FACULTÉ DES SCIENCES
SECTION DE MATHÉMATIQUES

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES
Section de mathématiques

Conference on Scientific Computing

Geneva
June 17 – 20, 2009

Celebrating Ernst Hairer's 60th birthday

Keynote speakers:

Assyr Abdulle
Michel Crouzeix
Martin Hairer
Marlis Hochbruck
Laurent Jay
Gustaf Söderlind
Uri Ascher
Nicola Guglielmi
Des Higham
Arieh Iserles
Chus Sanz-Serna
Antonella Zanna

http://www.unige.ch/math/hairer60/

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This conference is organized by
M. Gander, C. Lubich and G. Wanner

Conference on Scientific Computation

Geneva, Switzerland
June 17 – 20, 2009

Sponsored by:

Department of Mathematics
Faculty of Science
University of Geneva
L'Enseignement Mathématique
Stiftung der mathematischen Wissenschaften
Swiss Mathematical Society
Swiss National Science Foundation SNF
Swiss Academy of Sciences SAS

Organized by:

Martin Gander (Genève)
Christian Lubich (Tuebingen)
Gerhard Wanner (Genève)

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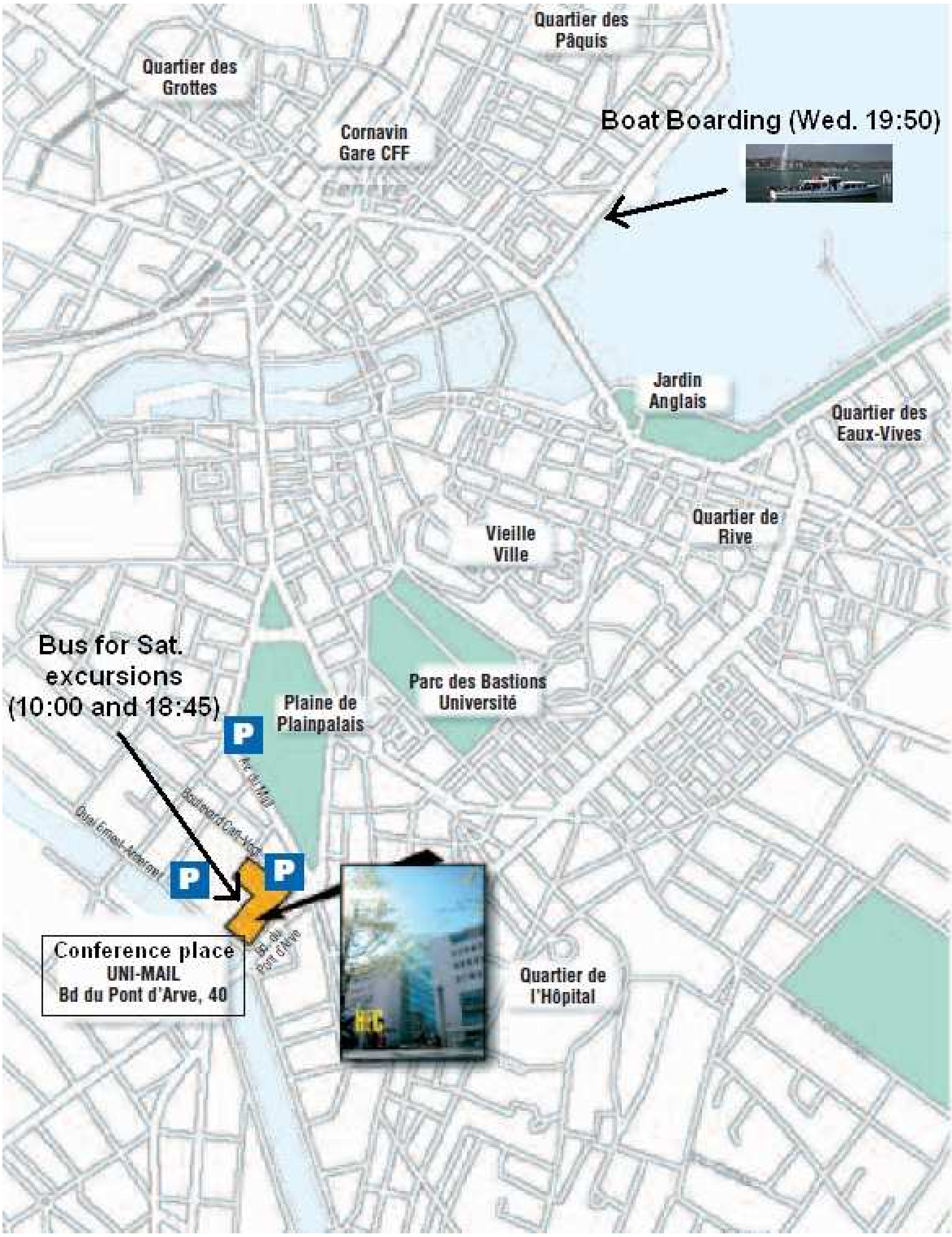
Ernst Hairer

born: June 19th, 1949 in Nauders, Austria



Quartier des Pâquis
Quartier des Grottes
Cornavin Gare CFF
Boat Boarding (Wed. 19:50)
Jardin Anglais
Quartier des Eaux-Vives
Quartier de Rive
Vieille Ville
Bus for Sat. excursions (10:00 and 18:45)
Plaine de Plainpalais
Parc des Bastions Université
P
P
P
Conference place
UNI-MAIL
Bd du Pont d'Arve, 40
Quartier de l'Hôpital

Timetable

Wednesday June 17th, 2009, morning

The conference takes place at UniMail in
lecture hall **S160** (plenary talks) and lecture halls **S160/R160/R170** (parallel sessions).
UniMail address: boulevard du Pont-d'Arve 40, 1205 Genève, Switzerland.

In front of **Room S160** 08:30 – 09:20	**Registration** (coffee, tea, juices, croissants, etc.)

Room S160 09:20 – 09:30	**Welcome** G. Wanner

Room S160	
Chair:	G. Wanner
09:30 – 10:15	**C. Sanz-Serna** (p. 36), B-series and multiscale methods

10:15 – 10:30	**Morning break (coffee, tea, juice)**

10:30 – 12:00	**Contributed talks (CT1)**
Room S160	
Chair:	G. Wanner
10:30 – 11:00	**J. Butcher** (p. 18), Order stars and order arrows
11:00 – 11:30	**P. Kaps** (p. 29), A DAE for skiing turns
11:30 – 12:00	**P. Rentrop** (p. 34), Wiener Calculus for Differential Equations with Uncertainties
12:00 – 12:30	**T. Jahnke** (p. 27), On hybrid stochastic-deterministic models for biochemical reaction kinetics

Timetable

Wednesday June 17th, 2009, afternoon

Room S160	
Chair:	C. Lubich
14:00 – 14:45	**A. Iserles** (p. 27), Asymptotic numerics of highly oscillatory equations

14:45 – 15:30	**Poster session**
In front of **Room S160**	**A. Eremin** (p. 22), Economic Dormand-Prince type embedded fifth order method for systems of special structure
	S. Guettel (p. 23), On the convergence of rational Ritz values
	D. Kumar (p. 30), Numerical treatment of singularly perturbed delay differential equations using B-Spline collocation method on Shishkin mesh
	I. Olemskoy (p. 33), Structural Approach to the Design of Explicit One-Stage Methods

15:30 – 17:30	**Concurrent sessions**
Room S160	Minisymposium (MS3): Geometric Integration of PDEs
Organizer:	D. Cohen
15:30 – 16:00	**J. Schweitzer** (p. 36), Numerical Simulation of Relativistic Laser-Plasma Interaction
16:00 – 16:30	**G. Dujardin** (p. 21), Long-time asymptotics of linear initial-boundary value problems with time-periodic boundary data
16:30 – 17:00	**C. Neuhauser** (p. 33), High-order time-splitting methods for Schrödinger equations
17:00 – 17:30	**L. Gauckler** (p. 22), Convergence of a split-step Hermite method for the Gross-Pitaevskii equation
Room R160	Minisymposium (MS7): Splitting Methods for Stiff and Nonstiff Problems
Organizers:	S. Descombes & M. Massot
15:30 – 16:00	**M. Duarte** (p. 20), New algorithms for multi-scale reaction waves simulation
16:00 – 16:30	**G. Vilmart** (p. 40), Splitting methods with complex times for parabolic equations
16:30 – 17:00	**C. Lubich** (p. 31), Splitting methods for nonlinear Schrödinger equations
17:00 – 17:30	**M. Thalhammer** (p. 39), Local error expansions for high-order exponential operator splitting methods
Room R170	Contributed talks (CT2)
Chair:	A. Iserles
15:30 – 16:00	**M. Demiralp** (p. 20), Random Sampling Fluctuation Free Multivariate Integration
16:00 – 16:30	**A. Rößler** (p. 35), Efficient Runge-Kutta methods for stochastic differential equations
16:30 – 17:00	**N. Yastrebova** (p. 42), Research of applicability of different fuzzy inference scheme's into the hierarchical fuzzy inference systems
17:00 – 17:30	**R. Jeltsch** (p. 28), High-order semi-Lagrangian numerical method for the Large-Eddy simulation of reactive flows

19:50	**Boat trip** on the lake of Geneva with "Star of Geneva" Boarding place: **quai 7** (opposite Hotel Beau-Rivage, 13 quai du Mont-Blanc) Return : about 22:00 NOTE: **Please bring your name tag** with you for verifications

Timetable

Thursday June 18th, 2009, morning

The conference takes place at UniMail in
lecture hall **S160** (plenary talks) and lecture halls **S160/R160/R170** (parallel sessions).
UniMail address: boulevard du Pont-d'Arve 40, 1205 Genève, Switzerland.

Room S160	
Chair:	G. Wanner
08:30 – 09:15	**D. Higham** (p. 25), The Opposite of Numerical Analysis
09:15 – 10:00	**M. Hochbruck** (p. 26), On the numerical solution of highly oscillatory problems arising in laser plasma interactions

10:00 – 10:30	**Morning break (coffee, tea, juice)**

10:30 – 12:30	**Concurrent sessions**
Room S160	Minisymposium (MS4): Hopf algebras in numerical analysis of ODEs
Organizers:	P. Chartier & A. Murua
10:30 – 11:00	**E. Celledoni** (p. 19), On B-series and their structure-preserving properties
11:00 – 11:30	**D. Manchon** (p. 31), Two Hopf algebras of trees interacting
11:30 – 12:00	**A. Murua** (p. 33), B-series and related expansions for highly oscillatory systems
Room R160	Contributed talks (CT3)
Chair:	M. Hochbruck
10:30 – 11:00	**M. Botchev** (p. 18), On unconditionally stable time integration schemes for Maxwell's equations
11:00 – 11:30	**M. Hönig** (p. 27), Regularization of nonlinear inverse problems by certain time integration schemes
11:30 – 12:00	**S. Karaa** (p. 29), The theta method revised
Room R170	Contributed talks (CT4)
Chair:	C. Sanz-Serna
10:30 – 11:00	**T. Udrescu** (p. 39), Adaptive wavelet-based approximation of the Chemical Master Equation
11:00 – 11:30	**K. Santugini** (p. 35), Rheologic modelization of a mixed nanotube/polymer fluid
11:30 – 12:00	**Y. Semerich** (p. 36), Numerical modeling of wave propagation in holey fibers by the R-functions method
12:00 – 12:30	**A. Yadaw** (p. 41), Comparative study of FDM, FEM and B-spline collocation method for singularly perturbed BVPs

Timetable

Thursday June 18th, 2009, afternoon

The conference takes place at UniMail in
lecture hall **S160** (plenary talks) and lecture halls **S160/R160/R170** (parallel sessions).
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Room S160	
Chair:	C. Lubich
14:00 – 14:45	**A. Abdulle** (p. 17), A posteriori error analysis of the finite element heterogeneous multiscale method
14:45 – 15:30	**G. Söderlind** (p. 38), Grid control in BVP solvers

15:30 – 16:00	**Afternoon break (coffee, tea, juice)**

16:00 – 17:30	**Concurrent sessions**
Room S160	Minisymposium (MS1): Control of ordinary differential equations
Organizers:	M. Chyba & J. Gergaud
16:00 – 16:30	**O. Junge** (p. 29), Discrete mechanics and optimal control
16:30 – 17:00	**E. Kostina** (p. 30), Direct multiple shooting methods for parameter estimation in dynamic processes
17:00 – 17:30	**P. Martinon** (p. 32), An improved switching detection for an optimal control problem with control discontinuities
Room R160	Contributed talks (CT5)
Chair:	A. Abdulle
16:00 – 16:30	**M. Hanke** (p. 25), Computational modelling of metabolism in mammalian cells
16:30 – 17:00	**I. Sgura** (p. 37), Numerical solution of singular ODE-BVPs arising in biomechanics
17:00 – 17:30	**O. Verdier** (p. 40), Normal forms for DAEs

Timetable

Friday June 19th, 2009, morning

The conference takes place at UniMail in
lecture hall **S160** (plenary talks) and lecture halls **S160/R160/R170** (parallel sessions).
UniMail address: boulevard du Pont-d'Arve 40, 1205 Genève, Switzerland.

Room S160	
Chair:	G. Wanner
08:30 – 09:15	**U. Ascher** (p. 18), Fast gradient descent and artificial time integration
09:15 – 10:00	**A. Zanna** (p. 42), Generalized polar coordinates on Lie groups

10:00 – 10:10	Group picture in UniMail main hall.

10:10 – 10:30	**Morning break (coffee, tea, juice)**

10:30 – 12:30	**Concurrent sessions**
Room S160	Minisymposium (MS5): IMEX (IMplicit-EXplicit) Runge-Kutta schemes
Organizer:	S. Boscarino
10:30 – 11:00	**I. Higueras** (p. 25), On stability issues for IMEX schemes applied to hyperbolic equations with stiff reaction term
11:00 – 11:30	**J. Verwer** (p. 40), Convergence and component splitting for Crank-Nicolson–leap-frog
Room R160	Minisymposium (MS8): Parallel methods for solving ODEs.
Organizer:	Damien Tromeur-Dervout
10:30 – 11:00	**D. Guibert** (p. 24), Parallel iterative time domain decompositions based on deferred correction methods for solving ODE systems
11:00 – 11:30	**M. Minion** (p. 32), A hybrid parareal-spectral deferred correction method
11:30 – 12:00	**P. Linel** (p. 30), Domain decomposition in time using symmetric integrators for solving ODEs
12:00 – 12:30	**T. Pham** (p. 34), Proper orthogonal decomposition for solving in parallel large system of stiff ODEs
Room R170	Contributed talks (CT6)
Chair:	U. Ascher
10:30 – 11:00	**R. Quispel** (p. 34), Geometric integration of differential equations
11:00 – 11:30	**V. Acary / B. Brogliato** (p. 17), Implicit Euler numerical simulation of sliding mode systems

Timetable

Friday June 19th, 2009, afternoon

The conference takes place at UniMail in
lecture hall **S160** (plenary talks) and lecture halls **S160/R160/R170** (parallel sessions).
UniMail address: boulevard du Pont-d'Arve 40, 1205 Genève, Switzerland.

Room S160	
Chair:	C. Lubich
14:00 – 14:45	**L. Jay** (p. 28), Lagrange-d'Alembert integrators for constrained systems in mechanics
14:45 – 15:30	**N. Guglielmi** (p. 23), On singular perturbations of neutral delay differential equations

15:30 – 16:00	**Afternoon break (coffee, tea, juice)**

16:00 – 18:00	**Concurrent sessions**
Room S160	Minisymposium (MS2): Discontinuous differential equations
Organizers:	A. Bellen & L. Lopez
16:00 – 16:30	**L. Dieci** (p. 20), Sliding modes in Filippov systems
16:30 – 17:00	**E. Usai** (p. 39), Real-time differentiation and system inversion via sliding modes
17:00 – 17:30	**N. Guglielmi** (p. 24), A regularization for discontinuous differential equations
17:30 – 18:00	**A. Caboussat** (p. 19), Coupling differential equations and constrained optimization: application to atmospheric chemistry
Room R160	Minisymposium (MS6): Innovative time integrators for fluid flow problems
Organizers:	O. Knoth & J. Wensch
16:00 – 16:30	**W. Hundsdorfer** (p. 26), Multirate and partitioned Runge-Kutta schemes for conservation laws
16:30 – 17:00	**M. Minion** (p. 32), Auxiliary variables and deferred corrections for divergence constrained flows
17:00 – 17:30	**A. St-Cyr** (p. 38), A linearly implicit time-integrator for a h-p adaptive geophysical fluid flow solver
17:30 – 18:00	**J. Wensch** (p. 41), Multirate time integration for conservation laws
Room R170	Contributed talks (CT7)
Chair:	A. Zanna
16:00 – 16:30	**A. El Boukili** (p. 21), Etching algorithms for process simulation of 3D MEMS-tunable devices
17:30 – 17:00	**S. Abbas** (p. 17), Almost periodic solutions of neutral functional differential equations
17:00 – 17:30	**Y. Skiba** (p. 37), Linear instability of ideal flows on a sphere
17:30 – 18:00	**J.-M. Ginoux** (p. 23), Differential geometry applied to dynamical systems

Timetable

Saturday June 20th, 2009

The conference takes place at UniMail in
lecture hall **S160** (plenary talks) and lecture halls **S160/R160/R170** (parallel sessions).
UniMail address: boulevard du Pont-d'Arve 40, 1205 Genève, Switzerland.

Room S160	
Chair:	G. Wanner
08:30 – 09:15	**M. Hairer** (p. 24), How hot can a heat bath get?
09:15 – 10:00	**M. Crouzeix** (p. 19), Some estimates in a non self-adjoint context

10:00	**Picnic on Salève + CERN Excursion by bus** Meeting place: North-West side (garden) of the University building (UNI-MAIL) Return: about 18:30, the bus brings you directly to the place of the birthday party **IMPORTANT NOTE** for Salève and CERN visit: You must bring your valid passport (or identity card), and bring some food for the picnic. Do not wear high heels or sandals, otherwise you will be refused entry into Cern. **Please bring your name tag** with you for verifications.

≈ 18:30	**Birthday party in the Geneva wine country** "Chez Dupraz" at Soral Village (10 km SW of city center) Caves des Chevalières, Claude Dupraz, viticulteur-oenologue chemin de Placet 8, 1286 Soral, tel. +41 22 756 15 66.
≈ 18:45	**Meeting place** for participants not joining the CERN visit: North-West side (garden) of the University building (UNI-MAIL) NOTE: **Please bring your tame tag** with you for verifications.

Abstracts

Almost periodic solutions of neutral functional differential equations.

Syed Abbas
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(contributed talk CT7)

In this talk we consider a non-autonomous neutral functional differential equation in a Banach space. Using the theory of semigroups of operators to evolution equations and Krasnoselskii's fixed point theorem we establish the existence and uniqueness of a mild almost periodic solution of the problem under consideration.

A posteriori error analysis of the finite element heterogeneous multiscale method

Assyr Abdulle
EPFL Swiss Federal Institute of Technology
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(invited talk)

In this talk we discuss a numerical method, the so-called finite element heterogeneous multiscale method (FE-HMM), for the simulation of partial differential equations with multiple scales.

In this method, the effective problem is directly discretized in a macroscopic finite element space. The fine-scales of the problem are accounted for in the macro-stiffness matrix by solving (on the fly) micro-problems in a scale-independent fixed-size domain within each macro-element.

After reviewing some a priori error estimates, we will present recent results on a posteriori error analysis of the FE-HMM obtained for multiscale elliptic problems.

Implicit Euler numerical simulation of sliding mode systems

Vincent Acary
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(contributed talk CT6)

(joint work with B. Brogliato)

In this paper it is shown that the implicit Euler time-discretization of some classes of switching systems with sliding modes, yields a very good stabilization of the trajectory and of its derivative on the sliding surface. Therefore the spurious oscillations which are pointed out elsewhere when an explicit method is used, are avoided. Moreover the method (an *event-capturing*, or *time-stepping* algorithm) allows for accumulation of events (Zeno phenomena) and for multiple switching surfaces (i.e., a sliding surface of codimension ≥ 2). The details of the implementation are given, and numerical examples illustrate the developments. This method may be an alternative method for chattering suppression, keeping the intrinsic discontinuous nature of the dynamics on the sliding surfaces. Links with discrete-time sliding mode controllers are studied.

Fast gradient descent and artificial time integration

Uri Ascher
University of British Columbia
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(invited talk)

The integration to steady state of many initial value ODEs and PDEs using the forward Euler method can alternatively be considered as gradient descent for an associated minimization problem. Greedy algorithms such as steepest descent for determining the step size are as slow to reach steady state as is forward Euler integration with the best uniform step size. But other, much faster methods using bolder step size selection exist. Various alternatives are investigated from both theoretical and practical points of view.

The steepest descent method is also known for the regularizing or smoothing effect that the first few steps have for certain inverse problems, amounting to a finite time regularization. We further investigate the retention of this property using the faster gradient descent variants in the context of two or three applications: denoising and deblurring of images, and shape optimization involving data inversion of elliptic PDEs. When the combination of regularization and accuracy demands more than a dozen or so steepest descent steps, the alternatives offer an advantage, even though (indeed because) the absolute stability limit of forward Euler is carefully yet severely violated.

On unconditionally stable time integration schemes for Maxwell's equations

Mike Botchev
University of Twente
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(contributed talk CT3)

(Based on joint work with Jan Verwer, CWI, the Netherlands.) We report on our recent research on time integration of Maxwell's equations discretized in space with Nedelec vector finite elements. Often, second-order time integration schemes are used, treating the curl terms explicitly and obeying the CFL stability restriction. However, unconditionally stable time integration may be attractive, for instance, when a strict CFL restriction is caused by local grid refinement. In this work we explore two possibilities for unconditionally stable time integration: the implicit trapezoidal rule implemented with preconditioned conjugate gradient solver and a second-order exponential scheme implemented with Krylov subspace techniques.

Order stars and order arrows

John Butcher
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(contributed talk CT1)

Order stars, introduced to the numerical analysis community thirty years ago, have had a profound and far-reaching effect on the way many stability and approximation questions are analysed and studied. In particular, many stability barriers can be proved easily as consequences of the order star approach. Order arrows represent a different way of looking at many of the same questions and they sometimes add a slightly different insight. Some aspects of these two theories will be discussed, with illustrations from stability barriers on both one-step and multistep families of methods.

Coupling differential equations and constrained optimization: application to atmospheric chemistry

Alexandre Caboussat
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(minisymposium MS2)

Ordinary differential equations are coupled with constrained optimization problems when modeling the thermodynamic equilibrium of a system evolving with time. Discontinuity points are created by the activation or deactivation of inequality constraints.

We develop a numerical framework based on an implicit Runge-Kutta method (RADAU5) for the solution of optimization-constrained differential equations, with application in particular to the modeling of atmospheric aerosol particles. We introduce numerical techniques for the detection of the events (activation and deactivation of constraints) based on dense output formulas, and continuation techniques.

We present numerical results for the simulation of the time-dependent equilibrium of organic atmospheric aerosol particles. Finally, we discuss the extension to populations of particles of different sizes.

This is joint work with C. Landry (EPFL) and E. Hairer.

On B-series and their structure-preserving properties.

Elena Celledoni
NTNU
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(minisymposium MS4)

B-series are a powerful tool in the analysis of Runge-Kutta numerical integrators and some of their generalizations ("B-series methods"). Recently there has been a lot of activity for characterizing B-series methods in terms of their ability of preserving invariants. The ultimate goal is to understand what is possible to achieve with B-series methods in terms of structure preservation, and also to design practical numerical methods with the desired properties. In particular we have been focusing on the study of the linear subspaces of energy- preserving and symplectic modified vector fields which admit a B-series, their finite dimensional truncations, and their dual spaces. The manifold of B-series conjugate to symplectic and conjugate to energy-preserving have been characterized. Joint work with R. McLachlan, R. Quispel and B. Owren.

Some estimates in a non self-adjoint context

Michel Crouzeix
Université de Rennes 1
michel.crouzeix@univ-rennes1.fr
(invited talk)

Spectral theory is a very efficient tool for estimating functions of a self-adjoint operator, but the situation is much more difficult if we consider non normal operators. We present some remarks which have been of use to us and illustrate them by some applications in numerical analysis.

Random Sampling Fluctuation Free Multivariate Integration

Metin Demiralp
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(contributed talk CT2)

This talk focuses on the integration of multivariate functions. To this end, we construct a formula which is a finite linear combination of the function values at certain points of the space of independent variables. The linear combination coefficients are determined by using the multivariate fluctuation free matrix representation. This representation approximates the matrix representation of the target multivariate function by the image of the independent variable matrix representations under that multivariate function. This approximation is based on a recently conjectured and proven theorem. The easiest form of the approximation is based on the Hilbert subspaces spanned by basis functions which can be expressed in terms of matrix direct products. This simplest case can be used for the construction of more general representations over certain desired Hilbert subspaces. Some illustrative examples will also be presented.

Sliding modes in Filippov systems

Luca Dieci
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(minisymposium MS2)

We consider discontinuous differential systems in the sense of Filippov. Our emphasis is on so-called sliding modes, and we propose some new ideas on sliding solutions on the intersection of several surfaces.

New algorithms for multi-scale reaction waves simulation

Max Duarte
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(minisymposium MS7)

Various domains such as combustion, environment modelization or even population dynamics generally use reaction-diffusion models with a large spectrum of time-scales. A complete numerical resolution of such problems by classical methods is often very expensive in computational time and resources. In this sense, operator splitting methods are preferred and are widely studied; nevertheless, recent introduction of time parallelization with parareal algorithms seems also to become a very promising and performing tool. The present work is devoted to the study of the combination of parareal algorithms and splitting methods applied to the simulation of multi-scale evolution problems, namely non-linear chemical waves. By taking into account theoretical aspects associated with the mathematical models and the numerical methods, we describe the influence of the multi-scale feature on the computational performances. This is joint work with M. Massot, S. Descombes, T. Dumont, V. Louvet and F. Laurent.

Long-time asymptotics of linear initial-boundary value problems with time-periodic boundary data

Guillaume Dujardin
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(minisymposium MS3)

This talk deals with the long-time behaviour of the exact solutions of linear evolution partial differential equations on the half line and on bounded intervals when the boundary data is time-periodic. Using a new integral representation method for the solutions of these problems introduced by A.S. Fokas, we present different kinds of asymptotic behaviours that occur and discuss the existence of asymptotic periodic profiles for the solutions of such linear PDEs. We illustrate our results with several numerical experiments in the case of the following linear Schrödinger equations :

$$\begin{cases} i\partial_t\varphi(t,x) + \partial_x^2\varphi(t,x) = 0 & (t,x) \in \mathbb{R}\times(0,+\infty) \\ \varphi(0,x) = \varphi_0(x) & x \in (0,+\infty) \\ \varphi(t,0) = f_0(t) & t \in \mathbb{R}, \end{cases}$$

and

$$\begin{cases} i\partial_t\varphi(t,x) + \partial_x^2\varphi(t,x) = 0 & (t,x) \in \mathbb{R}\times(0,L) \\ \varphi(0,x) = \varphi_0(x) & x \in (0,L) \\ \varphi(t,0) = f_0(t) & t \in \mathbb{R} \\ \varphi(t,L) = g_0(t) & t \in \mathbb{R}, \end{cases}$$

where f_0 and g_0 are smooth periodic functions of time.

Etching algorithms for process simulation of 3D MEMS-tunable devices

Abderrazzak El Boukili
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(contributed talk CT7)

Our focus is on domain decomposition methods together with developing advanced geometrical etching algorithms for etching simulation of complex 3d MEMS-tunable vertical cavity semiconductor optical amplifiers (VCSOAs). These algorithms are found to be simple, robust, and significantly reduce the overall run time of 3d MEMS-tunable device process simulations.

Long-wavelength VCSOAs devices are very attractive as they benefit from high coupling efficiency to optical fibers, and polarization independent gain. Creating a suitable and optimized geometry and mesh for mechanical and electrical simulations of MEMS-tunable VCSOAs is essential and in high demand from laser industries.

This presentation will describe in detail our contribution to improving and enhancing etching algorithms and using domain decomposition methods.

Economic Dormand-Prince type embedded fifth order method for systems of special structure

Alexey Eremin
Saint-Petersburg State University
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(poster)

Within the structural approach suggested by I. Olemskoy the embedded Dormand-Prince type method is suggested. The fifth order calculating scheme is constructed. A comparison to classical Dormand-Prince method is held, and shows the advantage in less right hand side evaluations for the new method.

The Euler method for nonlinear systems with discontinuous OSL right-hand sides - what is the sharp order?

Elza Farkhi
Tel-Aviv University
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(**cancelled talk**)

The classical error estimate of the Euler method for ODEs with Lipschitz continuous right-hand sides is O(h). If the nonlinear vector right-hand side is only one-sided Lipschitz (OSL), we can prove a square root of h error order (eventually extending the differential equation to a differential inclusion to ensure the existence of solutions). Is one half the sharp order of approximation in the OSL case? For a single differential equation the sharp estimate is O(h). What is the sharp order in general OSL systems with discontinuous right-hand sides?

Convergence of a split-step Hermite method for the Gross-Pitaevskii equation

Ludwig Gauckler
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(minisymposium MS3)

The Gross-Pitaevskii equation is a nonlinear Schrödinger equation used to describe Bose-Einstein condensates. In this talk, we discuss a discretization of the Gross-Pitaevskii equation by Strang splitting in time and Hermite collocation in space. We prove a second order error bound in L^2 for the semi-discretization error of the Strang splitting in time under suitable regularity assumptions on the exact solution. For the semi-discretization in space we show high order convergence, depending on the regularity of the exact solution. The analyses of the semi-discretizations in time and space are finally combined into an error analysis of the fully discrete method.

Differential geometry applied to dynamical systems

Jean-Marc Ginoux
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(contributed talk CT7)

This talk aims to present a new approach to Dynamical Systems Theory recently developed in a book published by World Scientific.

This book aims to present a new approach called Flow Curvature Method that applies Differential Geometry to Dynamical Systems. Hence, for a trajectory curve, an integral of any n-dimensional dynamical system as a curve in Euclidean n-space, the curvature of the trajectory - or the flow - may be analytically computed. Then, the location of the points where the curvature of the flow vanishes defines a manifold called flow curvature manifold. Such a manifold being defined from the time derivatives of the velocity vector field, contains information about the dynamics of the system, hence identifying the main features of the system such as fixed points and their stability, local bifurcations of codimension one, center manifold equation, normal forms, linear invariant manifolds (straight lines, planes, hyperplanes).

In the case of singularly perturbed systems or slow-fast dynamical systems, the flow curvature manifold directly provides the slow invariant manifold analytical equation associated with such systems. Also, starting from the flow curvature manifold, it will be demonstrated how to find again the corresponding dynamical system, thus solving the inverse problem.

On the convergence of rational Ritz values

Stefan Guettel
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(poster)

A constrained extremal problem from logarithmic potential theory is used to describe the convergence of rational Ritz values to the eigenvalues of a matrix. The resulting theory is useful to understand the superlinear convergence of rational Krylov approximations to matrix functions as, e.g., the matrix exponential function.

This poster summarizes joint work with Bernhard Beckermann, Michael Eiermann, Oliver Ernst and Raf Vandebril.

On singular perturbations of neutral delay differential equations

Nicola Guglielmi
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(invited talk)

In the context of the regularization of delay differential equations with state dependent delays it is natural to introduce singular perturbations.

In the talk I will consider two classes of singularly perturbed delay differential equations and discuss the properties of their solutions. In particular I shall analyze the convergence of the solutions when the parameter associated to the singular perturbation vanishes. In this way one can hope to define a weak solution of the problem and also to determine a modified system of differential equations for such weak solution.

Finally I shall discuss the numerical integration explaining some peculiar aspects concerned with both approaches.

This is joint work with Giorgio Fusco and Ernst Hairer.

A regularization for discontinuous differential equations.

Nicola Guglielmi
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(minisymposium MS2)

I will introduce a regularization for discontinuous differential equations based on an average in time of the vectorfield.

I will first discuss local existence of the solution of the regularized problem and then examine the behaviour of the solution as the regularization parameter tends to zero.

Some examples will illustrate the main features of the regularization considered.

Parallel iterative time domain decompositions based on deferred correction methods for solving ODE systems.

David Guibert
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(minisymposium MS8)

The development of large computational resources leads to search for parallel implementations not only based on space decompositions. In this talk we will propose to combine time domain decomposition and the simple deferred correction. The deferred correction [1] builds a perturbated problem which the exact solution is known. The defect difference between the perturbated solution and the solution of the original problem is computed by a process increasing the time accuracy at each iteration.

The iterative correction is computed sequentially at each time steps. To introduce parallelism, we gather the time steps into subdomains distributed among processors. A parallel pipe is then defined as: a processor computes its correction, sends it to the next subdomain and starts its next iteration. Hence a cyclic distribution of the time subdomains is introduced to reduced the startup of the first step of the iterated correction process. Numerical results and parallel efficiency will be presented.

[1] High-order multi-implicit spectral deferred correction methods for problems of reactive flow. A. Bourlioux, A. T. Layton, and M. L. Minion, J. Comput. Phys., 189(2):651 – 675, 2003.

How hot can a heat bath get?

Martin Hairer
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(invited talk)

We consider one of the simplest possible models of non-equilibrium statistical mechanics: two coupled oscillators in contact with two Langevin heat baths. The twist is that one of the heat baths is at "infinite" temperature in the sense that no friction acts on the corresponding degree of freedom. We explore the question of the existence of a stationary state in this situation and its properties if it exists. In particular, we will see that the question "Is the corresponding degree of freedom at infinite temperature?" can have a surprising variety of answers.

Computational modelling of metabolism in mammalian cells

Michael Hanke
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(contributed talk CT5)

A human cell consists schematically of an outer membrane, a cytoplasm containing a large number of organelles, a nuclear membrane, and finally the cellular nucleus. The organelle membranes create a complex and dense system of membranes throughout the cytoplasm. The mathematical description leads to a system of reaction-diffusion equations in a complex geometrical domain. If these structures are treated as separate subdomains, any model becomes computationally very expensive. In this talk, we will report on a homogenization approach to arrive at a manageable system of partial differential equations.

The Opposite of Numerical Analysis

Des Higham
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(invited talk)

Numerical analysts typically take a continuous object, such as a differential equation, and approximate it by a discrete object, such as a finite difference or finite element scheme. Many useful tools have been developed over the years to quantify how well the continuous can be approximated by the discrete. In this talk I will look at the opposite issue: here we have an underlying model that is inherently discrete, but in order to summarize its behaviour analytically or to make computer simulations feasible, we wish to approximate the model with a differential or integral equation. I will focus on two examples. First, I will look at random walks over small-world networks. Here the matrix equation that describes the expected number of steps on an excursion between randomly chosen nodes can be identified with a finite difference formula. The related integral equation may then be viewed as a 'mean field' approximation that allows the small-world cut-off to be characterized in the limit of large network size. Second, I will look at some very simple chemical reactions modeled in the discrete-space Markov jump framework. Here, the mean time for a species to exit prescribed upper and lower bounds can be viewed as a finite difference scheme for a two-point boundary ODE. The traditional convergence limit in numerical analysis then corresponds to the thermodynamic limit in physical chemistry. In both examples, standard numerical analysis tools for comparing discrete and continuous models must be adapted because (a) the underlying continuous problem is parameterized by the grid size and has a growing Lipschitz constant, and (b) convergence is typically relative rather than absolute.

On stability issues for IMEX schemes applied to hyperbolic equations with stiff reaction term

Inmaculada Higueras
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(minisymposium MS5)

Given the PDE

$$u_t + u_x = -\mu u(u-1)(u-\frac{1}{2}) \qquad 0 < x < 1 \qquad t > 0,$$

two main problems may arise when it is solved numerically: the presence of oscillations and a numerical delay in the shock profile.

In order to control numerical oscillations, explicit schemes require small stepsizes whereas, due to the convective derivative, implicit discretizations are not appropriate in general, and it might even be inviable in some cases. A way to overcome these difficulties is the use of IMplicit-Explicit schemes.

In this talk we show how to obtain numerical solutions free of oscillations using IMEX Runge-Kutta schemes. To obtain these results, we use the concept of region of absolute monotonicity for IMEX Runge-Kutta methods, developed in the context of Strong Stability Preserving (SSP) methods.

This is a joint work with R. Donat (Universidad de Valencia) and A. Martínez-Gavara (Universidad de Sevilla).

On the numerical solution of highly oscillatory problems arising in laser plasma interactions

Marlis Hochbruck
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(invited talk)

In this talk we discuss some recent developments for the numerical simulation of laser interactions with overdense plasmas at relativistic intensities. Our aim - together with our Theoretical Physics group - is to develop a full 3D hybrid code, where the beam of hot electrons is simulated using a standard particle in cell technique, while the cold background plasma is hydrodynamically simulated. Since the highest frequency arising in the problem results from the electron density, the new method should use time steps which are independent of the density.

In this presentation, we will focus on a subproblem of simulating reflections of a laser beam at the plasma barrier. We will present a mollified impulse method which can be used to overcome the limitation on the time steps. A few preliminary experiments with this method will be presented.

Multirate and partitioned Runge-Kutta schemes for conservation laws

Willem Hundsdorfer
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(minisymposium MS6)

Multirate schemes for conservation laws or convection-dominated problems seem to come in two flavors: schemes that are locally inconsistent, and schemes that lack mass-conservation. These two defects will be discussed for one-dimensional conservation laws.

Particular attention will be given to monotonicity properties of the multirate schemes, such as maximum principles and the total variation diminishing (TVD) property. The study of these properties will be done within the framework of partitioned Runge-Kutta methods.

(The talk is on a paper with co-authors Anna Mozartova and Valeriu Savcenco)

Regularization of nonlinear inverse problems by certain time integration schemes

Michael Hönig
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(contributed talk CT3)

In this talk we discuss the numerical realization of asymptotic regularization (Showalter's method) of inverse problems. Given a nonlinear inverse problem, the key idea of asymptotic regularization is that the solution of a certain evolution equation yields a stable approximation to the solution of the inverse problem for large time. 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.

Asymptotic numerics of highly oscillatory equations

Arieh Iserles
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(invited talk)

In this talk we introduce an approach, based on combination of asymptotic and numerical methodologies, for the computation of ODEs with rapidly oscillating forcing terms. We focus on a family of nonlinear second-order equations which appear in many applications and demonstrate that their solution can be expanded asymptotically employing modulated Fourier expansions. The calculation of expansion terms requires solely manipulation of non-oscillatory quantities, therefore is easily affordable and the cost is uniform in frequency.

On hybrid stochastic-deterministic models for biochemical reaction kinetics

Tobias Jahnke
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(contributed talk CT1)

Biochemical reaction systems are traditionally modelled by ordinary differential equations representing the concentrations of the species. The reaction-rate approach is computationally cheap, but becomes insufficient if some of the species contain only a very low number of particles, and if small-scale stochastic fluctuations can cause large-scale effects. This is the case, e.g., in gene regulatory networks where gene expression is regulated by a few activators or repressors, or in viral kinetics where the fate of very few infectious individuals decides whether the infection spreads over large parts of the population.

For such applications, the appropriate description is provided by stochastic reaction kinetics. Here, the system is represented by a time-dependent probability distribution $p(t, x_1, ..., x_d)$ which indicates the probability that at time t exactly x_i particles of the i-th species exist. It is well-known that p is the solution of the chemical master equation, but solving this equation numerically is only possible for rather small systems because the number of degrees of freedom grows exponentially with the number of species.

This difficulty has motivated a number of attempts to combine the simple deterministic approach with the precise but expensive stochastic kinetics. Several authors have proposed hybrid models in which only a part of the system is described by stochastic reaction kinetics, whereas the other part is represented by deterministic equations of motion. In this talk, the pros and cons of some of these hybrid methods will be discussed. Then, a new type of hybrid model which allows to overcome some of the drawbacks of the existing models will be derived.

Lagrange-d'Alembert integrators for constrained systems in mechanics

Laurent Jay
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(invited talk)

Numerical methods in discrete mechanics attempt to reproduce continuous concepts from mechanics at a discrete level. For example variational integrators for unconstrained Lagrangian systems satisfy a discrete Hamilton's variational principle, symplectic methods for Hamiltonian systems satisfy a discrete symplectic condition. In this talk we will consider Lagrangian systems with holonomic and nonholonomic constraints. Such systems can be expressed as overdetermined systems of differential-algebraic equations (DAEs) and they can be derived from the Lagrange-d'Alembert principle which is one of the most fundamental principles in classical mechanics. We define a new discrete Lagrange-d'Alembert principle for Lagrangian systems with constraints based on a discrete Lagrange-d'Alembert principle for forced Lagrangian systems. Constraints are considered as first integrals of the underlying forced Lagrangian system of ordinary differential equations. A large class of specialized partitioned additive Runge-Kutta (SPARK) methods satisfies the new discrete principle. We will show that symmetric Lagrange-d'Alembert SPARK integrators of any order can be obtained based for example on Gauss and Lobatto coefficients. We will also discuss how SPARK methods can be implemented efficiently.

High-order semi-Lagrangian numerical method for the Large-Eddy simulation of reactive flows

Rolf Jeltsch
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(contributed talk CT2)
Rolf Jeltsch (1), Julián T. Becerra Sagredo (2), Wesley P. Petersen (1), Jürg Gass (3)

(1) Seminar for Applied matheamtics, ETH Zurich
(2) Center for Energy Research, National University of Mexico, Temixco, Mexico
(3) Laboratory of Thermodynamics in Emerging Technologies, ETH Zurich

A high-order Semi-Lagrangian numerical method is developed for the simulation of a subsonic methane/air flame. The fluid is described by the Navier-Stokes equations for a mixture of ideal gases. Turbulence is modeled using Large-Eddy simulation (LES) together with a transport equation for the subgrid kinetic energy. For the chemical reactions we use an unsteady flamelet model based on transport equations for the mixture fraction and a reaction progress variable. This allows for extinctions and re-ignitions by not assuming fast chemistry nor steady flamelets.

To solve the resulting system of coupled transport equations a Semi-Lagrangian (FSL) method, known from climate modeling, is used. For the interpolations from the Lagrangian mesh points to a fix mesh an interpolation based on piece wise polynomials of degree 2m which are m-tmes differentiable are used. This interpolation is easy to implement, computations are fast. It is conservative, conservative and creates low or zero numerical diffusion and dispersion.

Finally the FSL method is used to simulate Sandia flame D. For the 3-d simulations a mesh in cylindrical coordinates is used where singular derivatives and high frequencies at the polar axis are controlled.

Discrete mechanics and optimal control

Oliver Junge
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(minisymposium MS1)

A new approach to the solution of optimal control problems for mechanical systems is proposed. It is based on a direct discretization of the Lagrange-d'Alembert principle for the system (as opposed to using, for example, collocation or multiple shooting to enforce the equations of motion as constraints). The resulting forced discrete Euler-Lagrange equations then serve as constraints for the optimization of a given cost functional. We analyze and numerically illustrate the method by several examples. This is joint work with Jerrold E. Marsden and Sina Ober-Bloebaum (both Caltech).

A DAE for skiing turns

Peter Kaps
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(contributed talk CT1)

The equation of motion for a model of a skier is given in descriptor form and solved by radau5.

The theta method revised

Samir Karaa
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(contributed talk CT3)

The θ-method is a well-known method for solving first-order ordinary differential equations. It is regarded as a weighted average method, and has a simple geometric interpretation. We propose a new formulation of the θ-method providing a general framework for studying stability, and allowing to select the values of the parameter θ that increase the order of accuracy. Based on the same idea, we develop a new technique for the derivation of linear multistep methods. We also derive new and general stability results for finite element θ-schemes. Parabolic and hyperbolic problems will be considered. Finally, we present a technique to improve the accuracy of the approximate factorization method originated by M. Beam and R. F. Warming.

Direct multiple shooting methods for parameter estimation in dynamic processes

Ekaterina Kostina
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(minisymposium MS1)

The quantitative validation of complex nonlinear differential equation models is a difficult task that requires the support by numerical methods for parameter estimation and the optimal design of experiments. The talk presents particularly efficient "direct all-at-once" methods for parameter estimation in dynamic systems. Special emphasis is placed on issues of robustness, i.e. how to reduce the sensitivity of the estimates with respect to measurement outliers. Real-life applications are discussed. The talk finally gives an outlook how the optimization instruments can be used for planning optimal experiments to maximize the information gain about parameters.

Numerical treatment of singularly perturbed delay differential equations using B-Spline collocation method on Shishkin mesh

Devendra Kumar
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(poster)

This paper is devoted to the numerical study for a class of boundary value problems of second-order differential equations in which the highest order derivative is multiplied by a small parameter ϵ and both the convection and reaction terms are with negative shift. To obtain parameter-uniform convergence, a piecewise uniform mesh (Shishkin mesh) is constructed, which is dense in the boundary layer region and coarse in the outer region. Cubic B-spline basis functions with fitted-mesh are considered in the procedure and yield a tridiagonal system which can be solved efficiently by using any well-known algorithm. A parameter-uniform convergence analysis of the method is given. The method is shown to have almost second-order parameter-uniform convergence. The effect of small delay δ on the boundary layer is also discussed. To demonstrate the performance of the proposed scheme several examples having boundary layers have been carried out. The maximum absolute errors are presented in tables.

Domain decomposition in time using symmetric integrators for solving ODEs.

Patrice Linel
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(minisymposium MS8)

We propose a time domain decomposition method that breaks the sequentiality of the integration scheme for system of ODEs. We transform the initial value problem into a boundary value problem using the symmetrization of the time interval. We then propose the Schwarz algorithm to deal with the domain decomposition. For systems of linear ODEs, the algorithm shows a linear convergence,thus the Aitken technique is used to accelerate the convergence of the solution at the boundaries of the domain. Another approach is then developed using a time-reversible integration scheme and a system of conditions satisfied by the solution at time boundaries. In case of non linear system of ODEs, the system of conditions is

solved by a Newton method. An implementation is briefly discussed and a number of examples are given to illustrate the success of the method.

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Splitting methods for nonlinear Schrödinger equations

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(minisymposium MS7)

We give an error analysis of Strang-type splitting integrators for nonlinear Schrödinger equations. For Schrödinger-Poisson equations with an H^4-regular solution, a first-order error bound in the H^1 norm is shown and used to derive a second-order error bound in the L_2 norm. For the cubic Schrödinger equation with an H^4-regular solution, first-order convergence in the H^2 norm is used to obtain second-order convergence in the L_2 norm. Basic tools in the error analysis are Lie-commutator bounds for estimating the local error and H^m-conditional stability for error propagation, where $m = 1$ for the Schrödinger-Poisson system and $m = 2$ for the cubic Schrödinger equation.

Two Hopf algebras of trees interacting

Dominique Manchon
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(minisymposium MS4)

We will show that the Connes-Kreimer Hopf algebra of rooted trees is a comodule Hopf algebra over another Hopf algebra of trees. This gives a Hopf algebra approach to the recent work of Ph. Chartier, E. Hairer and G. Vilmart on composition and substitution of B-series.

Numerical conservation of the Hamiltonian for an optimal control problem with control discontinuities

Pierre Martinon
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(minisymposium MS1)
Pierre Martinon (1) and Joseph Gergaud (2)

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Solving an optimal control problem with an indirect shooting method (based on Pontryagin's Minimum Principle) requires integration of an Initial Value Problem (IVP). When discontinuities of the right hand side are present, for instance due to control switchings, it is faster and more accurate to detect these events during the integration. However, the usual way to detect these discontinuities, based on the integrator's dense output, still causes some errors at the switchings that can be seen for instance on the Hamiltonian. We improve this detection in order to ensure that the switching point corresponds to the actual integration, which further improves the precision of the shooting method. These results are illustrated on a low thrust orbital transfer problem with up to 1500 control switchings.

Auxiliary variables and deferred corrections for divergence constrained flows

Michael Minion
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(minisymposium MS6)

A class of methods for the numerical solution of incompressible and low-Mach number flows based on a novel combination of deferred corrections and auxiliary variables is presented. Temporal integration is done using spectral deferred corrections which allow multiple terms in an equation to be treated either implicitly or explicitly and with different time steps and can easily be constructed to attain high formal order of accuracy. These methods are combined with a finite volume discretization of an auxiliary variable formulation of the equations of motion to produce higher-order accurate flow solvers. The key idea in auxiliary variable methods is to formulate an equation for a variable which does not have an explicit divergence constraint but from which the desired constrained velocity can be numerically extracted by the analog to the procedure used in projection methods. Examples from incompressible, 0-Mach number flows will be presented.

A hybrid parareal-spectral deferred correction method

Michael Minion
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(minisymposium MS8)

The parareal algorithm is an iterative method for the parallelization in the time direction of numerical methods for the solution of ordinary and partial differential equations. Each iteration of parareal consists of a parallel step, wherein each processor computes an accurate approximation to the solution using approximate initial data on a time interval, and a serial step which propagates a correction to the initial conditions

through the time domain. Two observations linking the parareal method and deferred correction methods will be explored: First, the serial step in the parareal algorithm can be interpreted as a particular choice of a deferred correction procedure. Second, rather than computing the accurate solution in the parallel step from scratch, the solution from the previous parareal iteration can be used as a predictor for a deferred correction procedure. These observations are used to construct a hybrid strategy combining features of both the parareal and spectral deferred correction methods which can significantly reduce the computational cost of the original parareal method. Numerical examples are presented to compare the effectiveness of the hybrid strategy.

B-series and related expansions for highly oscillatory systems

Ander Murua
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We consider highly oscillatory non-autonomous systems of ODEs. Although some of the ideas are also applicable to the multifrequency case, we focus on the case where the right-hand side is periodic in t. Several B-series-like formal expansions related to the highly oscillatory system are considered, that can be useful to study the solutions of the system, analyze existing methods, and design new special purpose integrators.

High-order time-splitting methods for Schrödinger equations

Christof Neuhauser
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(minisymposium MS3)

(joint work with M. Thalhammer)

In this talk, we discuss efficient numerical methods for the space and time discretisation of linear and nonlinear Schrödinger equations. As a model problem, we consider the Gross–Pitaevskii equation

$$\mathrm{i}\,\hbar\,\partial_t\psi(x,t) = \Big(-\tfrac{\hbar^2}{2\,m}\,\Delta + V(x) + \hbar^2 g\,\big|\psi(x,t)\big|^2\Big)\,\psi(x,t)\,, \qquad x\in\mathbb{R}^d, \quad t\ge 0,$$

which arises in quantum physics for the description of Bose–Einstein condensates. Our main concern is a theoretical analysis of numerical methods that are based on pseudospectral methods in space and higher-order exponential operator splitting methods in time. Numerical examples for systems of coupled Gross–Pitaevskii equations illustrate the theoretical results and the effectiveness of time-spitting pseudospectral methods compared to standard integrators in a long-term integration.

Structural Approach to the Design of Explicit One-Stage Methods

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(poster)

An explicit one-stage method is proposed for the numerical integration of systems of ordinary differential equations. A class of structural features of such systems is singled out. Economical numerical schemes from second up to fifth order of accuracy are constructed using these features at the algorithmic level.

Proper orthogonal decomposition for solving in parallel large system of stiff ODEs

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(minisymposium MS8)

We investigate the proper orthogonal decomposition (POD) as a useful tool in decoupling large dynamical systems suitable for parallel computing. POD is well known to be applied to model reduction for different applications. It is based on snapshots on iterated solutions and allows to generate a low dimensional space for the approximation of the solution. We will focus on the parallelism potential with decoupling dynamical systems into subsystems spread between processors.

We show a mathematical analysis to obtain a criterion on the error behavior in using POD in decoupling systems. Therefore we use this result is an error estimator for decoupling an ODE system. This error estimate under a residual form leads us to a criterion on how well the reduced model is still appropriated, and based on what we can get an idea when to exchange information between sub-systems. This method has been tested on several examples including stiff problems from PDEs. Numerical tests provide interesting results as well as great computing performance on parallel computers.

Geometric integration of differential equations

Reinout Quispel
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(contributed talk CT6)

Geometric integration is the numerical integration of a differential equation, while preserving one or more of its geometric/physical properties exactly, i.e. to within round-off error. Many of these geometric properties are of crucial importance in physical applications: preservation of energy, momentum, angular momentum, phase-space volume, symmetries, time-reversal symmetry, symplectic structure and dissipation are examples. In this talk we first present a survey of geometric numerical integration methods for differential equations, and then exemplify this by discussing symplectic vs energy-preserving integrators for ODEs as well as for PDEs.

Wiener Calculus for Differential Equations with Uncertainties

Peter Rentrop
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(contributed talk CT1)

During the last years the Polynomial Chaos of N. Wiener was revealed to be a cheap alternative to Monte-Carlo simulations. In stationary FEM the intrusive or nonintrusive approaches are still in discussion. The transient situation in ODEs or DAEs is open. The mathematics consists of orthogonal polynomial developments depending on a given distribution. The Martin Cameron Theorem requires bounded second moments. For time dependent uncertainties the Karhunen Loeve Theorem forms the base. Numerical experiments for the van der Pol equation with random parameter are presented.

IMEX schemes applied to the numerical solution of hyperbolic systems with stiff relaxation

Giovanni Russo
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(**cancelled talk**)

This talk is a review on the construction of IMEX schemes for the numerical solution of hyperbolic systems with stiff relaxation. In the limit of infinite stiffness, the relaxation reduces to an algebraic relation among the variables, that can be solved by expressing some unknowns in terms of the other. The system therefore reduces to a smaller quasilinear system. If a certain condition is satisfied, the solution of the original system also converges to the solution of the reduced system. A method of line approach based on high order finite difference discretization of the flux term reduces the PDE system to a large system of ordinary differential equation. Some IMEX discretizations are presented, obtained by combining an SSP explicit scheme with an L-stable implicit one. Such combination seems suitable for the numerical treatment of such systems. Some consideration about the stability of the schemes for convection-diffusion systems and for relaxation systems will be presented. Finally, the possibility of capturing the diffusion limit of the system by imposing suitable conditions on the coefficients of the IMEX scheme will be discussed.

Efficient Runge-Kutta methods for stochastic differential equations

Andreas Rößler
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(contributed talk CT2)

In the present talk, we consider stochastic differential equations (SDEs) driven by a multi-dimensional Wiener process. Since explicit solutions are only known in a very few cases, numerical solutions have to be calculated in many applications. Therefore, we introduce a new class of Runge-Kutta methods, which turns out to have significantly reduced computational complexity compared to well known Runge-Kutta schemes for SDEs. For this new class of Runge-Kutta methods, the computational effort depends only linearly on the dimension of the driving Wiener process while well known Runge-Kutta methods have a computational effort which depends quadratically on the dimension of the Wiener process. This improvement becomes apparent especially for high dimensional SDE systems. Further, order conditions for this new class of Runge-Kutta methods are calculated explicitly based on the multi-colored rooted tree analysis and some coefficients are presented as an example. Finally, the performance of the new Runge-Kutta methods is compared to some well known schemes by a simulation study.

Rheologic modelization of a mixed nanotube/polymer fluid

Kevin Santugini
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(contributed talk CT4)

Rheology is the study of materials having both liquid and solid properties such as visco elastic fluids, e.g. culinary preparations, cement, blood. In this presentation, we model the formation of a nanotube/polymer string.

B-series and multiscale methods

Chus Sanz-Serna
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(invited talk)

B-series were introduced 35 years ago by Ernst Hairer and Gerhard Wanner and have provided a universal tool to understand numerical methods for differential equations. In this talk I will show how to use them in the analysis of multiscale methods for highly oscillatory problems.

Numerical Simulation of Relativistic Laser-Plasma Interaction

Julia Schweitzer
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(minisymposium MS3)

In laser-plasma physics, many phenomena can be described by a nonlinear wave equation coupled to an equation for the plasma response. Since the interesting physical problems are huge, fast and efficient numerical solvers are required. In this talk, we present some advances on the numerical solution of these application problems.

Numerical modeling of wave propagation in holey fibers by the R-functions method

Yuriy Semerich
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(contributed talk CT4)

Microstructured optical fibers (MOFs) also called photonic crystal fibers or holey fibers are single material optical fibers with a periodic array of air holes running along their entire length [1]. MOFs have recently generated much interest thanks to the new ways provided to control and guide light. Many research efforts have been devoted to understanding the propagation characteristics of MOFs based on different numerical methods. This paper devoted to the numerical analysis of wave propagation in holey fibers by the R-functions method (RFM) [2]. The basic feature of the RFM is the construction of normalized boundary domain equations for geometric objects of complicated forms [3]. The mathematical model of the investigated processes is a boundary value problem for the Helmholtz equation. According to the RFM the solution of the problem constructed in analytical form by the sheaf of functions is called general structure of solutions (GSS), satisfying exactly the prescribed boundary conditions. Numerical realization of the elaborated method and an analysis of obtained results were conducted.

1. Bishnu P.P. Guided Wave Optical Components and Devices: Basics, Technology, and Applications. Elsevier, 2006.
2. Rvachev V.L. Theory of the R-functions and it's some applications. Nauk. dumka, Kiev, 1982 (in Russian).
3. Semerich Yu.S. The construction of loci with acyclical symmetry by the R-functions. Mathematical modelling and analysis, v. 10 (1), 2005, pp. 73-82.

Numerical solution of singular ODE-BVPs arising in bio-mechanics

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(contributed talk CT5)

We analyze a boundary value problem describing the rectilinear shear deformation of fiber reinforced materials, whose application is relevant in the biomechanics of soft tissues like tendons and muscles. The interesting feature of the problem is that the material models are governed by nonconvex constitutive equations. Hence, for some choices of the material parameters, multiple and non smooth solutions can exist. Since usual numerical methods for BVPs are devised for regular problems for which existence and uniqueness are guaranteed, they cannot provide good results in the present situations unless suitably modified. Moreoever, to our knowledge, only second-order two-point BVPs with singularities at either one or both of the boundary points have been investigated intensively in the numerical literature, but always in the assumption that the Lipschitz condition is satisfied.In this talk we present a numerical approach, recently introduced in [1], to face both the identification of the (unknown) singularity in the integration domain and the tracking of multiple solutions, in the case of Dirichlet and mixed boundary conditions. Energetic considerations coupled with suitable iterative techniques seem to be guidelines to devise good numerical approximations. It is worthing to note that these topics can also be of interest in the context of recent studies about the approximation of differential equations with non-smooth properties.

[1] M. Destrade, G. Saccomandi and I. Sgura (2009) ”Inhomogeneous shear of orthotropic incompressible non-linearly elastic solids: singular solutions and biomechanical interpretation”, International. Journal of Engineering Science, doi:10.1016 j.ijengsci.2008.12.016, in press

Linear instability of ideal flows on a sphere

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(contributed talk CT7)

A unified approach to the normal mode instability study of steady solutions to the vorticity equation governing the motion of an ideal incompressible fluid on a rotating sphere is considered. The four types of well-known solutions are considered, namely, the Legendre-polynomial (LP) flows, Rossby-Haurwitz (RH) waves, Wu-Verkley (WV) waves and modons. A conservation law for disturbances to each solution is derived and used to obtain a necessary condition for its exponential instability. By these conditions, Fjortoft average spectral number of the amplitude of an unstable mode must be equal to a special value. In the case of the LP flows or RH waves, this value is related only with the basic flow degree. For the WV waves and modons, it depends both on the basic flow degree and on the spectral distribution of the mode energy in the inner and outer regions of the flow. Peculiarities of the instability conditions for different types of modons are discussed. The new instability conditions specify the spectral structure of growing disturbances localizing them in the phase space. For the LP flows, this condition complements the well-known Rayleigh-Kuo and Fjortoft conditions related to the zonal flow profile. Some analytical and numerical examples are considered. The maximum growth rate of unstable modes is estimated too, and the orthogonality of any unstable, decaying and non-stationary mode to the basic flow is shown in the energy inner product. The analytical instability results obtained here can also be applied for testing the accuracy of computational programs and algorithms used for the numerical stability study. It should be stressed that Fjortoft spectral number appearing both in the instability conditions and in the maximum growth rate estimates is the parameter of paramount importance in the linear instability problem of ideal ideal flows on a sphere.

Grid control in BVP solvers

Gustaf Söderlind
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(invited talk)

Grid adaptation in two-point boundary value problems is usually based on mapping a uniform auxiliary grid to the desired nonuniform grid. Here this approach is used to construct a grid density function for the distribution of the grid points. Accuracy is controlled via a single parameter, the number N of points in the grid.

For any given grid, a solver provides a local error estimate, which is used by a feedback controller to adjust the grid density; this interaction continues until the error has been equidistributed, providing a Lagrangian minimax density.

Once the density function is determined, another control law determines N based on the prescribed tolerance and (possibly) a global error estimate. A complete control structure is presented, together with numerical tests that demonstrate the advantages of the control system within the bvpsuite solver, ceteris paribus, for a selection of problems and over a wide range of tolerances.

IMEX-RK approaches for the simulation of electrical activity in cardiac tissue

Raymond Spiteri
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(**cancelled talk**)

Mathematical models of electric activity in cardiac tissue typically involve ordinary differential equations (ODEs) that describe the ionic currents at the myocardial cell level. Generating an efficient numerical solution of these ODEs is a challenging task, and in fact the physiological accuracy of tissue-scale models is often limited by the efficiency of the numerical solution process. In this talk, I relate our experiences with the use of implicit-explicit Runge-Kutta (IMEX-RK) splitting methods for the numerical solution of 4 cardiac electrophysiological models. We find that variable step-size implementations of IMEX-RK methods that take advantage of Jacobian structure often outperform the methods commonly used in practice.

A linearly implicit time-integrator for a h-p adaptive geophysical fluid flow solver

Amik St-Cyr
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(minisymposium MS6)

A Jacobian-Free Rosenbrock W-method is employed to solve the compressible Euler equations in a parallel h-p adaptive discontinuous Galerkin solver. The latter is used in the simulation of atmospheric fluid flows and the W-method requires no Newton type iterations. Moreover W-methods enable the use of inexact Jacobians: various preconditioning can therefore be constructed.

Local error expansions for high-order exponential operator splitting methods

Mechthild Thalhammer
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(minisymposium MS7)

In this talk, I am concerned with high-order exponential operator splitting methods for the time-integration of abstract evolutionary problems. My main objective is the specification and inspection of a local error expansion; such an error expansion provides the basis for a convergence analysis of splitting methods when applied to nonlinear (stiff) differential equations. Compared to alternative representations of the local error that rely on the well-known Baker-Campbell-Hausdorf formula, recently exploited techniques provide optimal bounds with respect to the regularity requirements on the exact solution. Moreover, an alternative approach, particularly suitable for the investigation of evolutionary problems that involve critical parameters, will be discussed.

Adaptive wavelet-based approximation of the Chemical Master Equation

Tudor Udrescu
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(contributed talk CT4)

In the stochastic formulation of reaction kinetics, the time evolution of the probability distribution for a system of interacting molecular species is governed by the Chemical Master Equation (CME). This equation can be interpreted as a large system of ODEs or as a discrete time-dependent PDE. Solving the CME with standard methods is usually impossible as the number of degrees of freedom is far too large. In this talk, we propose the use of compactly supported orthogonal wavelets in order to avoid the "curse of dimensionality" that affects the CME. The solution is represented adaptively in a thresholded wavelet basis and only the essential degrees of freedom are propagated in each time step.

Real-time differentiation and system inversion via sliding modes

Elio Usai
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(minisymposium MS2)

The problem of differentiating a measured signal in real-time is a well-known ill-posed mathematical problem having many implications of practical relevance. One of them is related to the system inversion problem that can be stated as the evaluation of the input that causes the system output to exhibit some specific behavior. From a mathematical point of view it results in the evaluation of the function u(t) such that the solution of a (n)th-order differential equation coincides with some given function. Such a problem is the basis of model based fault detection schemes that can be used in industrial application in order to improve reliability. Actually it can be shown that the input reconstruction can be solved by means of multiple differentiation resorting to the concept of algebraic observability and considering the input as an additional state variable to be estimated. A great impulse to real-time differentiation has be given by the exploitation of Higher-Order Sliding Mode (HOSM) control techniques. By using the theory of discontinuous right-hand side differential equations it was shown that the differentiation problem can be regularized reducing it to an integration problem. Since the theoretic solution implies infinite frequency switching some limitation appears in real implementations. In the present paper the use of sliding differentiators embedded in input estimation schemes is presented. In particular two approaches are presented: the first based on algebraic observability and the second on a nonlinear observer. Applicative examples are reported to show the features of the proposed estimation schemes.

Normal forms for DAEs

Olivier Verdier
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(contributed talk CT5)

The study of DAEs usually starts with the linear case. In that case, the Kronecker normal form is used to define the index and explain the numerical difficulties arising when discretizing DAEs. However, the Kronecker normal form is not suitable for time dependent problems.

I will present a new normal form for linear DAEs that readily extends to the time dependent linear problems, and to a certain extent to nonlinear problems as well. It has also the benefit of providing simple explanations of the tractability and strangeness indices in the linear time-dependent case.

Convergence and component splitting for Crank-Nicolson–leap-frog

Jan Verwer
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(minisymposium MS5)

A new convergence condition is discussed for the Crank-Nicolson–Leap-Frog integration scheme. This convergence condition guarantees second-order temporal convergence uniformly in the spatial grid size for a wide class of implicit-explicit splittings. This is illustrated by successfully applying component splitting to first-order wave equations resulting in such second-order temporal convergence. Component splitting achieves that only on part of the space domain Crank-Nicolson needs to be used. This reduces implicit solution costs when for Leap-Frog the step size is severely limited by stability only on part of the space domain, for example due to spatial coefficients of a strongly varying magnitude or locally refined space grids.

Splitting methods with complex times for parabolic equations

Gilles Vilmart
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(minisymposium MS7)

(This is joint work with F. Castella, P. Chartier and S. Decombes. Similar results are derived independently by E. Hansen and A. Ostermann.)

Using composition procedures, we build up high order splitting methods to solve evolution equations posed in finite or infinite dimensional spaces. Since high-order splitting methods with real time are known to involve large and-or negative time steps, which destabilizes the overall procedure, the key point of our analysis is, we develop splitting methods that use complex time steps having positive real part: going to the complex plane allows to considerably increase the accuracy, while keeping small time steps; on the other hand, restricting our attention to time steps with positive real part makes our methods more stable, and in particular well adapted in the case when the considered evolution equation involves unbounded operators in infinite dimensional spaces, like parabolic (diffusion) equations.

Multirate time integration for conservation laws

Joerg Wensch
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(minisymposium MS6)

The simulation of atmospheric dynamics relies on the numerical solution of the Euler equations. These equations exhibit phenomena on different temporal scales. In the lower troposphere sound waves propagate approximately ten times faster than the advective velocities. Although sound waves play a minor role for numerical weather prediction, in recent years the interest in unfiltered models that exhibit these waves has been grown because filtering affects the dispersion relation for slower wave phenomena. An approach to overcome the CFL restriction caused by sound waves are split-explicit methods. By multirate techniques the terms relevant for sound waves are integrated by small time steps with a cheap time integration procedure, whereas the slow processes are solved by an underlying Runge-Kutta method using a larger macro step size. Nevertheless, even then sound waves pose a restriction on the macro step size. We generalize these methods, analyze order and stability of the generalized methods, and show how the stability barrier is improved by a factor of two for Runge-Kutta methods. When cyclic Runge-Kutta methods (Peer methods) are used as underlying method, a stronger relaxation of the stability barrier is obtained.

Comparative study of FDM, FEM and B-spline collocation method for singularly perturbed BVPs

Arjun Yadaw
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(contributed talk CT4)

A parameter-uniform numerical methods for a class of singularly perturbed one-dimensional parabolic reaction-diffusion problems with two small parameters on a rectangular domain are studied. Parameter-explicit theoretical bounds on the derivatives of the solutions are derived. The method comprises a standard implicit finite difference scheme to discretize in temporal direction on a uniform mesh by means of Rothe's method and finite element method in spatial direction on a piecewise uniform mesh of Shishkin type. The method is shown to be unconditionally stable and accurate of order $O(N^{-2}(\ln N)^2 + \Delta t)$. Numerical results are given to illustrate the parameter-uniform convergence of the numerical approximations.

Computing multiple solutions to the p-Henon equation

Zhong-hua Yang
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(**cancelled talk**)

The boundary value problems (BVP) of the p-Henon equation on the unit square and the unit disk are considered. The bifurcation method is used to compute the multiple positive solutions to the BVP of the p-Henon equation for different p, which appear in astrophysics ($p = 2$), pseudoplastic fluid and nonlinear elasticity ($p < 2$) and dilatant fluid ($p > 2$). Three algorithms are proposed and the multiple positive solutions are visualized.

Research of applicability of different fuzzy inference scheme's into the hierarchical fuzzy inference systems

Natalia Yastrebova
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(contributed talk CT2)
(Joint work with Sugeno, Mamdani, Larsen, Tsukamoto)

Hierarchical fuzzy inference systems became an active research field in recent years owing to their good capabilities for approximation and reduction of size for the base of rules in multi-dimension systems. I would like to describe architecture, advantages and disadvantages of hierarchical fuzzy inference systems on the basis of different fuzzy inference scheme's.

Generalized polar coordinates on Lie groups

Antonella Zanna
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(invited talk)

We present a new family of local coordinates on Lie groups (generalized polar coordinates) based on splitting. The splitting (at the algebra level) is derived using a sequence of nested sub-algebras obtained as the range of appropriate projection operators derived from involutive algebra automorphisms. Through the exponential map, the nested algebra-splitting defines a new family of coordinate maps on the underlying Lie group G. We also derive the formulas for the tangent coordinate maps and their inverses, necessary when solving ordinary differential equations on the group. The coordinate maps, tangent, and inverse tangent maps, can be computed efficiently for some low-rank splittings.

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Conference on Scientific Computing (17-20 June 2009)

Conference in honour of E. Hairer's 60th birthday

Program Summary

The conference takes place at UniMail in lecture hall **S160** (plenary talks) and **S160/R160/R170** (parallel sessions). UniMail address: boulevard du Pont d'Arve 40, 1205 Genève, Switzerland.

Wednesday 17th		Thursday 18th		Friday 19th		Saturday 20th	
8:30-9:20	Registration	8:30-09:15	D. Higham	8:30-09:15	U. Ascher	8:30-09:15	M. Hairer
9:20-9:30	Welcome						
9:30-10:15	C.Sanz-Serna	9:15-10:00	M. Hochbruck	9:15-10:00	A. Zanna	9:15-10:00	M. Crouzeix
10:15-10:30	Coffee Break	10:00-10:30	Coffee Break	10:00-10:30	Coffee Break	All day	Picnic on Salève and C.E.R.N. visit
10:30-12:30	CT1 (S160)	10:30-12:30	MS4/CT3/CT4 (S160/R160/R170)	10:30-12:30	MS5/MS8/CT6 (S160/R160/R170)		
12:30-14:00	Lunch	12:30-14:00	Lunch	12:30-14:00	Lunch		
14:00-14:45	A. Iserles	14:00-14:45	A. Abdulle	14:00-14:45	L. Jay		
14:45-15:30	Poster session	14:45-15:30	G. Söderlind	14:45-15:30	N. Guglielmi		
15:30-17:30	MS3/MS7/CT2 (S160/R160/R170)	15:30-16:00	Coffee Break	15:30-16:00	Coffee Break		
		16:00-18:00	MS1/CT5 (S160/R160)	16:00-18:00	MS2/MS6/CT7 (S160/R160/R170)		
At 19:50	boat excursion					At 18:30	conference dinner

List of Minisymposia
MS1: Control of ordinary differential equations (M. Chyba & J. Gergaud)
MS2: Discontinuous differential equations (A. Bellen & L. Lopez)
MS3: Geometric integration of PDEs (D. Cohen)
MS4: Hopf algebras in numerical analysis of ODEs (P. Chartier & A. Murua)
MS5: IMEX (IMplicit-EXplicit) Runge-Kutta schemes (S. Boscarino)
MS6: Innovative time integrators for fluid flow problems (O. Knoth & J. Wensch)
MS7: Splitting methods for stiff and nonstiff problems (S. Descombes & M. Massot)
MS8: Parallel methods for solving ODEs (D. Tromeur-Dervout)

NOTE: Please have your name tag with you for all excursion for verifications.
For Salève picnic and Cern visit:
Please bring your valid passport (or identity card), and bring some food for the picnic.
Do not wear high heels or sandals otherwise you will be refused entry into Cern.