturday lunch.

Computer access

Instructions about computers with passwords will be handed out at the registration desk. Please handle the password sheet responsibly. Wlan (Aalto open) is open access.

Social events

On Thursday at 17.00 the Get together will be held in the coffee room of the Institute (room U324 on the Building map).

On Friday at 17.30 there will be an occasion for sauna with refreshments at the roof-top sauna of the T-building. The roof-top sauna (number 30 on the map of Otaniemi) is located about 250 meters from the main building of Helsinki University of Technology. The conference dinner will follow there at 19.00.

Tourist information and activities in Helsinki

The city of Helsinki offers a lot to see and experience for visitors. The heart of Helsinki consists of Senate Square and Market Square. The National Museum of Finland, the Ateneum Art Museum as well as the Museum of Contemporary Art Kiasma are all within five minutes walking distance from there. Some of the other most popular sights in Helsinki include Suomenlinna Maritime fortress.

More information about activities in Helsinki can be found at

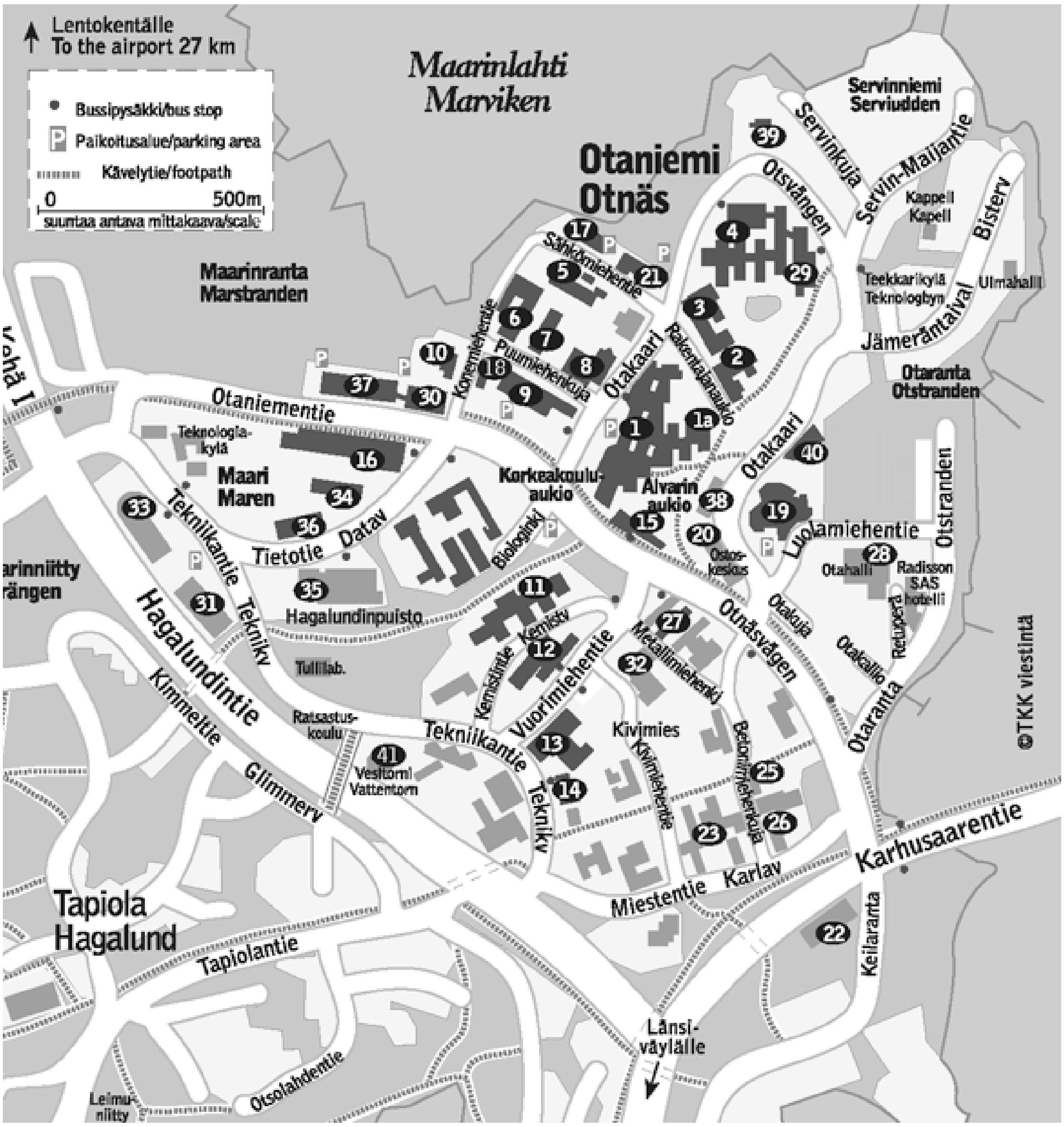
http://www.hel2.fi/tourism/en/matko.asp

The buses 102 and 103 commute between Otaniemi and downtown Helsinki.

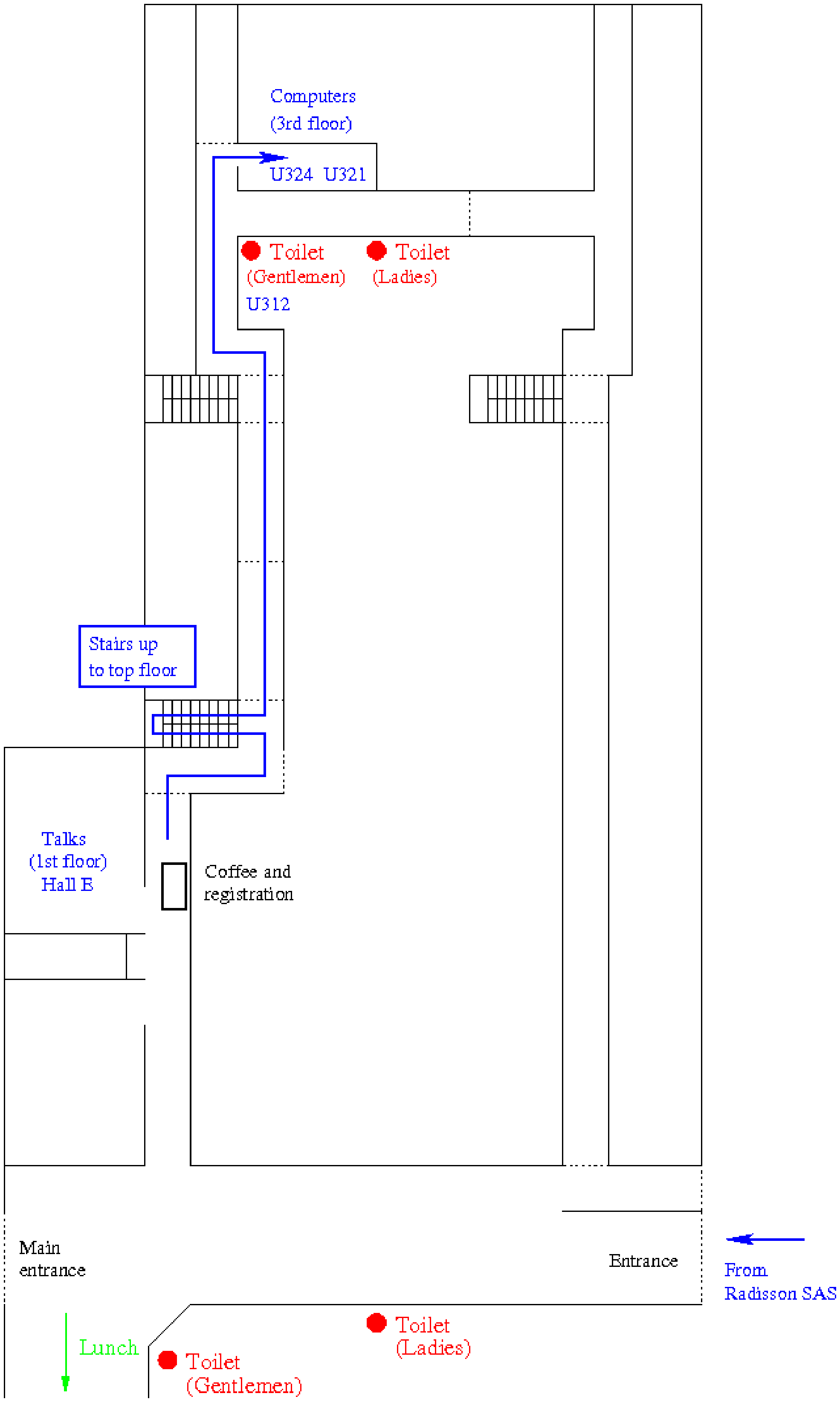
A note-worthy current event is APRIL JAZZ 2009, arranged April 22–26, in Espoo quite near Otaniemi.

http://www.apriljazz.fi/

2 Map of Otaniemi



3 Building map



4 Conference program

Thursday, April 23

10.00 Registration and coffee

10.30 Opening

10.40–12.00 Chair: Olavi Nevanlinna

Christian Lubich, University of Tübingen:
Modulated Fourier expansions for weakly nonlinear wave equations

Sebastian Reich, University of Potsdam:
Hybrid Monte Carlo and Metropolis adjusted time-stepping methods for classical mechanics subject to fluctuation-dissipation terms

12.00 Lunch

13.20–14.40 Chair: Marlis Hochbruk

Willy Govaerts, University of Gent:
Basic models for cell cycle controls from a dynamic viewpoint

Erik Van Vleck, University of Kansas:
Exponential dichotomy, matrix decompositions, and Newton's method

14.40 Coffee

15.20–16.00 Chair: Chuz Sanz-Serna

Gennady Leonov, St Petersburg University:
Hidden oscillations

Marianna Khanamiryan, University of Cambridge:
Quadrature methods for highly oscillatory dynamical systems

17.00–19.00 Get together

Friday, April 24

9.10–10.30 Chair: Luca Dieci

Ben Leimkuhler, University of Edinburgh:
Controlled Variable Molecular Dynamics

Anders Szepessy, KTH Stockholm:
Accuracy of molecular dynamics simulations

10.30 Coffee

11.00–12.20 Chair: Bernd Krauskopf

Chus Sanz-Serna, Universidad de Valladolid:
Computational experiences with multiscale methods for problems with fast oscillations

Marlis Hochbruck, University of Düsseldorf:
Regularization of nonlinear inverse problems by certain time integration schemes

12.20 Lunch

13.30–14.50 Chair: Christian Lubich

Alexander Ostermann, University of Innsbruck:
Convergence analysis of splitting methods

Reinout Quispel, La Trobe University:
Geometric numerical integration of differential equations

14.50 Coffee

15.20–16.40 Chair: Gennady Leonov

Etienne Emmrich, Technische Universität Berlin:
Stability and convergence of time discretisation methods for nonlinear evolution problems

Philip Aston, University of Surrey:
Integration methods using vector norms for computing Lyapunov exponents

17.30 Sauna with refreshments

19.00–23.00 Dinner (casual, buffet)

Saturday, April 25

9.10–10.30 Chair: Reinout Quispel

Dimitri Breda, Università di Udine:
Numerical computation of Lyapunov exponents for delay differential equations

Bernd Krauskopf, University of Bristol:
Computing the symbolic dynamics of heteroclinic orbits of the Lorenz system

10.30 Coffee

11.00–12.20 Chair: Anders Szepessy

Sergei Pilyugin, St Petersburg University:
Approximate trajectories for set-valued mappings and differential inclusions

Nikolay Kuznetsov, St Petersburg University:
Period doubling bifurcation in discrete phase-locked loop

12.20 Lunch at Dipoli

13.30–14.50 Chair: Ben Leimkuhler

Olavi Nevanlinna, TKK Helsinki *Computing the spectrum and representing the resolvent*

Luca Dieci, Georgia Tech:
Sliding modes in Filippov systems

14.50 Closing

5 List of participants

Organizers

Timo Eirola, TKK Helsinki
Olavi Nevanlinna, TKK Helsinki

Speakers

Philip Aston, University of Surrey
Dimitri Breda, Università di Udine
Luca Dieci, Georgia Tech
Etienne Emmrich, Technische Universität Berlin
Willy Govaerts, University of Gent
Marlis Hochbruck, University of Düsseldorf
Marianna Khanamiryan, University of Cambridge
Bernd Krauskopf, University of Bristol
Nikolay Kuznetsov, St Petersburg University
Ben Leimkuhler, University of Edinburgh
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Christian Lubich, University of Tübingen
Olavi Nevanlinna, TKK Helsinki
Alexander Ostermann, University of Innsbruck
Sergei Pilyugin, St Petersburg University
Reinout Quispel, La Trobe University
Sebastian Reich,University of Potsdam
Chus Sanz-Serna, Universidad de Valladolid
Anders Szepessy, KTH Stockholm
Erik Van Vleck, University of Kansas

Organizing committee

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Kurt Baarman, TKK Helsinki
Mikko Byckling, TKK Helsinki
Marita Katavisto, TKK Helsinki
Santtu Ruotsalainen, TKK Helsinki
Suvi Törrönen, TKK Helsinki

6 Abstracts

Modulated Fourier expansions for weakly nonlinear wave equations

Christian Lubich[1]

[1] University of Tübingen

ABSTRACT

Nonlinearly perturbed wave equations show unexpected long-time properties regarding the almost-preservation of actions and slow energy exchange between modes. This behaviour can be explained, both for the analytical problem and for symplectic numerical discretizations, using the technique of modulated Fourier expansions.

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Hybrid Monte Carlo and Metropolis adjusted time-stepping methods for classical mechanics subject to fluctuation-dissipation terms

Sebastian Reich[1]

[1] University of Potsdam

ABSTRACT

Markov chain Monte Carlo (MCMC) methods are often the method of choice when it comes to sample for a high dimensional probability distribution function (PDF). While MCMC method offer great flexibility and can be widely applied, they also often suffer from a high correlation between samples which leads to a slow exploration of phase space. The hybrid Monte Carlo method (HMC) is an attractive variant of MCMC because it allows, in principle, to take large steps in phase space. The key underlying idea is to formulate a Hamiltonian system which possesses the desired PDF as an invariant. While this leads to a 100 % acceptance rate in theory, numerical implementations reduce the acceptance rate with increasing system size and large discretization parameters.

In my talk I will first provide a brief introduction the HMC and related methods. I will then show how the inherent geometry of the underlying Hamiltonian system and its numerical approximation can be used to avoid a reduction in the acceptance rates even for highly non-local proposal steps. Finally, I will discuss in as far HMC and related Metropolis corrected time-stepping methods can be interpreted as statistically correct implementations of Langevin and Nose-Hoover dynamics.

Basic models for cell cycle controls from a dynamical viewpoint

Willy Govaerts[1] (joint work with Virginie De Witte and Leila Kheibarshekan)

[1] University of Gent

ABSTRACT

A recent application field of bifurcation theory is in modelling the cell cycle. We refer in particular to the work of J.J. Tyson and B. Novak, which is based on extensive experimental work, in particular on budding yeast, fission yeast and egg cells. The fundamental idea is that the cell cycle is not a periodic orbit, but an alternation between two self-maintaining stable steady states of a system of kinetic equations.

Several aspects of these models deserve close attention. For example, the limit point curves in the two-variable model behave in an ungeneric way under variation of the natural parameters and the hysteresis loop in the model is not the usual loop caused by the existence of a codimension-2 cusp point.

We also find that orbits homoclinic-to-saddle-node (HSN) in the three-variable model die in a non-central orbit homoclinic-to-saddle-node (NCH) under a natural parameter variation. The range of existence of these orbits is crucial for the structural stability of the important behavioural aspects of the model.

Since the cell cycle is not just a periodic orbit in a dynamical system, the question arises what it really is and how the models can be studied computationally. One possibility is to see it as a boundary value problem, another one is to see it as a fixed point of a map. Whatever the object is, it clearly needs a form of stability.

We will discuss some of the above issues.

Exponential Dichotomy, Matrix Decompositions, and Newton's Method

Erik Van Vleck[1]

[1] University of Kansas

ABSTRACT

In this talk we develop new methods for determining exponential dichotomies of linear time varying differential equations. The techniques are based upon continuous matrix factorizations (SVD and QR) and rely upon having integral separation or more generally stable Lyapunov exponents. A perturbation theory is developed by formulating a zero finding problem and applying a version of the classical Newton-Kantorovich Theorem.

Hidden oscillations

Leonov G.A.[1], Kuznetsova O.A., Seledzhi S.M.

[1] Department of Applied Cybernetics
Faculty of Mathematics and Mechanics
Saint-Petersburg State University
leonov@math.spbu.ru

ABSTRACT

The methods of Lyapunov quantities and harmonic linearization, numerical methods, and the applied bifurcation theory together discover new opportunities for analysis of "hidden" oscillations of control systems. In the present work these opportunities are demonstrated. New methods for calculation of Lyapunov quantities and for asymptotic integration are applied for localization of small and large limit cycles in two dimension autonomous systems. Here the autonomous quadratic system is reduced to the Lienard equation and by the latter the two- dimensional domain of parameters, corresponding the existence of four limit cycles: three "small" and one "large", was evaluated. New method, based of harmonic linearization, for "construction" of periodic solutions is suggested. For non-autonomous control systems ¯lter hypothesis, Aizerman and Kalman problems are considered.

Quadrature methods for highly oscillatory dynamical systems

Marianna Khanamiryan[1]
[1] University of Cambridge
Department of Applied Mathematics and Theoretical Physics
Wilberforce Road, Cambridge CB3 0WA, United Kingdom
Email: M.Khanamiryan@damtp.cam.ac.uk

ABSTRACT

The talk will address the issues of numerical approximations of dynamical systems in presence of high oscillation. For the systems of highly oscillatory ordinary differential equations given in the vector form $\mathbf{y}' = A_\omega \mathbf{y} + \mathbf{f}$, where A_ω is a constant nonsingular matrix, $\|A_\omega\| \gg 1$, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\mathbf{f}$ is a smooth vector-valued function and ω is an oscillatory parameter, we show how an appropriate choice of quadrature rule improves the accuracy of numerical approximation as $\omega \to \infty$. We present a *Filon*-type method to solve highly oscillatory linear systems and WRF method, a special combination of the *Filon*-type method and the *waveform methods*, for nonlinear systems. The work is accompanied by numerical examples.

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Controlled Variable Molecular Dynamics

Ben Leimkuhler[1]

[1] University of Edinburgh

ABSTRACT

For molecular dynamics to be useful for recovering macroscopically-relevant information (e.g. thermodynamic averages), it must be regulated by auxiliary control laws such as thermostats (for temperature) and barostats (for pressure). In this talk I will discuss some examples of such controls, focusing primarily on thermostats. Ergodicity is always a crucial issue in molecular dynamics; I will discuss mixed stochastic-dynamic methods which enhance sampling efficiency.

Accuracy of molecular dynamics simulations

Anders Szepessy[1]
[1] KTH Stockholm

ABSTRACT

I will show that Born-Oppenheimer, Smoluchowski, Langevin and Ehrenfest dynamics are accurate approximations of time-independent Schrödinger observables for a molecular system, in the limit of large ratio of nuclei and electron masses, without assuming that the nuclei are localized to vanishing domains. The derivation, based on characteristics for the Schrödinger equation, bypasses the usual separation of nuclei and electron wave functions and gives a different perspective on initial and boundary conditions, caustics and irreversibility, the Born-Oppenheimer approximation, computation of observables, stochastic electron equilibrium states and symplectic simulation in molecular dynamics modeling.

Computational experiences with Multiscale Methods for problems with fast oscillations

Chus Sanz-Serna[1]

[1] Universidad de Valladolid

ABSTRACT

I will report on my experience with the use of heterogeneous multiscale methods to follow the slow dynamics of problems whose solutions consist of both slowly and rapidly oscillating components. Among the issues considered, I will include (i) relating the values of the micro and macrostates of the system (ii) the design on new filters/mollifiers (iii) the implementation of the technique in conjunction with standard software.

Regularization of nonlinear inverse problems by certain time integration schemes

Marlis Hochbruck[1]

[1] University of Düsseldorf

ABSTRACT

In this talk we discuss the numerical realization of asymptotic regularization (Showalter's method) of inverse problems. Given a nonlinear inverse problem $F(u) = y^\delta$, the key idea of asymptotic regularization is that the solution $u(t)$ of the evolution equation $u'(t) = F'(u(t))^*(y^\delta - F(u(t)))$, $u(0) = u_0$ yields a stable approximation to the solution of the inverse problem for *large* t. Application of standard integration schemes yield well known regularization methods. For example, the explicit Euler method and the linearly implicit Euler method are equivalent to Landweber and Levenberg-Marquardt regularization, respectively.

Further, we discuss the regularization properties of the Levenberg-Marquardt method and of the exponential Euler method applied to the Showalter equation. In particular, we will present a variable step size analysis which allows to prove that optimal convergence rates are achieved under suitable assumptions on the initial error.

This is joint work with Michael Hönig and Alexander Ostermann.

Convergence analysis of splitting methods

Alexander Ostermann[1]

[1] Institut für Mathematik, Universität Innsbruck
Technikerstraße 13, A-6020 Innsbruck, Austria

ABSTRACT

In recent years there has been a lot of progress in better understanding the convergence properties of splitting methods for evolution equations involving unbounded operators. Most of the available analysis is based on semigroup theory and usually involves the variation-of-constants formula. In this talk we will introduce a simple framework which is based on discrete evolution operators and φ-functions thereof. This framework allows to obtain (optimal) convergence rates for a variety of dimension splittings of parabolic problems. Moreover, it can be used to analyse high-order exponential operator splitting methods for parabolic problems. The talk is based on recent results that have been obtained jointly with Eskil Hansen from Lund University.

Geometric Numerical Integration of Differential Equations

Reinout Quispel[1]

[1] La Trobe University

ABSTRACT

Stability and convergence of time discretisation methods for nonlinear evolution problems

Etienne Emmrich[1]

[1] Technische Universität Berlin

ABSTRACT

Many time-depending problems in science and engineering can be described by the initial-value problem for a nonlinear evolution equation of first order. In this talk, we present new results on the convergence of the temporal semi-discretisation by several standard methods on uniform and non-uniform time grids.

The evolution equation under consideration is assumed to be governed by a time-depending operator that is coercive, monotone, and fulfills a certain growth and continuity condition. Strongly continuous perturbations are also studied.

By employing algebraic relations, which reflect the stability of the numerical method, and based upon the theory of monotone operators, the convergence of piecewise polynomial prolongations of the time discrete solutions towards a weak solution is shown. The analysis does not require any additional regularity of the exact solution. The results apply to several fluid flow problems such as incompressible non-Newtonian shear-thickening fluid flow.

Integration Methods Using Vector Norms for Computing Lyapunov Exponents

Philip J Aston[1], with Michael Dellnitz[2]
[1] University of Surrey
[2] University of Paderborn

ABSTRACT

Lyapunov exponents are usually computed using time averaging over a long orbit. However, there are a number of problems with this approach. An alternative approach that we consider is to use integration with respect to the invariant measure which overcomes all the pitfalls of the time averaging approach.

We previously considered a sequence of integrals involving a matrix norm which converge to the dominant Lyapunov exponent. We now extend this work by considering a sequence of integrals involving a vector norm, where the Jacobian matrix is multiplied by a fixed vector that we can choose. We prove convergence results for this sequence of integrals and show that particular choices of the fixed vector will give particularly good results. This approach is illustrated with some examples.

Numerical computation of Lyapunov exponents for delay differential equations

Dimitri Breda[1]

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ABSTRACT

The study of the asymptotic behavior of nonautonomous linear systems arising from linearization around chaotic orbits offers good prospects for understanding complex nonlinear dynamics. Knowledge of the Lyapunov exponents (and other stability spectra) plays a central role in this context and several computational techniques have been established to address the problem in finite dimension, i.e. for Ordinary Differential Equations (ODEs), basically originating from the successive re-orthonormalization of an initial small sphere of realizations in the phase space. In this talk we briefly recall the ideas behind QR-based methods for approximating the Lyapunov spectrum of ODEs and then present how they can be used in the infinite-dimensional case represented by Delay Differential Equations (DDEs). The aim of the work is to develop a first systematic study (i.e. analyzing theoretical foundations, implementation and convergence) of a numerical scheme for DDEs not being a mere adaptation of ODEs methods. This is a joint work in progress with Luca Dieci from Georgia Institute of Technology (Atlanta, GA - USA) and Erik Van Vleck from Department of Mathematics, Kansas University (Lawrence, KS - USA).

Computing the symbolic dynamics of heteroclinic orbits of the Lorenz system

Bernd Krauskopf[1] with Hinke Osinga[1] and Eusebius Doedel[2]
[1] University of Bristol
[2] Concordia University

ABSTRACT

The Lorenz manifold is the 2D stable manifold of the origin of the famous Lorenz system. We consider here its intersections with the 2D unstable manifolds of the secondary equilibria or periodic orbits of saddle type (also known as the template of the Lorenz system). We compute both these manifolds and consider their intersection curves, which are structurally stable heteroclinic connections from the origin to the secondary equilibria. We numerically find 512 of these heteroclinic orbits and continue them in the Reynolds number parameter of the Lorenz system. This allows us to show how the symbolic dynamics of these heteroclinic orbits is associated with the symbolic dynamics of codimension-one homoclinic orbits of the origin, at which they originate and terminate.

Approximate trajectories for set-valued mappings and differential inclusions

Sergei Yu. Pilyugin[1], with Janosch Rieger[2]
[1] St. Petersburg State University
[2] Bielefeld University

ABSTRACT

We study the problem of shadowing and inverse shadowing for dynamical systems generated by set-valued mappings. The problem is solved for contractive mappings. We introduce new hyperbolicity conditions for several classes of set-valued mappings (including, for example, polytope-valued ones) and show that these conditions imply the Lipschitz shadowing and inverse shadowing. The same problem is considered for T-flows of differential inclusions.

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Period doubling bifurcation in discrete phase-locked loop

Kudryashova E.V., Kuznetsov N.V.[1]

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Faculty of Mathematics and Mechanics
Saint-Petersburg State University
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ABSTRACT

Mathematical model of discrete phase-locked loop (DPLL) with sinusoidal characteristic of phase discriminator is considered. The Feigenbaum effect for nonunimodal maps which describe such DPLL is investigated by theoretical approach and numerical calculations. Bifurcation parameters of period doubling bifurcation are calculated.

Computing the spectrum and representing the resolvent

Olavi Nevanlinna[1]

[1] TKK Helsinki

ABSTRACT

We discuss computing the spectrum of a bounded operator and representing its resolvent operator. The results include a general convergence theorem for the polynomial convex hull of the spectrum and explicit representations for the resolvent outside. The results are formulated and proved in general Banach algebras.

Sliding Modes in Filippov Systems

Luca Dieci[1], with Luciano Lopez[2]
[1] School of Mathematics, Georgia Tech
[2] Univ. of Bari

ABSTRACT

In this talk we consider discontinuous differential systems in the sense of Filippov. Our emphasis is on so-called sliding modes. We review existing theory and propose some new ideas both on regularization techniques and on sliding modes integration on several surfaces. If time remains, we will also discuss linearized stability analysis in this context. Illustrative numerical examples will also be given.

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ISBN 978-951-22-9868-6 (print)
ISBN 978-951-22-9869-3 (PDF)
ISSN 0784-6460 (print)
ISSN 1797-5875 (PDF)