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Plenary Talks

Splitting methods for autonomous and non-autonomous perturbed systems

S. Blanes

Universidad Politécnica de Valencia, Spain

An important number of differential equations originated from as diverse research areas as celestial mechanics, quantum mechanics, Hybrid Monte Carlo, parabolic problems or some eigenvalue problems can be considered as perturbations of problems whose solutions are exactly solvable (or can be easily and accurately approximated). For the numerical integration of these equations it is usually convenient to solve separately the perturbation and the dominant part, and then to consider appropriate compositions of their flows. An efficient method for a given problem must take into account the relevant aspects of the problem. For example:

– The size of the perturbation.
– The accuracy of the desired solution.
– The length of the time integration.
– Is the perturbation exactly solvable? or, can we use a low order numerical approximation for this part?
– Do the flows admit negative time steps? and, can we use complex coefficients having positive real part?
– Is the dominant part explicitly time dependent?
– Etc.

In this talk we present our recent works on the search of methods for these problems (a new way to get the order conditions, the analysis of the conditions to be solved by the coefficients in each case, and to find the explicit coefficient for the methods). The performance of the methods is illustrated on several numerical examples.

Computing Operator Determinants and Preconditioning Riemann-Hilbert Problems – A Numerical Analyst's Encounter with Mathematical Physics

F. Bornemann

Technische Universität München, Germany

The numerical evaluation of operator determinants, originally born out of an attempt to validate some highly structured differential equations calculations, has become a popular tool in areas of Mathematical and Theoretical Physics dealing with integrable systems; e.g., it was recently used by S. Nishigaki to calculate the 'pion decay constant' of certain QCD-like theories. We review some of this development, tell an amusing story about the numerical evaluation of higher-order derivatives and its relation to a problem in graph theory, and end by showing how all this generalizes to the preconditioning of matrix-valued Riemann-Hilbert problems.
Partly joint work with my PhD student Georg Wechslberger (TU München).

Plane wave stability of the split-step Fourier method for the nonlinear Schrödinger equation

L. Gauckler[a], *E. Faou*[b] *and Ch. Lubich*[c]

[a] Technische Universität Berlin, Germany

[b] INRIA & ENS Cachan Bretagne & ENS Paris, France

[c] Universität Tübingen, Germany

The cubic nonlinear Schrödinger equation has solutions that are plane waves. In the talk we will discuss the stability of these solutions and the stability of their numerical approximation.

We first study the stability of plane waves in the exact solution. We show orbital stability of plane waves over long times. In the second part of the talk we study a very popular method for the numerical discretization of the nonlinear Schrödinger equation, the split-step Fourier method. This method combines a Fourier spectral method in space with a splitting integrator in time. We will pursue the question whether the stability of plane waves in the exact solution transfers to this numerical discretization.

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Convergence of an ADI splitting for Maxwell's equations

M. Hochbruck, T. Jahnke and R. Schnaubelt

Karlsruhe Institute of Technology, Germany

Maxwell's equations provide the foundation for the theory of electromagnetism, and solving these equations numerically is an important task in many applications. For problems posed on a cuboid or on $\mathbb{R}^3$, the alternating direction implicit method proposed by Zheng, Chen, and Zhang (2000) is particularly attractive, because this method is unconditionally stable and computationally cheap. The main idea is, roughly speaking, to decompose the Maxwell operator in such a way that the sub-flows can be propagated in a stable and efficient way.
In this talk, second-order convergence for the semi-discretization in time is shown in the framework of operator semigroup theory. The proof is based on results concerning the regularity of the Cauchy problems of the sub-flows, which then allow to apply an abstract convergence proof by Hansen and Ostermann [1].
Before the error analysis, well-posedness of Maxwell's equations on cuboids and on $\mathbb{R}^3$ will be discussed.

References

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On solving highly oscillatory ODE problems

A. Murua

Universidad del País Vasco, Spain

In this talk, we are interested in studying the solutions of highly oscillatory systems of ordinary differential equations and constructing and analyzing numerical integrators for such problems. We present the approach developed in [1, 2, 3, 4, 5], where standard combinatorial-algebraic tools for analysing numerical integrators for non-oscillatory ODEs are adapted to the highly oscillatory context. We explore in which extent our approach for analysing the solutions of highly oscillatory problems can by used to construct actual numerical integrators tailored for such problems by treating in some detail several examples that fit in our framework.

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Weighted Essentially Non-Oscillatory limiters for Runge-Kutta Discontinuous Galerkin Methods

J. Qiu

School of Mathematical Sciences, Xiamen University, China

In the presentation we will describe our recent work on a class of new limiters, called WENO (weighted essentially non-oscillatory) type limiters, for Runge-Kutta discontinuous Galerkin (RKDG) methods. The goal of designing such limiters is to obtain a robust and high order limiting procedure to simultaneously obtain uniform high order accuracy and sharp, non-oscillatory shock transition for the RKDG method. We adopt the following framework: first we identify the "troubled cells", namely those cells which might need the limiting procedure; then we replace the solution polynomials in those troubled cells by reconstructed polynomials using WENO methodology which maintain the original cell averages (conservation), have the same orders of accuracy as before, but are less oscillatory. These methods work quite well in our numerical tests for both one and two dimensional cases, which will be shown in the presentation.

Off-Label Uses for ODE Methods: Randomization

R.D. Skeel and Y. Fang

Purdue University, United States

One of the most demanding calculations is to generate a single instance of a point in a high-dimensional configurational space from a specified probability distribution (with an unknown normalizing prefactor). (Being able to generate a dozen independent samples would solve grand challenge problems, such as protein folding.) Direct methods for doing this are impractical: one has to resort to using an iterative process known as a Markov chain Monte Carlo method, which converges only in the limit to the prescribed distribution. Such methods crawl through configuration space step by step, with acceptance of a step based on a Metropolis(-Hastings) criterion. An acceptance rate of 100% is possible in principle by embedding configuration space in a higher-dimensional phase space and using ODEs. In practice, numerical integrators must be used, lowering the acceptance rate, but at the same time allowing long moves. This is the essence of *hybrid Monte Carlo* methods. Presented is a general framework for constructing such methods under relaxed conditions.

Computational Methods for Bayesian Inverse Problems

A. Stuart

University of Warwick, United Kingdom

Many problems in the physical sciences require the determination of an unknown field from a finite set of indirect measurements. Examples include oceanography, oil recovery, water resource management and weather forecasting. The Bayesian approach to these problems is natural for many reasons, including the under-determined and ill-posed nature of the inversion, the noise in the data and the uncertainty in the differential equation models used to describe complex mutiscale physics. The object of interest in the Bayesian approach is the posterior probability distribution on the unknown field.
However the Bayesian approach presents a computationally formidable task as it results in the need to probe a probability measure on function space. The talk will start by briefly overviewing the state-of-the-art in MCMC methods for the exploration of such probability measures [1]. It will then highlight two classes of methods which aim to simplfy the computational task based on approximating the probability measure by a Dirac measure or by a Gaussian. The motivation for doing this is partly related to the idea of Bayesian posterior consistency: the fact that, in the large data or small noise limits, the posterior distribution concentrates near the true value of the unknown field underlying the data [2].
The idea of approximating the posterior measure by a Dirac is the maximum a posteriori (MAP) estimator which, in words, computes the mostly likely point under the posterior probability distribution. It will be shown how to make sense of this idea in infinite dimensions, resulting in a problem from the calculus of variations; posterior consistency of the MAP estimator will also be studied [3]. We will then study approximation of the posterior measure by a Gaussian, looking for the closest Gaussian with respect to the Kullback-Leibler divergence. Again we show how to make sense of this in infinite dimensions, and we describe computational methods for the problem, based on the Robbins-Monro algorithm [4].

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Minisymposia Talks

MS01 – Molecular Dynamics

Organized by: Benedict Leimkuhler and Carsten Hartmann

On the use of Bayes theorem for estimating free energies from adaptively biased simulations

M. Athènes, L. Cao, M.C. Marinica, G. Stoltz and T. Lelièvre

CEA Saclay, Service de Recherches de Métallurgie Physique, France

An important task of molecular simulation is the computation of free energy profiles $A(\zeta)$ where ζ is a control parameter acting on a multi-particle system. Among free-energy techniques, adaptive methods introduce an external bias to minimize the time spent sampling regions of the free energy that have already been visited. The time-dependent bias may be added to the potential or to the force governing the dynamics. We show how the biasing force can be efficiently constructed using an extended form of Bayes theorem.

A meshfree discretization of optimal control problems with applications in Molecular Dynamics

R. Banisch and C. Hartmann

Freie Universität Berlin, Germany

Rare but important transition events between long lived states are a key feature of many molecular systems. In many cases the computation of rare event statistics by direct molecular dynamics (MD) simulations is infeasible even on the most powerful computers because of the immensely long simulation timescales needed. Recently a technique for spatial discretization of the molecular state space designed to help overcome such problems, so-called Markov State Models (MSMs), has attracted a lot of attention. We introduce a novel approach to using MSMs for the efficient solution of optimal control problems that appear in Molecular Dynamics applications where one desires to optimize molecular properties by means of external controls. The discretization is both meshfree and structure-preserving. It will be illustrated with some numerical examples.

Structure preserving integration of constrained multirate systems

S. Leyendecker[a] *and S. Ober-Blöbaum*[b]

[a] Chair of Applied Dynamics, University of Erlangen-Nuremberg, Germany

[b] University of Paderborn, Germany

Mechanical systems with dynamics on varying time scales, e.g. including highly oscillatory motion, impose challenging questions for numerical integration schemes. Tiny step sizes are required to guarantee a stable integration of the fast frequencies. However, for the simulation of the slow dynamics, integration with a larger time step is accurate enough. Here, small time steps increase integration times unnecessarily, especially for costly function evaluations. For systems comprising fast and slow dynamics, multirate methods integrate the slow part of the system with a relatively large step size while the fast part is integrated with a small time step [1, 2]. A particular challenge is the treatment of the coupling between slow and fast dynamics, e.g. via potentials or holonomic constraints. In this talk, a multirate integrator is derived in closed form via a discrete variational principle, resulting in a symplectic and momentum preserving multirate scheme [3].

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Robust and efficient configurational molecular sampling via Langevin Dynamics

Ch. Matthews and B. Leimkuhler

University of Edinburgh, United Kingdom

Efficient algorithms are of paramount importance in computationally-intensive disciplines such as molecular dynamics. In this talk, we compare a wide variety of numerical methods for solving the stochastic differential equations often encountered in molecular dynamics. We analyse methods based on the application of deterministic impulses, drifts, and Brownian motions in some combination. In computed simulations of alanine dipeptide (both solvated and unsolvated), higher accuracy is obtained without loss of computational efficiency, while allowing large timestep, and with no impairment of the conformational sampling rate. Efficiency improvements of 25% or more in practical timestep size are achieved in vacuum, and with reductions in the error of configurational averages of a factor of ten or more attainable in solvated simulations at large timestep.

Mathematical analysis of accelerated dynamics

T. Lelièvre

CERMICS, École des Ponts Paris Tech, France

We will present some mathematical analysis of accelerated dynamics techniques which have been proposed by A.F. Voter in the late nineties: the parallel replica method, the hyperdynamics and the temperature accelerated dynamics. The analysis strongly relies on the notion of quasi-stationary distribution.
These are joint works with D. Aristoff, C. Le Bris, M. Luskin, F. Nier and D. Perez.

References

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Linear response theory and optimal control for a molecular system under nonequilibrium conditions

H. Wang[a], *C. Hartmann*[a] *and C. Schuette*[b]

[a] Freie Universität Berlin, Germany

[b] Freie Universität Berlin & Zuse Institute Berlin, Germany

In this talk, we propose a straightforward generalization of linear response theory to systems in nonequilibrium that are subject to nonequilibrium driving. We briefly revisit the standard linear response result for equilibrium systems, where we consider Langevin dynamics as a special case, and then give an alternative derivation using a change-of-measure argument that does not rely on any stationarity or reversibility assumption. This procedure moreover easily enables us to calculate the second order correction to the linear response formula (which may or may not be useful in practice). Furthermore, we outline how the novel nonequilibrium linear response formula can be used to compute optimal controls of molecular systems for cases in which one wants to steer the system to maximize a certain target expectation value. We illustrate our approach with simple numerical examples.

Using Coarse Grained Models to Speed Convergence to the Minimum Energy Pathway

J. Weare, B. Qiu, S. Kale, M. Saunders, B. Roux and A. Dinner

University of Chicago, United States

For large complex systems interrogation of the reaction mechanism by straightforward simulation is often impossible due to the presence of a vast range of time scales. For this reason, efficient techniques that focus on discovery of the reaction pathways are important. Unfortunately in large complex systems discovery of these pathways can itself be prohibitively expensive. In this work we develop a technique for discovery of the minimum energy pathway (and other pathwise descriptions of reactions) that uses inexpensive, coarse grained models to accelerate convergence. In most practical settings the reaction pathway corresponding to the coarse grained model does not accurately describe the reaction of interest. Nevertheless, by carefully arranging the calculation, the coarse grained system can be used to accelerate convergence to the MEP of a more expensive, more accurate, model. We demonstrate the effectiveness of this approach on several test problems.

MS02 – Recent Trends in Lattice Boltzmann Methods: Boundary Conditions and Applications

Organized by: Matthias Ehrhardt and Salvador Izquierdo

Introduction to Lattice Boltzmann Method and Recent Trends

A. Bartel and D. Heubes

University of Wuppertal, Germany

In computational fluid dynamics often complex physical fluid properties (like multiphase, multicomponent, chemical reaction, multiphysics) need to be taken into account. Furthermore, boundaries or obstacles with complex fluid interaction occur. Classically, the Navier-Stokes equations would be needed to be supplemented with corresponding mathematical models.

The lattice Boltzmann method (LBM) uses a particle approach in which these complex phenomena can be relatively easily represented on the basis of particle interaction.

In this talk, the basic ideas of LBM will be explained including boundary conditions. We give a mathematical interpretation of the algorithms as certain quadrature rules. Furthermore, we report on certain recent trends such as multiphysical systems, fluid structure interaction and transparent boundaries.

Challenges in boundary conditions for CFD simulations using lattice Boltzmann methods

S. Izquierdo[a] *and N. Fueyo*[b]

[a] Universidad de Zaragoza and Instituto Tecnológico de Aragón, Spain

[b] Universidad de Zaragoza, Spain

The lattice Boltzmann (LB) method has reached enough maturity to be an alternative for current industrial CFD simulations. However, one of the essential points of the method, the boundary conditions, is the subject of a variety of approaches, which are not always consistent with the target macroscopic equations. We present a systematic review of these approaches to define boundary conditions in LB methods. Two partially-solved challenges are analyzed: suppression of reflecting waves in steady and unsteady simulations, and implementation of Neumann boundary conditions. Based on their conclusions we will discuss how to provide practical solutions for present challenges, such as the definition of boundary conditions for complex fluids.

High order boundary conditions for Lattice Boltzmann Schemes

M.M. Tekitek[a], *F. Dubois*[b] *and P. Lallemand*[c]

[a] University Tunis ElManar, Tunisia

[b] CNAM, LMSSC, Paris, France

[c] CNRS, Paris, France

Our communication will be divided into two parts. In the first part, we show that it is possible to get the macroscopic fluid equations of lattice Boltzmann schemes with an external force using Taylor expansion. In a second part of our contribution, we validate this general expansion by a detailed application to boundary conditions.

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Non-Reflecting Boundary Conditions for the Lattice Boltzmann Method

D. Heubes, A. Bartel and M. Ehrhardt

University of Wuppertal, Germany

In this talk, we present different approaches of non-reflecting boundary conditions for the lattice Boltzmann method (LBM). One approach is based on a hyperbolic PDE formulation of the fluid's motion. There Dirichlet conditions at the artificial boundaries are computed using an analysis of characteristics. Then, the Dirichlet conditions are transferred to the LBM framework. Our procedure can be seen as a generalized LODI (local one dimensional inviscid) approach.
In addition, we present our recent results of another approach, where a non-reflecting boundary condition is directly derived on the discrete level. Under the assumption of a simplified collision operator we compute an exact boundary condition on the discretized level for a one dimensional setting. This formulation depends on all previously computed values at the boundary. Based on the exact formulation, we aim at techniques to get practical and efficient boundary conditions.

Asymptotic analysis of LB for fluid-structure interaction: boundaries, forces and coupling schemes

A. Caiazzo

WIAS Berlin, Germany

Recent development of LB schemes offer a variety of algorithms to incorporate different boundary conditions and deal with the fluid-solid interactions. We discuss some of these issues from the point of view of asymptotic analysis [1, 2], in particular discussing the consistency of the conditions at the fluid-solid interface for no-slip conditions, immersed boundary approaches, Lees-Edwards boundaries and force evaluation via Momentum-Exchange [3, 4]. Finally, asymptotic analysis of coupling scheme will be discussed.

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Numerical lifting for Lattice Boltzmann models

Y. Vanderhoydonc and W. Vanroose

Universiteit Antwerpen, Belgium

In this contribution we give an overview of various lifting strategies for Lattice Boltzmann models (LBMs). A lifting operator finds for given macroscopic variables the corresponding distribution functions, mesoscopic variables of the LBM. There are several applications where macroscopic variables need to be mapped to these distribution functions. For example, starting a LBM from given macroscopic initial conditions includes some arbitrariness. The initialization of the LBM then requires a lifting operator. Another application of a lifting operator is found in coupled LBM and macroscopic partial differential equation (PDE) models, where one part of the domain is described by a PDE while another part is modeled by a LBM. Such a hybrid coupling results in missing data at the interfaces between the different models. The lifting operator provides the correct boundary conditions for the LBM domain at the interfaces. [1] contains an overview of the different lifting strategies.

References

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Lattice Boltzmann Simulations of Soft Matter Interfaces

J. Harting, S. Frijters, F. Günther, B. Kaoui and T. Krüger

TU Eindhoven, Netherlands

Interfaces are ubiquitous in soft matter systems and appear in various shapes and sizes. Prominent examples are vesicles, capsules, and biological cells. Other classes of fluid-fluid interfaces can be found in emulsions, foams, and liquid aerosols. We investigate the underlying physical properties of soft matter interfaces by combining a multiphase lattice Boltzmann solver for the involved fluids with molecular dynamics or immersed boundary methods to describe (colloidal) particles or deformable membranes. An overview on recent applications will be given ranging from rheological and structural properties of particle stabilized fluid interfaces and emulsions towards microfluidic transport of vesicles and biological cells.

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Real world CFD applications on GPGPU based LBM with local grid-refinement

M. Geier, M. Schönherr and M. Krafczyk

TU Braunschweig, Germany

In order for the lattice Boltzmann method to be applicable to real world CFD applications the code needs to be flexible and efficient at the same time. It has to support off-grid boundary conditions to fit arbitrary geometrical constrains with a Cartesian mesh and local grid-refinement is necessary to enhance the resolution in areas of higher gradients. It is essential that grid-refinement and off-grid boundaries work seamlessly and efficiently together. In this contribution we present an LBM implementation for GPGPUs based on the sparse EsoTwist data structure. EsoTwist combines streaming and collision into a single step and requires only one set of variables. It allows for a random access order to the lattice notes and is hence completely thread-safe and suitable for many-core implementations. Grid-refinement and boundary conditions are designed to be as compact as possible in order to work efficiently with the EsoTwist data structures without compromising accuracy.

MS03 – Computational and stochastic methods in inverse problems

Organized by: Uri Ascher and Sebastian Reich

Stochastic algorithms for inverse problems involving PDEs and many measurements

U. Ascher, F. Roosta-Khorasani and K. van den Doel

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Inverse problems involving systems of partial differential equations (PDEs) and many experiments are very expensive to solve numerically. The mere evaluation of a misfit function often requires hundreds and thousands of PDE solves. We develop and assess dimensionality reduction methods, both stochastic and deterministic, to reduce this computational burden. Highly efficient variants of the resulting algorithms are identified and demonstrated in the context of the famous DC resistivity and EIT problems.

Mass Conservation and Positivity Preservation with Ensemble-type Kalman Filter Algorithms

T. Janjic Pfander[a], *D.B. McLaughlin*[b], *S.E. Cohn*[c] *and M. Verlaan*[d]

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This paper considers incorporation of constraints to enforce physically-based conservation laws in the ensemble Kalman filter. In particular, equality and inequality constraints are used both to conserve mass and to maintain positivity through measurement updates. In order to ensure mass conservation, a projection matrix that corrects for localization effects is constructed. In order to maintain both mass conservation and positivity preservation through the analysis step, we construct two data assimilation algorithms based on quadratic programming and ensemble Kalman filtering. We demonstrate the benefits of imposing these constraints in two simple experimental setups: a solid body rotation experiment and idealized problems of environmental pollution. The results show clear improvements in both analyses and forecasts, particularly in the presence of localized features.

Exploiting Shape Hessians in PDE constrained Shape Optimization

V. Schulz

Trier University, Germany

Shape optimization problems are a special kind of inverse problems which involve a somewhat "exotic" differential calculus - especially in the case of PDE constrained shape optimization. Second order computational optimization methods are rarely applied in that field. In this talk, we discuss, how nevertheless so-called shape Hessians can be exploited for convergence aceleration and try to pave the way for Newton-like approached based on a Riemannian interpretation of shape optimization problems.

Can Localization Lift the Curse of Dimensionality for Particle Filters?

S. Reich[a] *and Y. Cheng*[b]

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The optimal way of incorporating observations into dynamical models, also known as filtering or data assimilation, can be quite easily done in theory by combining the model dynamics with an application of Bayes' formula. Particle methods come into play as a way to approximate the true filtering solution. The downside is that the number of particles needed to come close to the analytic solution grows exponentially with the model dimension, which is also known as the curse of dimensionality. This problem can in principle be addressed by the concept of localization, which takes advantage of the spatial structure of the state space and transforms a global problem to local problems. This concept has yet to be transferred to particle filters, which we do by using methods from optimal transportation.

Consistent inference for coarse-grained models from multiscale data

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Imperial College London, United Kingdom

Most dynamical systems in the natural sciences are characterized by the presence of processes that occur across several length and time scales. Examples include the atmosphere-ocean system, biological systems, materials and molecular dynamics. Typically only the dynamics at the macroscopic scale is of interest. While multiscale methods (e.g. homogenization) provide the analytical framework for the rigorous derivation of effective coarse-grained dynamical systems, statistical inference for these multiscale systems (i.e. identifying parameters in the coarse-grained system from data of the macroscopic component) remains far from being straightforward. In

particular, standard statistical techniques such as maximum likelihood become biased due to the multiscale error. In this talk we will introduce a novel class of estimators for multiscale diffusions that do not suffer from this bias. In addition to presenting rigorous convergence results, we will present several illustrative examples.

A combined registration-segmentation model for filtration estimation in the kidney

A. Zanna[a], *E. Hodneland*[b] *and E. Hanson*[a]

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[b] Department of Biomedicine, University of Bergen, Norway

In this talk we propose a combined registration-segmentation method for motion correction and parameter estimation for the kidney applied to dynamic contrast-enhanced MR images of the kidney. The motion correction is performed using normalized gradients as data term in the registration and a Mahalanobis distance from the segmented phases to a training set to supervise a segmentation. By applying this framework to input 4D image time series we conduct simultaneous motion correction and two-phase segmentation into renal cortex and background. The resulting time series are then used to estimate kidney perfusion.

MS04 – Time integration of partial differential equations

Organized by: Alexander Ostermann

Variational discretization of wave equations on evolving surfaces

Ch. Lubich and D. Mansour

Universität Tübingen, Germany

A linear wave equation on a moving surface is derived from Hamilton's principle of stationary action. The variational principle is discretized with functions that are piecewise linear in space and time. This yields a discretization of the wave equation in space by evolving surface finite elements and in time by a variational integrator, a version of the leapfrog or Störmer–Verlet method. We study stability and convergence of the full discretization in the natural time-dependent norms under the same CFL condition that is required for a fixed surface. Using a novel modified Ritz projection for evolving surfaces, we prove optimal-order error bounds. Numerical experiments illustrate the behavior of the fully discrete method.

A numerical analysis of parabolic differential equations on evolving surfaces

D. Mansour

Universität Tübingen, Germany

A linear parabolic partial differential equation on a moving surface is discretized in space by the evolving surface finite element method. Discretization in time is done by implicit Runge–Kutta methods, aiming for higher-order accuracy in time and unconditional stability of the fully discrete scheme. Thanks to the properties of the spatial semi-discretization, the latter is established for algebraically stable and stiffly accurate Runge–Kutta methods. Under sufficient regularity conditions, optimal-order error estimates in the natural time dependent norms are shown. Numerical experiments are presented to confirm some of the theoretical results.

Implicit Runge-Kutta schemes and discontinuous Galerkin methods for Maxwell's equations

T. Pazur and M. Hochbruck

Karlsruhe Institute of Technology, Germany

Maxwell's equations can be considered as an abstract initial value problem

$$u'(t) = Au(t) + f(t), \qquad u(0) = u_0$$

on a suitable Hilbert space H. In this talk we first present an error analysis for Gauß and Radau collocation methods applied to this abstract problem. Our error analysis is based on energy technique discussed in [1]. For s-stage collocation methods we obtain an order reduction to order $s + 1$ instead of the classical order $2s$ and $2s - 1$ for Gauß and Radau collocation methods, respectively.
Next we discretize Maxwell's equations in space using the discontinuous Galerkin method and then apply a collocation method to integrate the semidiscrete problem in time. We can prove that the full discretization error is of size $\mathcal{O}(h^{p+1/2} + \tau^{s+1})$, where h denotes maximum diameter of the finite elements and τ denotes the time step. Finally, we illustrate our theoretical results by numerical experiments.

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Numerical approximation of Turing patterns in a reaction-diffusion model for electrodeposition

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We describe the dynamics of metal growth by electrodeposition by a reaction-diffusion PDE system that allows spatial pattern formation through Turing instability [1]. Oscillating Turing patterns arise if a forcing frequency is applied [2]. Numerical approximation of Turing patterns is a challenging task: high accuracy in space and long-time integration are needed, in the forced model highly oscillatory solutions are expected. We perform space semi-discretization by high order finite difference ECDFs. For time discretization, we introduce a test equation and define its stability region in terms of reaction and diffusion time scales. We present a stability analysis for Crank-Nicolson, IMEX 2-SBDF, ADI schemes. We approximate both stationary and oscillating Turing patterns by ADI-ECDF since do not require stepsize restrictions [3, 4]. New results will be presented related to Turing-Hopf instability, which can yield patterns oscillatory in space and time.

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On Schrödinger, Strang and Strichartz

T. Jahnke, M. Hochbruck and R. Schnaubelt

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Exponential operator splitting is a very efficient and well established approach for solving time-dependent Schrödinger equations. It is well known that the Lie-Trotter splitting and the Strang-Marchuk splitting converge with order 1 and 2, respectively, if the initial data and the potential are sufficiently regular. However, the necessary regularity assumptions for the potential are too restrictive in many applications.
In this talk, Strichartz estimates are used to prove new error bounds for exponential splitting methods applied to the linear Schrödinger equation on $\mathbb{R}^d$ (with moderate $d \in \mathbb{N}$). These error bounds show convergence of both methods under weaker assumptions, but the classical orders are reduced by a factor which depends on the regularity of the potential and the dimension d. For smooth potentials, the classical orders of convergence are recovered.

An investigation of Strang and high order splitting schemes for Vlasov-type equations

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In astro- and plasma physics the behavior of a collisionless plasma is modeled by the Vlasov equation coupled to an appropriate model of the electromagnetic field. For such a system Strang splitting is the most common integration method described in the literature.
We provide a rigorous convergence analysis for the Strang splitting scheme in the case of Vlasov-type equations; this analysis is conducted in an abstract framework which includes the above mentioned applications. In addition,

we show convergence of a full discretization for the electrostatic case, where this scheme is combined with a discontinuous Galerkin approximation in space.
Due to the fact that the Strang splitting scheme, in general, is not symmetric, a straightforward extension to higher order methods, using composition, is not possible. To remedy this, we propose and analyze an explicit method which retains all favorable properties of the Strang splitting scheme.

References

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Efficient time integration of the Klein-Gordon equation in the non-relativistic limit regime

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We consider the Klein-Gordon equation in the non-relativistic limit regime, i.e. the speed of light c formally tending to infinity. Due to the highly-oscillatory nature of the solution in this regime, its numerical simulation is very delicate. Here we will construct an asymptotic expansion for the exact solution in terms of the small parameter c^{-2}. We will see that for sufficiently smooth initial values this asymptotic expansion exists up to an arbitrary order, and can be reconstructed by superposing highly-oscillatory terms to cascaded solutions of c-independent Schrödinger-like systems. The numerical advantage is that the high-oscillations in the exact solution can be filtered out explicitly and the numerical task reduces to solving the non-oscillatory Schrödinger-like limit systems, which can be carried out very efficiently without any additional time-step restriction.

Finite-difference schemes with splitting and discrete TBCs for the 2D Schrödinger equation in a strip

A. Zlotnik

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The splitting technique is widely used to simplify solving of the TD Schrödinger and related equations [1] which are so important in various fields. We apply the Strang-type splitting in potential to the Crank-Nicolson and

Numerov-Crank-Nicolson schemes for the 2D TD Schrödinger in a strip with the discrete transparent boundary conditions (DTBC). We prove the uniform in time L^2-stability and the uniqueness of solutions.
We also need to study the splitting schemes on an infinite mesh in the strip and derive the uniform in time L^2-stability and the mass conservation law. The DTBC operator is written in terms of the discrete convolution in time and the discrete Fourier expansion in direction y perpendicular to the strip. Effective direct algorithms using FFT in y are developed to implement the schemes for general potential. Promising numerical results on the tunnel effect for some barriers and the practical error analysis in C and L^2 norms are given.

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On construction of customized efficient exponential integrators for large stiff systems of ODEs

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The flexibility of the exponential propagation iterative (EPI) methods framework allows construction of exponential schemes with improved computational efficiency. We present three classes of EPI methods of Runge-Kutta type (EPIRK) – nonsplit, split and hybrid integrators. We discuss the design principles that let us develop efficient schemes of high order with low number of stages and, consequently, reduced computational cost for a given problem. Further improvements in efficiency are derived from development of adaptive Krylov and parallel versions of EPIRK integrators. A new MPI-based software package that includes implementation of exponential methods for serial and parallel computational platforms will be presented. Using a suite of test problems we illustrate performance advantages of the new schemes and software by comparing them with other exponential and implicit methods including the popular CVODE package.

Exponential B-series: The stiff case

V.T. Luan and A. Ostermann

Department of Mathematics, University of Innsbruck, Austria

For the purpose of deriving the order conditions of exponential Runge–Kutta and exponential Rosenbrock methods, we extend the well-known concept of B-series to exponential integrators. As we are mainly interested in the stiff case, Taylor series expansions have their limitations. Our approach is based on the variation-of-constants formula which allows us to treat semilinear problems, where the stiffness comes from the linear part. By truncating the arising exponential B-series to a certain order (which requires regularity of the considered exact solution) we are able to identify the sought-after order conditions. In particular, we show how the stiff order conditions of arbitrary order can be obtained in a simple way from a set of recursively defined trees.

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Projected explicit Lawson methods for the integration of Schrödinger equation

B. Cano[a] *and A. González-Pachón*[b]

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In this talk we will prove that explicit Lawson methods, when projected onto one of the invariants of nonlinear Schrödinger equation (norm) are also automatically projected onto another invariant (momentum) for many solutions. As this procedure is very cheap and geometric because two invariants are conserved, we will show that it offers an efficient tool to integrate some solutions of this equation till long times. On the other hand, we will show a detailed study on the numerical performance of these methods against splitting ones, with fixed and variable stepsize implementation.

References

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Exponential type integrators for abstract quasilinear parabolic equations with variable domains

C. González

Universidad de Valladolid, Spain

In this talk, I propose an exponential explicit integrator for the time discretization of quasilinear parabolic problems. My numerical scheme is based on Runge-Kutta methods. In an abstract formulation, the initial-boundary value problem is written as an initial value problem on a Banach space X

$$u'(t) = A\big(u(t)\big)u(t) + b(t), \quad 0 < t \leq T, \qquad u(0) \text{ given}, \tag{1}$$

involving the sectorial operator $A(v) : D(v) \to X$ with variable domains $D(v) \subset X$ with regard to $v \in V \subset X$. Under reasonable regularity requirements on the problem, I analyze the stability and the convergence behaviour of the numerical methods.

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MS05 – Oscillatory Hamiltonian systems

Organized by: Christian Lubich

Multi-revolution composition methods for highly oscillatory differential equations

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[c] Université de Genève, ENS Cachan, Antenne de Bretagne and INRIA Rennes, France

We introduce a new class of multi-revolution composition methods (MRCM) for the approximation of the N^{th}-iterate of a given near-identity map. When applied to the numerical integration of highly-oscillatory systems of differential equations, the technique we propose benefits from the properties of standard composition methods: it is intrinsically geometric and well-suited for Hamiltonian or divergence-free equations for instance. We prove error estimates with error constants that are independent of the oscillatory frequency. Numerical experiments, in particular for the nonlinear Schrödinger equation, illustrate the theoretical results, as well as the efficiency and versatility of the methods.

Control of parasitic oscillations in linear multistep methods

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Université de Genève, Switzerland

Due to the presence of parasitic roots in symmetric linear multistep methods, the numerical solution of differential equations gives rise to non-physical oscillations. Although these oscillations have a small amplitude in the beginning, they can grow exponentially with time and soon dominate the error in the numerical approximation. Certain symmetric multistep methods for second order differential equations have the feature that these oscillations remain bounded and small (below the discretization error of the smooth solution) over very long time intervals. We extend former results for second order Hamiltonian equations to systems with holonomic constraints (index 3 differential-algebraic equations). The technique of proof is backward error analysis combined with modulated Fourier expansions.
The presented results have been obtained in collaboration with Christian Lubich and Paola Console.

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Highly oscillatory ODEs with irregular oscillators

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There exist several robust computational approaches to ODEs with regular highly oscillating forcing terms, not least HMM and asymptotic expansions. However, once we consider irregular oscillators and allow for the presence of stationary points, very little exists in terms of either theory or numerical practice. In this talk we develop a general asymptotic expansion in this situation. Each n-th term in this expansion can be computed as a highly oscillatory integral over n-dimensional simplexes.

A Multiscale Method for Highly Oscillatory Dynamical Systems Using a Poincaré Map Type Technique

R. Tsai, B. Engquist and S.J. Kim

The University of Texas at Austin, United States

We propose a new multiscale method for computing the effective behavior of a class of highly oscillatory ordinary differential equations (ODEs). Without the need for identifying hidden slow variables, the proposed method is constructed based on the following ideas: a nonstandard splitting of the vector field (the right hand side of the ODEs); comparison of the solutions of the split equations; construction of effective paths in the state space whose projection onto the slow subspace has the correct dynamics; and a novel on-the-fly filtering technique for achieving a high order accuracy. Numerical examples are given.

Integrating Highly-Oscillatory Mechanical Systems with Solution-Dependent Frequencies

D. Weiss

Karlsruhe Institute of Technology, Germany

The talk is about the application of several integrators to highly-oscillatory mechanical systems with solution-dependent frequencies. As an example we use the stiff spring double pendulum: two mass points are attached serially by stiff springs to one another. The numerical behaviour of several integrators such as FLAVORS, the impulse method, and the mollified impulse method is studied. It is explained that a correct approximation of the actual motion relies on an almost-invariance property of the actions in the system. This almost-invariance property also guarantees the existence of an underlying effective system, which is derived. The analysis is done using canonical transformations proposed by K. Lorenz and Ch. Lubich (see [1, 2]).

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MS06 – Markov Chain Monte Carlo and related dynamic sampling methods

Organized by: Tony Lelièvre

Convergence of the Wang-Landau algorithm

G. Fort[a], *B. Jourdain*[b], *E. Kuhn*[c], *T. Lelièvre*[b] *and G. Stoltz*[b]

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[c] INRA unité MIA, France

We analyse the convergence properties of the Wang-Landau algorithm. This sampling method belongs to the general class of adaptive importance sampling strategies which use the free energy along a chosen reaction coordinate as a bias. Such algorithms are very helpful to enhance the sampling properties of Markov Chain Monte Carlo algorithms, when the dynamic is metastable. The convergence of Wang-Landau is established as well as a Central Limit Theorem.

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Optimal scaling of the transient phase of Metropolis Hastings algorithms

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We consider the Random Walk Metropolis algorithm on $\mathbb{R}^n$ with Gaussian proposals, and when the target probability measure is the n-fold product of a one dimensional law. It is well-known that, in the limit n tends to infinity, starting at equilibrium and for an appropriate scaling of the variance and of the timescale as a function of the dimension n, a diffusive limit is obtained for each component of the Markov chain. We generalize this result when the initial distribution is not the target probability measure. The obtained diffusive limit is the solution to a stochastic differential equation nonlinear in the sense of McKean. We prove convergence to equilibrium for

this equation. We discuss practical counterparts in order to optimize the variance of the proposal distribution to accelerate convergence to equilibrium. Our analysis confirms the interest of the constant acceptance rate strategy (with acceptance rate between 1/4 and 1/3).

Numerical Analysis of Gaussian Random Field Generators

T. Shardlow

University of Bath, United Kingdom

We look at sampling Gaussian random fields with the eyes of a numerical analyst and consider the error analysis of some established algorithms. In particular, we consider the circulant embedding and turning bands method, along with methods based on the Wiener–Khintchine theorem and the Karhunen–Loeve expansion.

Gibbs Sampling for Hierarchical Bayesian Inverse Problems

A. Stuart, S. Agapiou, J. Bardsley and O. Papaspiliopoulos

University of Warwick, United Kingdom

I will describe properties of a Gibbs sampler applied to a hierarchical Bayesian formulation of the linear inverse problem. Emphasis will be placed on the insight obtained from formulation of the problem in an infinite dimensional setting and this insight will be used to study convergence properties of Gibbs sampler, based on a splitting into the unknown functions and the hyper-paremeters, as the computational mesh is refined. Posterior consistency properties will also be exhibited, in the small noise limit.

MS07 – Multiphase Flows: Analysis, Numerics and Optimization

Organized by: Malte Braack and Andreas Prohl

On energy-stable schemes for a Vesicle Membrane phase-field model

F. Guillen-Gonzalez[a] *and G. Tierra*[b]

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[b] University of Notre Dame, United States

In this talk we extend the ideas to approximate Allen-Cahn and Cahn-Hilliard equations giving in [2, 4, 3], to design efficient numerical schemes for a physically motivated model given in [1], concerning the behavior of the deformation of vesicle membranes coupled with incompressible flow fields. The model is based on the diffuse-interface phase-field strategy, satisfying a dissipative energy law. The system is completed with two constraints, fixing the volume and surface of the vesicle membranes.
We study the Vesicle Membrane model and analyze two different ideas to impose the volume and surface constraints (by means of either Lagrange multipliers or penalization), arriving at two different problems. We provide one energy-stable numerical scheme for each problem, with a linear approximation for the Lagrange multipliers case and a non-linear approach of the penalized problem.

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Finite element discretization of a phase field model for incompressible fluid flow with variable density and viscosity

L. Banas

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Accurate simulation of flow of mixtures of immiscible and incompressible fluids is of interest for a variety of scientific and industrial problems. We present a finite element approximation for a system of Cahn-Hilliard and Navier-Stokes equations with a non-smooth potential which can be used to describe the flow of multiple immiscible and incompressible fluids with different densities and viscosities. We discuss advantages of the method and its usefulness for porous media flow and optimal control applications.

Structure Preserving Discontinuous Galerkin methods in space and time for Allen-Cahn equation

A. Sariaydin, B. Karasözen and M. Uzunca

Institute of Applied Mathematics, Middle East Technical University, Ankara, Turkey

Gradient flow equations like Allen Cahn and Cahn-Hilliard are characterized by the energy decreasing property. We apply space-time discontinuous finite elements to preserve the energy decreasing property in the discretized form. For discretization in space, we use the interior penalty method discontinuous Galerkin method [1]. The semi-discretized system is solved by the discontinuous Galerkin-Petrov method [2], which is preserving the energy decreasing property and is A-stable. Numerical results for Allen-Cahn equation with Neumannn and periodic boundary conditions confirm the theoretical results.

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Optimal control of incompressible two-phase flows

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We consider an optimal control problem of two incompressible and immiscible Newtonian fluids. The motion of the interface between these fluids can be captured by a phase field model or level set model. Both methods are subject of this talk. The state equation includes surface tension and is discretized by a discontinuous Galerkin scheme in time and a continuous Galerkin scheme in space. In order to resolve the interface propagation we also apply adaptive finite elements in space and time. We derive first order optimality conditions including the adjoint equation which is also formulated in a strong sense. The optimality system on the discrete level is solved by Newton's method. In the numerical example we compare level sets with a phase field model.

On solvability of lubrication systems modelling evolution of two immiscible viscous thin liquid films

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Existence of global nonnegative weak solutions is proved for coupled one-dimensional lubrication systems that describe evolution of nanoscopic bilayer immiscible thin polymer films and take account of Navier-slip or no-slip conditions at both liquid-liquid and liquid-solid interfaces. In addition, in the presence of attractive van der Waals and repulsive Born intermolecular interactions existence of positive smooth solutions is shown.

Phase field models for two phase flows with phase transition

D. Kroener and M. Kraenkel

University of Freiburg, Germany

For the numerical simulation of two phase flows with phase transition we consider two different mathematical models. The first one is based on the Navier-Stokes-Korteweg model. In this case the interface between the two phases are not sharp. The width of the interface is proportional to a parameter δ which occurs in the momentum equation. Now it turns out that (at least in the stationary case) the pressure jump is proportional to this parameter δ. This is not in agreement with physical experience. Therefore we have replaced this Navier-Stokes-Korteweg model by a diffuse phase field model. In that case it can be shown that the jump conditions are correct in the limit $\delta \to 0$. For this phase field model, which is based on results of Alt, Witterstein and Dreyer, we

have developed a Discontinuous Galerkin method for two phase flows in two space dimensions. Several numerical test cases have been considered and the results will be shown in this contribution.

MS08 – Splitting Methods

Organized by: Fernando Casas

Splitting Methods for High-Precision Integration in Dynamical Astronomy

A. Farres, S. Blanes, F. Casas, J. Laskar and A. Murua

Universite de Bourgogne, France

In this talk we will present new families of splitting methods designed for the numerical integration of near-integrable Hamiltonian systems, with a particular interest on planetary N-body problems. We will use a Newtonian model for the motion of the planetary system and perform an extensive comparison between various high-order symplectic splitting methods. The comparisons will be made in both, Jacobi and Heliocentric coordinates.

Multi-revolution composition methods for time-dependent Schrödinger equations

M. Thalhammer

University of Innsbruck, Austria

In this talk, the error behaviour of the recently introduced multi-revolution composition methods is analysed for a class of highly oscillatory evolution equations posed in Banach spaces. The scope of applications in particular includes time-dependent linear Schrödinger equations, where the realisation of the composition approach is based on time-splitting pseudo-spectral methods. The theoretical error bounds for the resulting space and time discretisations are confirmed by numerical examples.

This is joint work with Philippe Chartier and Florian Méhats.

Splitting methods for Schrödinger equations in imaginary time

Ph. Bader[b], *S. Blanes*[c] *and F. Casas*[a]

[a] Universitat Politècnica de València, Spain

[b] Institut de Matemàtiques i Aplicacions de Castelló, Universitat Jaume I, Castellón, Spain

[c] Instituto de Matemática Multidisciplinar, Universitat Politècnica de València, Spain

An efficient method to compute the eigenstates of the Schrödinger equation is the propagation in imaginary time. The separability of the Hamiltonian makes the problem suitable for the application of splitting methods. High order fractional time steps of order greater than two necessarily have negative steps and can not be used for this class of diffusive problems. However, there exist methods which use fractional complex time steps with positive real parts which can be used with only a moderate increase in the computational cost. We analyze the performance of this class of schemes and propose new methods which outperform the existing ones in most cases. If the gradient of the potential is available, methods up to fourth-order with real and positive coefficients exist. We also explore this problem class and present highly optimized sixth order schemes for near integrable systems using positive real part complex coefficients with and without modified potentials.

References

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On some splitting methods involving high order derivatives

F. Casas

Universitat Jaume I, Spain

In this talk we review some splitting schemes for Hamiltonian systems of the form $H(q,p) = T(p) + V(q)$, with $T(p)$ quadratic in momenta, which involve the flow associated with the bracket $[V,[T,V]]$ alongside the potential $V(q)$. In this way second order derivatives of the potential have to be computed at each step along the integration interval. Some new methods involving even higher order derivatives of the potential are considered. Methods within this class require less stages than standard splitting schemes to achieve high order of accuracy. We analyze the applicability of the new methods to specific problems where the evaluation of the nested brackets is not particularly costly.

MS09 – Software issues

Organized by: Francesca Mazzia and Luis Rández

Refinements in the Approximate Matrix Factorization for the time integration of advection-diffusion-reaction PDEs

S. González Pinto, D. Hernández Abreu and S. Pérez Rodríguez

Universidad de La Laguna, Spain

The numerical integration of PDEs of Advection Diffusion Reaction type in several spatial variables in the MoL framework is considered. The spatial discretization is based on Finite Differences and the time integration is carried out by using splitting techniques applied to some Rosenbrock-type methods. The focus is to provide a way of making some refinements to the usual Approximate Matrix Factorization (AMF), here considered as the splitting technique to solve the large linear systems of equations. The AMF-refinements allow to recover the convergence order of the underlying method and in some cases to enlarge the linear stability regions and the Courant numbers with regard to the standard AMF-scheme. Most of these methods belong to the class of the W-methods. A few numerical experiments on some important 2D and 3D non-linear PDE problems with applications in Physics are presented. The development of some integration codes (in Fortran, Matlab, R) is in progress.

Automated design and analysis of ODE solvers

D. Ketcheson[a] *and M. Parsani*[b]

[a] King Abdullah University of Science and Technology - KAUST, Saudi Arabia

[b] NASA Langley, United States

Decades of research have led to a wealth of detailed knowledge about properties of numerical ODE solvers – their accuracy, stability, efficiency, structure preservation, and so forth. The process of applying this knowledge to the study of existing methods and the design of new ones can be fully automated. I will describe ongoing efforts to create a software laboratory whose ultimate goal is to tell you everything you might want to know about a given method, help you select an appropriate method for a given problem, or even design a new method that is particularly effective for a given problem. Some examples will be given to demonstrate the power of these tools in the context of applications like compressible fluid flow.

References

[1] D.I. Ketcheson, *NodePy software version 0.4*, `http://numerics.kaust.edu.sa/nodepy/`

[2] D.I. Ketcheson, M. Parsani and A. Ahmadia, *RK-Opt software version 0.4*, http://numerics.kaust.edu.sa/RK-Opt/

[3] D.I. Ketcheson, Umair bin Waheed, *A theoretical comparison of high order explicit Runge-Kutta, extrapolation, and deferred correction methods*, http://arxiv.org/abs/1305.6165, submitted.

[4] M. Parsani, D.I. Ketcheson, and W. Deconinck, *Optimized explicit Runge-Kutta schemes for the spectral difference method applied to wave propagation problems*, SIAM J. Sci. Comput. 35(2): A957-A986.

daePAD – a DAE solver based on Projectors and AD

R. Lamour

Humboldt University of Berlin, Germany

The code *daePAD* integrates IVPs of DAEs. It determines the index of the DAE pointwise, calculates consistent initial values and discovers singularities. Therefore, the code overcomes the weakness of existing tools.
We approximate the solution of IVPs for DAEs by truncated Taylor series using algorithmic differentiation (AD). In fact, AD provides a suitable framework, especially for the computation of the differentiations.
The tractability index concept is applied with all its fascinating properties. The matrix sequence provides, with its invariant ranks, a way of index determination and a monitor for singularities. For linear DAEs, the computed projectors allow a decomposition into the inherent ODE and assignments to the algebraic and higher index components, respectively. Thus, for nonlinear DAEs the iterations of a Newton-Kantorovich method are explicitly present.
The code is realized in Matlab using the AD tool INTLAB.
Illustrating examples complement the talk.

Numerical Solution of Initial and Boundary Value Problems in the open source software R: Packages deTestSet and bvpSolve

F. Mazzia[a], *J.R. Cash*[b] *and K. Soetaert*[c]

[a] Dipartimento di Matematica, Università di Bari, Italy

[b] Imperial College London, United Kingdom

[c] Royal Netherlands Institute of Sea Research (NIOZ), Netherlands

In this talk we present the R packages deTestSet and bvpSolve for the numerical solution of initial and boundary value problems. The R package deTestSet is derived from the Test Set for Initial Value Problem Solvers available at http://www.dm.uniba.it/∼testset which includes documentation of the test problems, experimental results from a number of proven solvers, and Fortran subroutines providing a common interface to the defining problem functions. Many of these facilities are now available in the R package deTestSet, which comprises an R interface to the test problems and to most of the Fortran solvers [1, 3, 4]. The R package bvpSolve includes an R interface to well known Fortran solvers and a set of challenges test problems [1, 2].The packages deTestSet and bvpSolve

are free software distributed under the GNU General Public License, as part of the R open source software project.

References

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[3] K. Soetaert, J.R. Cash and F. Mazzia, *deTestSet: Testset for differential equations*. 2011, `http://CRAN.R-project.org/package=deTestSet`. v. 1.0.

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Numerical methods with LaTeX

L. Randez[a], *J.L. Varona*[b], *J.I. Montijano*[a] *and M. Perez*[a]

[a] Universidad de Zaragoza, Spain

[b] Universidad de La Rioja, Spain

In this talk we present several ways to use numerical methods inside LaTeX documents employing free software. First, we show the use of `python` and `SAGE` in LaTeX files with the large number of associated numerical libraries. Also we present the extension of TeX known as LuaTeX. The main goal of LuaTeX is to execute scripts written in the general purpose programming language called `Lua`.
Finally, we show how to produce interactive pdf documents from LaTeX by using embedded `javascript`, noting that we need only the free software `Acroread` to read this class of documents.

Solving Network DAEs with Python

C. Tischendorf, S. Baumanns, L. Jansen and M. Matthes

Humboldt University of Berlin, Germany

The dynamic modelling and simulation of flow networks (gas networks, water networks, electronic circuits, blood circuits) leads to Differential-Algebraic Equations (DAEs). Depending on the (lumped or distributed) modelling of each network element the DAEs may result from space discretized PDAEs and be, therefore, highly dimensional. It leads to the demand for an efficient network DAE solver.
We discuss several solver issues as a network parser generating a stable DAE formulation and allowing a fast function evaluation as well as a modular implementation of integration methods, nonlinear solvers and linear

solvers. In particular, we address the need of a hybrid linear solver combining direct and iterative methods. Finally, we present a Python implementation for solving network DAEs. It includes a Python solver for DAEs of the form

$$f(\frac{\mathrm{d}}{\mathrm{d}t}d(x,t),x,t)=0.$$

Deferred correction based on exponentially fitted mono-implicit Runge-Kutta methods

M. Van Daele and D. Hollevoet

Ghent University, Belgium

Deferred correction [1] is a well-known approach to the numerical solution of general first order systems of nonlinear two-point boundary value problems. A well-known code built on this technique is TWPBVP.
The idea behind (iterated) deferred correction is to (iteratively) correct for the smooth errors of the discretization algorithm. This is also the original idea behind exponential fitting methods. Exponential fitting [2] is a procedure that produces variants of classical methods, aimed to solve problems with exponential (or in the complex case oscillating) solutions more efficiently.
In this talk, the combination of exponential fitting and deferred correction based on mono-implicit Runge-Kutta methods is discussed. Particular attention is given to the parameter selection of the exponentially fitted deferred correction schemes to annihilate or minimize the leading error term. Several algorithms are discussed and illustrated with numerical results.

References

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Solving Optimal Transport Problems Using Python

J. Van lent

University of the West of England, Bristol, United Kingdom

In the eighteenth century the mathematician and engineer Gaspard Monge considered the problem of finding the best way of moving a pile of material from one site to another. This optimal transport problem has since found a wide range of applications such as mesh generation, moving mesh methods, image registration, image morphing, optical design, cartograms, probability theory and many more. In this talk, I will introduce the optimal transport problem and its links to nonlinear optimisation, nonlinear partial differential equations and linear programming.

I will illustrate how to use Python and libraries for scientific computing and visualisation such as Numpy, Scipy and Matplotlib to implement and analyse numerical methods for optimal transport problems.

MS10 – Numerics for Stochastic Differential Systems

Organized by: Evelyn Buckwar

Energy-preserving integrators for stochastic Poisson systems

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A new class of energy-preserving numerical schemes for stochastic Hamiltonian systems with non-canonical structure matrix (in the Stratonovich sense) is proposed. These numerical integrators are of mean-square order one and also preserve quadratic Casimir functions. In the deterministic setting, our schemes reduce to methods proposed in [2] and [1].

References

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Regularity and convergence rates for SDEs with non-globally Lipschitz coefficients

S. Cox[a]*, M. Hutzenthaler*[b] *and A. Jentzen*[a]

[a] ETH Zürich, Switzerland

[b] University of Frankfurt, Germany

Consider the following SDE in $\mathbb{R}^d$:

$$dX_t = A(X_t)\,dt + B(X_t)\,dW_t, \quad t > 0; \quad X_0 = x \in \mathbb{R}^d, \tag{SDE}$$

where W is an m-dimensional standard Brownian motion, and $A : \mathbb{R}^d \to \mathbb{R}^d$ and $B : \mathbb{R}^d \to \mathbb{R}^{d\times m}$ are continuous mappings.
The classical results concerning convergence rates for temporal approximations of this SDE (e.g., convergence rates for the Euler scheme) require the coefficients A and B to be globally Lipschitz continuous. However, many SDEs arising from financial and physical models do not have globally Lipschitz continuous coefficients.

In joint work with Martin Hutzenthaler and Arnulf Jentzen, we consider the regularity of the solution to the SDE with respect to the initial value x, for certain types of SDEs with non-globally Lipschitz continuous coefficients. We use this to prove convergence rates for approximations.

The Numerical Approximation of Stochastic Evolution Equations in Banach spaces

E. Hausenblas[a] *and S. Cox*[b]

[a] Montanuniversity Leobenh, Austria

[b] ETH Zürich, Switzerland

The topic of my talk will be the numerical approximation of stochastic evolution equations in Banach spaces. Here we will consider Wiener and/or Levy noise.

On the use of discrete forms of the Itô formula

C. Kelly[a], *G. Berkolaiko*[b], *E. Buckwar*[c] *and A. Rodkina*[a]

[a] University of the West Indies, Jamaica

[b] Texas A & M University, United States

[c] Johannes Kepler University, Austria

A discrete form of the Itô formula was introduced in a 2009 paper by Appleby et al [1] for the purpose of deriving sharp a.s. asymptotic stability conditions for a scalar stochastic difference equation of the form produced by an Euler-Maruyama discretisation of an SDE with nonlinear coefficients.
The formula has proved flexible, and has since found application in the a.s. asymptotic stability analysis of linear systems with a.s. stabilising and destabilising perturbations under θ-Maruyama discretisation (see [2]).
We anticipate that versions of this discrete Itô formula will find wider application in the field of stochastic numerical analysis. However, the original 2009 proof contains an implicit assumption that must be carefully revisited each time the formula is adapted for a new discretisation method or test system. In this talk we explore the nature of this assumption and how it may be dealt with.

References

[1] J. A. D. Appleby, G. Berkolaiko and A. Rodkina, *Non-exponential stability and decay rates in nonlinear stochastic difference equation with unbounded noise*, Stochastics: An International Journal of Probability and Stochastic Processes, 81:2 (2009), pp. 99–127.

[2] G. Berkolaiko, E. Buckwar, C. Kelly and A. Rodkina, *Almost sure asymptotic stability analysis of the θ-Maruyama method applied to a test system with stabilising and destabilising perturbations*. LMS Journal of Computation and Mathematics, 15 (2012), pp. 71–83.

Weak convergence in second moments for linear SPDEs

R. Kruse[a], *A. Andersson*[b] *and S. Larsson*[b]

[a] ETH Zürich, Switzerland

[b] Chalmers University of Technology, Sweden

In numerical analysis of stochastic differential equations (SDEs) one usually differentiates between the so called strong and weak convergence. While the first notion ensures a good pathwise approximation of the SDE, a weakly convergent scheme only gives a good approximation of the law of the exact solution. Strong convergence implies weak convergence and, by a rule of thumb, the order of weak convergence is up to twice the order of strong convergence.

In this talk we confirm this rule for an Euler Galerkin finite element approximation of a linear stochastic PDE and a certain class of test functions, which ensures the so called convergence in second moments. The main feature of our analysis is that we avoid the classical ansatz relying on the associated Kolmogorov's backward equation. Instead we follow a more direct approach with Gronwall's lemma.

If time permits we indicate several possible ways to generalize this approach to semilinear SPDEs and a richer class of test functions.

Integrating factor methods for stochastic differential equations

A. Kværnø[a] *and K. Debrabant*[b]

[a] Norwegian University of Science and Technology, Norway

[b] Department of Mathematics and Computer Science, University of Southern Denmark, Denmark

The integrating factor methods, also called the Lawson methods, are well known techniques for solving stiff, semi-linear differential equations. The main idea behind the method is to use a change of variables to remove the explicit dependence on the stiff, linear part of the differential equation. In this talk, we will present some such methods for stochastic differential equations and discuss their stability properties.

Stability analysis for stiffly accurate SRK methods

A. Rößler[a], *D. Küpper*[b] *and A. Kværnø*[c]

[a] Universität zu Lübeck, Germany

[b] Technische Universität Darmstadt, Germany

[c] Norwegian University of Science and Technology, Norway

In the present talk, we deal with the numerical solution of stochastic differential-algebraic equations (SDAEs) of index one that are driven by a scalar Brownian motion. Recently, a class of stiffly accurate stochastic Runge-Kutta (SRK) methods has been proposed for the strong numerical solution. These SRK methods turned out to attain strong order one if they are applied to SDAEs and they are easy to implement. Considering this class of implicit SRK methods, we present some special families of approximation schemes that possess very good stability properties if their mean-square stability is analysed.

References

[1] D. Küpper, A. Kværnø and A. Rößler, *A Runge-Kutta method for index 1 stochastic differential-algebraic equations with scalar noise*, BIT Numerical Mathematics, Vol. 52, No. 2, (2012), pp. 437–455.

An adaptive time stepping method for SDEs

T. Shardlow[a] *and P. Taylor*[b]

[a] University of Bath, United Kingdom

[b] University of Manchester, United Kingdom

We use rough path theory to understand an adaptive time stepping strategy for the pathwise approximation of SDEs.

MS11 – Structure preserving numerical methods

Organized by: Colin Cotter and Onno Bokhove

Compatible Space-Time Finite Element Discretizations for Wave Tanks

O. Bokhove[a], *E. Gagarina*[b] *and J. van der Vegt*[b]

[a] University of Leeds, United Kingdom

[b] University of Twente, Netherlands

The numerical modeling of nonlinear waves is often adequately done using conservative, Hamiltonian fluid dynamics, even in the presence of some forcing and damping. For two laboratory experiments such a non-autonomous Hamiltonian/variational framework is relevant: a) maritime engineering tests investigating rogue wave formation, also in model wave tanks, and b) wave-sloshing validations in a table-top Hele-Shaw cell with breaking waves. Wave-makers and linear momentum damping make these otherwise autonomous systems non-autonomous. We developed a compatible time-discontinuous Galerkin finite element discretization of geometric/variational dynamics. These discretizations are based on using a non-conservative product flux for the classical p dq/dt-term in the canonical variational principle. The challenge of finding compatible schemes for certain (forced/damped) fluid systems in space and time will also be highlighted.

Analysis of Compatible Discrete Operator Schemes for Stokes problem on Polyhedral Meshes

J. Bonelle[a] *and A. Ern*[b]

[a] EDF R&D - CERMICS, École des Ponts Paris Tech, France

[b] CERMICS, École des Ponts Paris Tech, France

Compatible Discrete Operator (CDO) schemes belong to the class of compatible (or mimetic, or structure-preserving) schemes. Their aim is to preserve key structural properties of the underlying PDE. This is achieved by distinguishing topological laws and constitutive relations. CDO schemes are formulated using discrete differential operators for the topological laws and discrete Hodge operators for the constitutive relations.
CDO schemes have been recently analyzed in [1] for elliptic problems. We first review the main results in this case. Design properties for discrete Hodge operators leading to stability and P_0-consistency are identified. We also highlight links between CDO schemes and existing schemes in the litterature [2, 3].
Then, we derive CDO schemes for Stokes flows that are closely related to the recent work of Kreeft and Gerritsma [4]. Finally, we present numerical results on 3D test cases.

References

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Mimetic Finite Element methods applied to the Shallow Water Equations

A. McRae and C. Cotter

Imperial College London, United Kingdom

In the context of weather forecasting, the evolution of the ocean and atmosphere is governed by the Navier-Stokes equations. The shallow water equations are a simplification of the full equations that are relevant for atmosphere/ocean modelling. The analytic shallow water equations conserve several physically meaningful quantities, such as the total energy and entropy within the system. In this talk, I will present a discretisation of the shallow water equations, based on mimetic finite elements, which reproduces many of the same conservation properties. This is achieved through using distinguished choices of function spaces. The function spaces are linked by differential operators, which allows some operations to be represented exactly. This leads to discrete equivalents of identities such as 'div-curl = 0' and 'curl-grad = 0', which turn out to be fundamental in proving the discrete conservation properties.

Structure-preserving discretization of continuum theories

D. Pavlov[a], *M. Desbrun*[b], *E. Gawlik*[c], *P. Mullen*[b] *and J. Marsden*[b]

[a] Imperial College London, United Kingdom

[b] California Institute of Technology, United States

[c] Stanford University, United States

In this talk I will describe several discrete models of infinite dimensional systems which preserve underlying geometric structures. This work started with development of the first variational integrator for Euler fluids. Since then, our methods have been developed further and are now applicable to a great variety of infinite-dimensional systems, such as magnetohydrodynamics or complex fluids. I will discuss our new approach to

discretization based on ideas of noncommutative geometry. One of the goals of this work is creating a new model of discrete differential geometry that leads to a structure preserving discretization of general relativity.

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MS12 – Geometric and Algebraic Methods for Differential Equations

Organized by: Brynjulf Owren

B-series - 50 years and still young

H.Z. Munthe-Kaas

University of Bergen, Norway

In 1963 three remarkable papers were published in three different mathematical disciplines. We all know John Butcher's celebrated paper on coefficients for the study of Runce-Kutta methods, initiating the theory of B-series and their applications in numerical analysis. The same year E.B. Vinberg approached the same mathematical structure from a differential geometric point of view, studying flat and torsion free connections on a manifold. In the very same year M. Gerstenhaber approached the subject from a third route, via algebraic homology theory. In this talk we will see that after 50 years, B-series is still a very active area of research. We will present some very new unpublished results, and may touch upon both connections on manifolds and homologic algebra. Indeed, B-series is an important mathematical tool with possible applications beyond numerical analysis.

Which methods have a B–Series expansion?

O. Verdier[a] *and H. Munthe-Kaas*[b]

[a] Umeå University, Sweden

[b] University of Bergen, Norway

Runge–Kutta methods are *affine equivariant* (they are compatible with affine variable transformations), and *local* (they depend only on an infinitesimal neighbourhood of every point). The same holds for B-Series in general. We address the following question:

are B–Series the only affine equivariant and local methods?

The answer turns out to be true in one dimension, and *false* in more dimensions.
The methods which are affine equivariant and local, however, *almost* have a B–Series expansion. This observation leads to a new family of methods, which contains Runge–Kutta methods. Those methods have advantages over Runge–Kutta methods: for instance, they can potentially be volume preserving, whereas B–Series are known not to be.
We will explain what Runge–Kutta methods, B–Series, equivariance and locality mean in detail, so no prerequisite is required to attend the talk.

Algebraic structures related to stochastic differential equations

K. Ebrahimi-Fard[a], *C. Curry*[b], *S.J.A. Malham*[b] *and A. Wiese*[b]

[a] Instituto de Ciencias Matemáticas - ICMAT, Madrid, Spain

[b] Heriot-Watt University, Edinburgh, Reino Unido

In this talk we report on recent work exploring algebraic structures related to stochastic differential equations. This comprises in particular the notion of quasi-shuffle products in the context of the algebra of semimartingales.

Approximation of Hamiltonian systems using a variational approach

S. Amat[a], *M.J. Legaz*[a] *and P. Pedregal*[b]

[a] Universidad Politécnica de Cartagena, Spain

[b] Universidad de Castilla-La Mancha, Spain

Hamiltonian systems are related with numerous areas of mathematics and have a lot of application branches, such as classical and quantum mechanics, statistics, optical, astronomy, molecular dynamics, plasma physics, etc. In general, the integration of these systems needs the use of geometric integrators. In this talk, we introduce a new variational approach for models which are formulated naturally as conservative systems of ODEs, most importantly Hamiltonian systems. Our variational method for Hamiltonian systems, which is proposed here, is in some sense symplectic and energy preserving. We analyze the new approach both theoretically and numerically.

Volume preserving numerical methods and generating forms

A. Zanna, *H. Xue and O. Verdier*

Department of Mathematics, University of Bergen, Norway

In this talk, we consider the problem of constructing volume-preserving maps (ultimately, numerical integrators) for divergence-free differential equations. We study the problem using the technique of differential forms and generating functions (generating forms), paying particular attention to the simplest nontrivial case that differs from the symplectic case, i.e. $n = 3$. We propose a classification other than that of [1], who classified the generating equations, compatibility conditions and twist condition for volume forms. From our classification, we identify classes of generating forms that have a closed-form solution. Connections are made to the theory of discrete Lagrangians [2], and we identify a new type of generating equations that are not known in the context of symplectic maps.

References

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Preserving first integrals with symmetric Lie group methods

E. Celledoni, B. Owren and H. Marthinsen

Norwegian University of Science and Technology, Norway

We give a short introduction to Lie group methods. A selection of applications of Lie group integrators are discussed. Finally, the notion of discrete gradient methods is generalised to Lie groups, integrators on cotangent bundles of Lie groups are also discussed. This work is based on two recent papers in collaboration with Håkon Marthinsen and Brynjulf Owren.

References

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Integral preserving methods on moving grids

B. Owren and S. Eidnes

Norwegian University of Science and Technology, Norway

Integral preserving schemes for ODEs can be derived by means of for instance discrete gradient methods. For PDEs, one may first discretize in space by e.g. finite differences and then apply an integral preserving method for the corresponding ODEs. For PDEs discretized on moving grids, the situation is more complicated, it is not even clear exactly what we mean by an integral preserving scheme in this setting. In this talk we propose a definition and then we derive a way to preserve integrals according to this definition. We show numerical examples for the KDV and BBM partial differential equations.

Recent results on Kahan's method

R. Quispel

La Trobe University, Australia

We present some recent results on the method of Kahan.

MS13 – Discontinuous dynamical systems: theory and numerical methods

Organized by: Luciano Lopez and Cinzia Elia

A novel method to compute Lyapunov exponents of switched linear systems (I)

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For a given finite set of matrices $\mathcal{G} = \{C_1, \ldots, C_m\}$, where $C_i \in \mathbb{R}^{d,d}$, $i = 1, \ldots, m$, we consider the switched linear system of ODEs $\dot{x}(t) = C(u(t))x(t),\ x(0) = x_0$, where $x(t) \in \mathbb{R}^d$, $u : \mathbb{R} \longrightarrow \{1, \ldots, m\}$ is a piecewise constant control function and $C(i) = C_i$.
We propose a novel method for the approximation of the upper Lyapunov exponent and, under suitable assumptions, of the lower Lyapunov exponent which is based on the computation of the joint spectral radius and lower spectral radius of a sequence of discretized systems obtained by forcing the switching instants to be multiple of $\Delta^{(k)}t$, where $\Delta^{(k)}t \to 0$ as $k \to \infty$.
In the first talk we shall give general ideas to bound the Lyapunov exponents. In the second talk we shall provide details about the approximation of the joint (lower) spectral radius.

A novel method to compute Lyapunov exponents of switched linear systems (II)

M. Zennaro[a] *and N. Guglielmi*[b]

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Optimal adaptive approximation of a class of non-autonomous IVPs with unknown singularities

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The numerical solution of singular initial-value problems in ODEs leads to many interesting theoretical questions. For example, there arise problem of finding strict bounds on error and information cost for algorithms that solve such problems. Optimality of used algorithms is also of interest. We present recent theoretical results concerning the solution of a class of scalar non-autonomous equations with separated variables and unknown singularities. In the case when the right-hand side function has two singularities (which leads to four unknown 'events' in the two-dimensional space), we show the construction of an algorithm that automatically takes care of the singularities. It adaptively modifies the mesh points to preserve the optimal error known for the regular case. Lower bounds in the case of more than two singularities will also be discussed.

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A Filippov sliding vector field on a codimension 2 surface. Theoretical justifications

C. Elia[a], *L. Dieci*[b] *and L. Lopez*[a]

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[b] Georgia Institute of Technology, United States

We consider sliding motion on a codimension 2 discontinuity surface Σ. We characterize the case of Σ being attractive in finite time upon sliding and we justify, under this assumption, the use of a given Filippov vector field on Σ.

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Runge-Kutta methods for the numerical solution of discontinuous systems of Filipov's type

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In this work we consider the numerical solution of initial value problems of ODEs with discontinuous right-hand side. In particular we are interested in the integration of Filipov's type systems where sliding behaviour on the discontinuity surface is allowed. We show how Runge-Kutta methods can be adapted to the solution of this class of problems, with the minimum information about the problem provided by the user. Some numerical experiments using the well known DOPRI5(4) scheme are presented.

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Numerical solution of fractional differential equations with discontinuous right–hand side

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Recently, a growing interest has been shown in the study of fractional differential equations (FDEs) with discontinuous right–hand side and their applications in sliding mode control.
This talk concerns with the numerical solution of discontinuous FDEs; after studying, for some test problems, the finite–time convergence of the true solution on the sliding surface, we describe two methods for FDEs obtained by generalizing, in different ways, the classical implicit Euler method.
An interesting result allows to show that different methods derived from the same implicit Euler method behave in a different way when applied to discontinuous problems and just the method devised in the framework of the *fractional linear multistep methods* inherit the chattering–free character of the original method [1]. We focus the attention on this method, which allows finite–time stabilization on the sliding surface, study its main properties and present test problems.

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One-sided numerical methods to locate event points in discontinuous ODEs

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We present a numerical approach to treat discontinuous differential systems of ODEs of the type: $x' = f_1(x)$ when $h(x) < 0$ and $x' = f_2(x)$ when $h(x) > 0$, and with $f_1 \neq f_2$ for $x \in \Sigma$, where $\Sigma := \{x : \ h(x) = 0\}$ is a smooth co-dimension one discontinuity surface. Often, f_1 (f_2) cannot be evaluated when $h(x) > 0$ ($h(x) < 0$) and for this reason, we consider numerical schemes which do not require f_1 above Σ (respectively, f_2 below Σ). The use of explicit schemes allows us to avoid the evaluation of the numerical solution in the forbidden region (see [1, 2]) but can produce oscillations of the numerical solution around the event point on the discontinuity surface. A penalty technique, for the stepsize, can produce a sequence of numerical solutions which approach Σ from one-side only.
We remark that in this talk we restrict attention only to accurately locate the event point where a trajectory reaches Σ.

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MS14 – Efficient computation of matrix functions for exponential and trigonometric integrators

Organized by: Volker Grimm

Rational L_∞ approximations to the matrix cosine

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In applications, many processes are described by second order differential equations and the exact solution for these equations is given in terms of the matrix functions sine and cosine. Among the most competitive algorithms for computing these functions are Padé approximations [1]. Here we focus on two classes of matrices, positive and Hermitian. We present intervals of applications for rational L_∞ approximations of various degrees and tolerances for these types of matrices in the lines of [2].

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A Parallel Rational Krylov Subspace Method for the Approximation of φ-Functions in Exponential Integrators

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The efficient approximation of the matrix φ-functions is an important task in the application of exponential integrators. Recent advances have shown that rational Krylov methods have a great advantage over standard Krylov methods for large matrices A with a huge field-of-values in the left complex half-plane.

We consider the approximation of $\varphi(A)v$ in the space

$$\text{span}\left\{(z_{-m}I - A)^{-1}v, \ldots, (z_mI - A)^{-1}v\right\}$$

with equidistant poles on the line $\text{Re}(z) = \gamma > 0$. It is possible to solve the occurring linear systems in parallel by using a suitable parallel implementation. In this way, we achieve a significant speed-up compared to a serial implementation.
We present error bounds that predict a uniform convergence. This is a fundamental property for the successful application of this parallel rational Krylov method in exponential integrators. The advantages and efficiency of our method are illustrated by several numerical experiments.

Recent advances of Leja interpolation

P. Kandolf[a], *M. Caliari*[b], *A. Ostermann*[a] *and S. Rainer*[a]

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[b] Università di Verona, Italy

Exponential integrators require a reliable and efficient implementation of the action of the matrix exponential and related φ functions. In this work we consider the Leja method for performing this task. We give an overview on recent developments with a closer look on a new a posteriori error estimate. A numerical comparison of a revised implementation to other methods from the literature is presented.
For the new error estimate we define the notion of a residual based estimate where the residual is obtained from differential equations defining the φ functions. For the numerical investigation of the newly defined error estimate as well as the comparison of the Leja interpolation we rely on test examples from spatial discretizations of time dependent partial differential equations. The experiments show that our new error estimate is robust and that the Leja interpolation performs very well in comparison to other methods.

A moment-matching Arnoldi method for phi-functions

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We consider a new Krylov subspace algorithm for computing expressions of the form $\sum_{k=0}^{p} h^k \varphi_k(hA)w_k$, where $A \in \mathbb{R}^{n\times n}$, $w_k \in \mathbb{R}^n$, and φ_k are matrix functions related to the exponential function. Computational problems of this form appear when applying exponential integrators to large dimensional ODEs in semilinear form $u'(t) = Au(t) + g(u(t))$. Using Cauchy's integral formula we give a representation for the error of the approximation and derive a priori error bounds which describe well the convergence behaviour of the algorithm. In addition an efficient a posteriori estimate is derived. Numerical experiments in MATLAB illustrating the convergence behaviour are given.

MS15 – Multiscale modelling: numerical methods and applications

Organized by: Konstantinos Zygalakis and Assyr Abdulle

Multiscale image based modelling of two phase flow in soil

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Processes governing fluid flow in soil and the water uptake by plant roots are inherently multiscale. The internal pore structure of soil aggregates and the wider pore space between them contribute to the global behaviour of soils. Using homogenization we approximate the effects of soil structure on the global flow properties by considering three scales. The behaviour of the soil aggregate is determined by considering a sub sample of the aggregate structure and a representative boundary region. This allows an aggregate scale hydraulic conductivity and a set of boundary conditions to be determined. A second level of averaging allows the macroscopic behaviour of a collection of aggregates to be obtained. Application of this process to X-ray CT images of real soil allows us to answer fundamental questions regarding the interaction of roots in soil and feeds back into the resolution driven imaging of soils by providing a lower limit to the scale of features which affect flow properties.

Multiscale Problems in Fluctuating Hydrodynamics

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Thermal fluctuations have been incorporated into the classical equations of fluid dynamics, however, the resulting systems of stochastic PDEs are very difficult to handle. I will focus on the problem of diffusive mixing of fluids, and demonstrate that accounting for the spectrum of the thermal velocity fluctuations is crucial in simulating even the simplest diffusive processes in realistic liquids. Comparisons between hard-particle molecular dynamics and fluctuating hydrodynamics finite-volume solvers show a good agreement. Due to extreme time scale separation between mass and momentum diffusion (a factor of 400 in water, for example), even finite-volume simulations become impractical. It is therefore necessary to use a seamless multiscale method to reduce the stiffness, or to directly model the limiting dynamics obtained from adiabatic mode elimination. I will describe and compare these approaches both analytically and numerically.

Optimal control of multiscale systems: an approach using logarithmic transformations

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Computing optimal controls of multiscale systems is often prohibitive, especially in high dimensions. A way out is to replace the equations of motion by reduced-order models that do not contain the microscales and which can be obtained by, e.g., homogenisation or averaging. But even though the reduced model may be a good approximation if the controls are known, the question is whether one can also compute an optimal control from it that approximates the optimal control of the original system. In most cases the answer is no, but for a certain class of multiscale diffusions this questions can be answered in the affirmative. The talk will be about this particular class of stochastic control problems that are linear quadratic in the control (though nonlinear in the states) and can be transformed to a control-free problem by a logarithmic transformation. We give a theoretical foundation of the method and discuss several numerical examples and applications.

A MsFEM approach à la Crouzeix-Raviart for problems on perforated domains

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The Multiscale Finite Element Method (MsFEM) is a Finite Element type approximation method for multiscale PDEs, where the basis functions used to generate the approximation space are specifically adapted to the problem at hand. Many ways to define these basis functions have been proposed. Here, we introduce and analyze a specific MsFEM variant, in the spirit of Crouzeix-Raviart elements, where the continuity of the solution accross the mesh edges is enforced only in a weak sense [1, 2].
Our motivation stems from our wish to address multiscale problems for which implementing flexible boundary conditions on mesh elements is of particular interest. A prototypical situation is that of perforated media, where the accuracy of the numerical solution is generically very sensitive to the choice of values of the basis functions on the boundaries of elements. The Crouzeix-Raviart type elements we construct then provide an advantageous flexibility, as shown by our numerical results.

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Weak second order mean-square stable integrators for stiff stochastic differential equations

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We present two families of integrators for stiff Itô stochastic differential equations which exhibit simultaneously favourable mean-square stability properties and weak second order of accuracy. The first integrators are implicit with respect to the drift function and are shown to be mean-square A-stable for the usual complex scalar linear test problem with multiplicative noise. The second integrators are fully explicit and still have extended mean-square stability domains. These constructions inspired the design of a "swiss-knife" integrator for stiff diffusion-advection-reaction problems with noise.

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Numerical studies of homogenization under a fast cellular flow

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We discuss the problem of a particle diffusing in the presence of a fast two dimensional cellular flow in a finite domain. If the flow amplitude A is held fixed and the number of cells L^2 goes to infinity, then the problem homogenizes, while if L is held fixed and A goes to infinity the solution averages along stream lines. More interesting is the case of the double limit when both L and A go to infinity, and this is the limit in which we focus here. In particular, in the first part of the talk we review some well-known results related to homogenization for Stochastic Differential Equations (SDEs) and discuss different approaches for calculating the effective diffusion matrix. We then describe the construction of numerical integrators used in our numerical investigations and finish the talk by presenting some numerical results for the double limit, focusing on the sharp transition between the homogenization and the averaging regimes when $A = L^4$.

MS16 – DAEs and PDAEs: Analytical aspects, numerics and applications

Organized by: Ricardo Riaza and Caren Tischendorf

Functional-analytic aspects of DAEs

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The great progress of the theory of PDEs during the twentieth century, both the analytical and the numerical parts, are unthinkable without the achievements and contributions of the functional analysis emerging at that time. In contrast, so far, the impact of functional-analytic ideas in the theory of DAEs is weak. The field of DAEs is widely dominated by standard ODE tools and geometric approaches. The functional-analytic character of DAEs is hardly developed so far; by now, an adequate sophisticated characterization has not been accomplished. What's more, one might find seemingly conflicting assertions.
We consider operators associated with linear and nonlinear DAEs acting in various Banach and Hilbert spaces. We ask for settings such that the DAE operator becomes bounded or closed with dense domain. Then we investigate whether a DAE operator has a closed range and whether it is a Fredholm operator. Furthermore, we discuss consequences for the approximate solution.

Convergence issues of DAEs with non-constant constraints

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Two of the best known DAE solver packages are DASSL and RADAU. While RADAU is based on the Radau IIA method, DASSL uses BDF-methods to solve a DAE. The BDF-methods as well as the Radau IIA method may fail to provide a convergent numerical solution for linear DAEs with time depending constraints. In particular these methods do not converge if applied to the following well known example:

$$\begin{aligned} x_1' + \eta t x_2' + (1+\eta) x_2 &= 0, \\ x_1 + \eta t x_2 &= e^{-t}, \end{aligned}$$

with $\eta < -0.5$, [1]. While other prominent methods like Lobatto IIIA share the same convergence problem we present a class of discontinuous collocation methods which overcomes this weakness.

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Characterizing DAE circuit models via mixed determinantal expansions

I. García de la Vega and R. Riaza

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An index characterization is essential to make a correct numerical treatment of any kind of DAE and, in particular, of DAE-based circuit models. Beyond the passive setting, an index characterization has been achieved for nodal models by performing a Maxwell-type determinantal expansion of the nodal admittance matrix. Nevertheless, this characterization precludes current-controlled resistors and topological degeneracies. Overcoming these restrictions entails studying matrices with a more complex structure: in this communication we enlarge the scope of former results by extending Maxwell's determinantal expansions to these so-called *mixed* matrices. As a byproduct, we address other related problems in circuit theory.
Research supported by Project MTM2010-15102 of Ministerio de Ciencia e Innovación, Spain, and by SisDAC Research Group and Depto. de Matemática Aplicada a las Tecnologías de la Información, ETSI Telecomunicación, Universidad Politécnica de Madrid.

Collocation for Singular BVPs in ODEs with Unsmooth Data

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We deal with BVPs for systems of ODEs with singularities. Typically, such problems have the form

$$z'(t) = \frac{M(t)}{t} z(t) + f(t, z(t)), \;\; t \in (0, 1], \quad B_0 z(0) + B_1 z(1) = \beta,$$

where B_0 and B_1 are constant matrices which are subject to certain restrictions for a well-posed problem. Here, we focus on the linear case where the function f is unsmooth, $f(t) = g(t)/t$. We first deal with the analytical properties of the problem – existence and uniqueness of smooth solutions.
To solve the problem numerically, we apply polynomial collocation and for the linear IVPs, we are able to provide the convergence analysis. It turns out that the collocation retains its high order even in case of singularities, provided that the analytical solution is sufficiently smooth. We illustrate the theory by numerical experiments; the related tests were carried out using the MATLAB code `sbvp` [1].

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Projection techniques for higher index DAEs revisited

M. Arnold

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The numerically stable time integration of higher index DAEs is based on analytical transformations before time discretization. It is well known that this *index reduction* may result in the drift-off effect that characterizes the numerically observed violation of the original constraints of the higher index problem. Projection steps are a standard technique to avoid the drift-off effect in the numerical solution without deteriorating the order of convergence.
The combination of direct time discretization of higher index DAEs and projection steps may, however, result in order reduction. This undesired behaviour will be studied for an index-3 Lie group integrator for constrained mechanical systems that suffers from order reduction and spurious oscillations in a transient phase after each projection step. Furthermore, we discuss how to avoid this order reduction and the spurious oscillations by a systematic perturbation of starting values.

Diagnosis of Singular Points of DAEs

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At a singular point of a DAE, the IVP fails to have a unique solution. All results concerning the existence and uniqueness of the IVP trace back to the Picard-Lindelöf-Theorem, whereas for DAEs the implicit function theorem is used. Proven results are given for so-called regularity-regions, that can be characterized considering linearized problems.

Automatic (or Algorithmic) Differentiation (AD) opens new possibilities to realize an analysis of DAEs and to monitor the assumptions of regularity regions. We present how the index determination, the computation of consistent initial values, and the diagnosis of singular points can be reliably undertaken for DAEs up to index three. The approach uses the projector based analysis for DAEs employing AD. Different approaches are considered and illustrated by some examples, with particular emphasis on electrical circuits containing controlled sources.

A different look at DAEs

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By examining an error functional associated in a natural way with a given DAE, we propose to design some simple and flexible numerical schemes to approximate the solutions. We will show various explicit examples of the performance of the method. In addition, we would also like to examine what consequences of a more analytical nature one can derive through this approach. This perspective has already been explored for regular ODEs, so that this contribution is an attempt to extend those ideas for DAEs.

MS17 – Numerical approximation of nonlinear waves

Organized by: Angel Durán and Vassilios Dougalis

Theory and numerical analysis of systems of KdV-equations

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Systems of nonlinear dispersive wave equations arise in various physical contexts. Some of these have been shown to provide reasonably good models of real phenomena. This lecture will review recent work in this area focused upon a paradigm problem. We will see that systems can throw up a larger variety of phenomena than do the associated single equations.

Fast and accurate computation of solitary waves to the free surface Euler equations

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Among different kinds of special solutions, solitary waves play the central role in the nonlinear science. These solutions are very common in optics, plasma physics, but also in the hydrodynamics. In the present study we propose a fast and accurate numerical method to compute solitary wave solutions to the free surface Euler equations. It is based on the conformal mapping technique combined with an efficient Fourier-type pseudo-spectral method. The resulting nonlinear equation is solved using the Petviashvili iterative scheme. Our computational results are finally compared to some existing approaches such as the Tanaka method and the high order asymptotic expansion of Longuet-Higgins & Fenton (1974).

Error estimates for Galerkin-Finite element methods for the shallow water equations

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We analyze the standard Galerkin-finite element method for a simple initial-and boundary-value problem for the Shallow Water equations and their symmetric version in one space dimension. We prove error estimates for the semidiscrete problems for uniform and quasiuniform meshes, and also for their temporal discretization by the Shu-Osher third order RK method. We also discuss other types of boundary conditions and present results of relevant numerical experiments.

Numerical dynamic detection, generation and simulation of solitary waves for nonlinear wave equations

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There exist different techniques in the literature to obtain numerically solitary waves of nonlinear wave equations. In this work, we focus on the one known as iterative cleaning [3, 4]. It is based on numerical simulations of initial conditions that evolve with time into a single main pulse or train of pulses along with dispersive tails, and uses cleaning techniques in order to obtain a numerical approximation of a solitary wave. The main disadvantage of this method is that it is used in a specific way for each numerical experiment, determining in a manual way suitable times and regions for the cleaning of the numerical solution, which implies a lot of work.
As an alternative, we propose a completely automatic algorithm that detects and generates solitary waves in an efficient and dynamic way [2]. It is based on a cleaning technique [1] and an efficient integration of the problem that checks symmetry conditions and the preservation of the velocity of the wave.

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Instability of the split-step and related methods near localized solutions of nonlinear Schrödinger equations

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The split-step method (SSM) is widely used for numerical solution of nonlinear evolution equations, e.g., the generalized NLS:

$$iu_t + u_{xx} + (V(x) + 2|u|^2)u = 0.$$

We will show how SSM's instability is analyzed using a modified linearized NLS for a high-wavenumber numerical error. For example, for the SSM which uses the finite-difference solution of its dispersive step, this modified linearized NLS is:

$$i\psi_t + \delta\psi - \alpha\psi_{\chi\chi} + V(\epsilon\chi)\psi + 2|u_{\rm sol}(\epsilon\chi)|^2(2\psi + \psi^*) = 0,$$

where ψ is proportional to the numerical error. We will show how the instability differs for a stationary, moving, and oscillating background pulse.
We will also highlight differences between instabilities of the finite-difference and Fourier implementations of the SSM, and then discuss how these results can be used to predict the instability of the integrating factor and exponential time differencing methods.

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On the derivation of energy-preserving H^1-Galerkin schemes for Hamiltonian partial differential equations

Y. Miyatake and T. Matsuo

University of Tokyo, Japan

In this talk, we propose an energy-preserving finite element method for Hamiltonian PDEs. As is well known, energy-preserving integrators often give qualitatively nice solutions, and on the other hand, H^1-formulations are generally preferred in the finite element discretizations from the practical point of view.

A difficulty arises in the attempt of combining these two concepts, when the structure of the equation is complicated. For example, for the equation which has higher order derivatives, we usually consider a mixed formulation so that the equation can be formulated in H^1 space. However, this generally destroys the structure of the equation.
Our method successfully solves such a difficulty, and is applicable to not only a wide variety of Hamiltonian PDEs but also dissipative PDEs. We can adopt the discrete gradient method for finding fully discrete schemes. The new method can be combined also with symplectic time discretizations.

Long wave models and pressure evaluation for surface waves on shear flows

H. Kalisch and A. Ali

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The effect of background vorticity on the pressure beneath steady long gravity waves at the surface of a fluid is investigated. In particular, we derive a model equation and a formula for the pressure in a flow with constant vorticity. The model equation was previously found by Benjamin [2], and is given in terms of the vorticity ω_0, and three parameters Q, R and S representing the mass flux, total head and momentum flux, respectively.
The focus of this work is on the reconstruction of the pressure from solutions of the model equation and the behavior of the surface wave profiles and the pressure distribution as the strength of the vorticity changes. In particular, it is shown that strong enough vorticity can lead to non-monotone pressure profiles under the wave. As already indicated in [4], it is also possible for the fluid pressure near the wavecrest to be below atmospheric pressure.

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On some systems for internal wave propagation

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We consider a system of Benjamin-Ono type for the propagation of internal waves over a horizontal bottom and a rigid lid. First we study the existence of solitary waves by numerical means while in a special case we present analytical formulas of solitary waves that decay with a polynomial order. An efficient numerical method for the integration of the specific system will be introduced and checked with several experiments, including solitary-wave interactions and stability. Some comparisons with the classical Benjamin-Ono equation will also be made.

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MS18 – Mathematical Models and Numerical Methods for Image Processing

Organized by: Eduardo Cuesta

Denoising an image by denoising its curvature image

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In this talk we argue that when an image is corrupted by additive noise, its curvature image is less affected by it, i.e. the PSNR of the curvature image is larger. We speculate that, given a denoising method, we may obtain better results by applying it to the curvature image and then reconstructing from it a clean image, rather than denoising the original image directly. Numerical experiments confirm this for several PDE-based and patch-based denoising algorithms.

A nonconvex model for image segmentation

B. Coll, J. Duran and C. Sbert

Department of Mathematics and Computer Science, University of Balearic Islands, Spain

In this paper, we study the problem of unsupervised segmentation through the minimization of energies composed of a quadratic data-fidelity term and a nonconvex regularization term. Since probably the greatest amount of information in an image is contained in the edges of the objects, we give some conditions for the design of an edge-preserving regularization. We show that, under those edge-preserving conditions, the functional can be rewritten in a dual formulation as a weighted total variation and thus, Chambolle's projection algorithm applies. This leads to design an efficient algorithm based on alternate minimizations on the two variables. Experimental results are presented and show the effectiveness and the efficiency of the proposed algorithm.

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Image processing and non–local continuous models

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In this talk non-local PDE's models of Volterra type [1]

$$\mathbf{u}(t) = \mathbf{u}_0 + \int_0^t \mathbf{K}(t-s)A\mathbf{u}(t)ds, \quad t \geq 0, \tag{1}$$

are considered in the context of image processing. In (1) $\mathbf{u}_0$ stands for the original image vector–arranged, $\mathbf{u}(t)$ stands for the evolved $\mathbf{u}_0$ at time stage t, A is a linear operator (typically a discrete 2D-Laplacian), and $\mathbf{K}(t)$ is a convenient convolution kernel.
The models (1) are linear, and well-posedness and stability are guaranteed under very general conditions on $\mathbf{K}(t)$. The talk will discuss the adaptation of (1) to image processing problems. It will focus on scale–space properties, the preservation of relevant quantities, and the comparison with local nonlinear PDE–based models recently proposed in the literature [2].

Acknowledgement: The authors have been supported by MICINN project MTM2010-19510/MTM.

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A basic diffusion model on Grassmannians for simultaneous Detection, Segmentation and Restoration in Video mini-sequences

J. Finat, E. Cuesta, A. Duran, A. Hurtado and R. Martinez

MoBiVAP Research Group at University of Valladolid, Spain

Noise and aliasing are two very common problems in Image Processing [2]. Both of them are irregularly distributed and very often their local behavior follows different patterns. To minimize adverse effects of noise and aliasing, it is necessary to recover well defined regions without degrading boundaries. First issue concerns to global aspects of image segmentation related to minimization of convex functionals having in account an adaptive behavior in terms of anisotropic diffusion. Second issue involves to the preservation of true edges (very often degraded or missing) in terms of regularization operators. In this work we develop an approach based in the use of grassmannians [1] which involves to a multivector representation of meaningful data (which are represented as points of a grassmannian) and their tracking along a mini-video sequence in terms of shifted means to identify tangent space to the grassmannian in order to have a robust initialization (Lipschitz).

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Second-order Riemannian Active Contours for Image Segmentation

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[a] Universidad Politécnica de Madrid, Spain

[b] Universidad Complutense de Madrid, Spain

This work aims at providing algorithms for geodesic active contours optimization based on second-order approximations of functionals. In contrast to the standard approach based on gradient schemes, that define a time-continuous curve evolution that must be discretized, we propose algorithms that are intrinsically time-discrete. To this purpose, we obtain the second-order approximation of the Riemannian curve energy and length and show how the extrema of these approximations can be characterized by means of linear second order differential equations. Moreover, we prove that the solution of the equations for the length functional is given by a simple closed-form expression, while the damped case requires the solution of a second-order ordinary differential equation that can be considered as a generalization of the classical equation defining the Jacobi fields along the curve.

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Discrete gradient methods in image processing

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[b] La Trobe University, Australia

In PDE-based image diffusion, gradient systems are widely used to denoise, regularise, and, in general, to enhance images. For these applications, preservation of the gradient structure in the discretisation is much more important than, for example, higher order of the integration scheme. We will discuss some results, that indicate, that discrete gradient methods can outperform standard methods in these applications.

Some Nonlinear Diffusions inspired by the Perona-Malik equation

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[b] Yale School of Medicine, United States

[c] University of Southern Mississippi, United States

Two regularizations of the Perona-Malik equation will be described which allow for some mathematical analysis and for implementations which exhibit some desirable properties. Mathematical and experimental results will be discussed.

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MS19 – Recent advances on parareal algorithms

Organized by: Frédéric Legoll and Yvon Maday

Introduction to the minisymposium and to the parallelisation in time algorithms

Y. Maday

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In the same spirit as the domain decomposition methods in space, time domain decomposition methods are based on a decomposition of the time interval, and then each solution trajectory is solved simultaneously in all the time subintervals using an iteration on the initial condition over each subinterval. The parareal algorithm proposed in 2001 by Lions, Maday and Turinici allowed to highlight the interest in the parallelisation in this direction. There are now several successful implementations together with convergence results that illustrate the interest of the parallelization in time is for problems when very many processors are available. The speedup — even though not so impressive than with parallelization in space for the plain approach — allows to reach real time leading to the name parareal (parallel in real time) of the new algorithm from 2001.

Now the method is more mature, it appears better like a large framework that allows to propose new ideas working on different aspects of the different ingredients of the method. This symposium will allow to first present the frame of the parareal approach and then illustrate its application on very large problems together with attempts to cure some problems of the original algorithms and also how to combine those iterations with others in order to achieve the plain speedup available by the given number of processors.

A study of parareal applications to advanced operation scenario simulations of fusion plasma

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Operation scenario simulations play a significant role in the construction as well as operation of fusion experiments. This work explores the applicability of the Parareal algorithm [1] to such simulations, using the CORSICA [2, 3] code as a test case. CORSICA is an advanced free-boundary equilibrium and transport simulation code used to study scenarios in burning plasma experiments. The "Parareal Framework" developed at ORNL has been used for the implementation. In the past the algorithm has been applied to multiple problems including fully developed plasma turbulence [5]. CORSICA introduces new challenges. These are quasi steady states with

intermittent events resulting from MHD activity, pellet injection or an introduction of ELMs. The algorithm involves a predictor-corrector technique. This work studies the extent of the crudeness of the coarse solver when applying the algorithm. Its successful implementation makes time efficient simulations of ITER-like plasmas more tractable.

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An adjoint approach for stabilizing the parareal method for hyperbolic problems

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[b] Universite Pierre et Marie Curie, France

[c] EPF Lausanne, Switzerland

The parareal method provides opportunities for achieving higher efficiency in parallel computing. However, it is known to be unstable for hyperbolic problems, which play an important role in large scale and long time simulations of wave phenomenon. Specifically, when the coarse resolution is not fine enough, the solution blows up during intermediate iterations. It is challenging to stabilize the parareal method for hyperbolic problems with unrestricted coarse step size. The main reason for the instability is that condition numbers of underlying propagation matrices become too large so that the coarse solver fails in precondition. Motivated by this, we incorporate the adjoint problem into better iterative strategies like the conjugate gradient method, so that the A-norm errors strictly decrease in terms of iterations. Details of the new approach, as well as numerical results of first- and second-order wave equations and the Burgers' equation, will be presented.

Parallel-in-time integrators for Hamiltonian systems

F. Legoll, X. Dai, C. LeBris and Y. Maday

CERMICS, École des Ponts Paris Tech, France

In this talk, we will describe some recent advances for the integration of Hamiltonian systems using parareal-type algorithms. In this specific context, structure-preserving algorithms are preferably employed, because they show interesting numerical properties, in particular excellent preservation of the total energy of the system. We will describe here several structure-preserving variants of the original plain parareal algorithm. Numerical tests on several model systems illustrate the properties of the proposed algorithms over long integration times.

This is joint work with X. Dai (Univ. Paris 6 and Chinese Academy of Sciences), C. Le Bris (ENPC and INRIA) and Y. Maday (Univ. Paris 6 and Brown Univ.).

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An intermediate state method for the time-parallelized solving of optimal control problems

J. Salomon

CEREMADE, Université Paris-Dauphine, France

In this talk, we present a general approach to parallelize efficiently optimal control solvers. This method, first introduced in 2006, is based on the introduction of intermediate states that enables to decompose the original optimality system into similar sub-systems that can be treated independently using standard solvers. We present a recent improving on the method that makes it fully efficient and discuss the role of the solver used in parallel.

A novel, semilagrangian, coarse solver for the parareal technique and its application to 2D drift-wave (BETA) and 5D gyrokinetic (GENE), turbulence simulations

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[c] Max-Planck-Institut fur Plasmaphysik EURATOM-IPP, Garching, Germany

In this work, we apply parareal [1] to convection dominated problems. In particular, to a 2D drift waves case using BETA code and in a 5D gyrokinetic simulation using GENE code. Partial success was previously reported [2] but, here, a new and promissing coarse solver based on semilagrangian time advance is proposed and tested on both kind of simulations. The advantage of the semilagrangian solver is that it can be split into a piece that can run in parallel (the computation of the interpolation coefficients) and a piece that is computed serially (the application of the coefficients over the convected field). The second piece is the time limiting part (due to its sequential character) but can be computed much faster than the fine solver.

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A parareal multiscale coupling of finite element and Lattice Boltzmann methods

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[c] CMCS, Lausanne, Switzerland & MOX, Modeling and Scientific Computing, Milano, Italy

We present a new numerical procedure for the simulation of time-dependent problems based on the coupling between the finite element method and the Lattice Boltzmann method. The two methods are regarded as macroscale and mesoscale solvers, respectively. The procedure is based on the parareal paradigm and allows for a truly multiscale coupling between two numerical methods having optimal efficiency at different space and time scales. The main motivation, among other, is that one technique may be more efficient, or physically more appropriate or less memory consuming than the other depending on the target of the simulation and/or on the sub-region of the computational domain. We detail the theoretical and numerical framework for linear parabolic

equations. We show various numerical examples that will validate the proposed procedure and illustrate its advantages. Finally some recent extensions will be discussed.

A micro-macro parareal algorithm: application to singularly perturbed ordinary differential equations

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[b] CERMICS, École des Ponts, Paris Tech, France

We introduce a micro-macro parareal algorithm for the time-parallel integration of multiscale-in-time systems. The algorithm first computes a cheap, but inaccurate, solution using a coarse propagator (simulating an approximate slow macroscopic model), which is iteratively corrected in parallel using a fine-scale propagator (accurately simulating the full microscopic dynamics). We provide a numerical analysis of the algorithm for a prototypical example of a micro-macro model, namely singularly perturbed ordinary differential equations.

MS20 – Variational Techniques in Structure-Preserving Methods for Partial Differential Equations

Organized by: Takaharu Yaguchi and Christopher J. Budd

Predictor corrector algorithm with the discrete variational derivative method

D. Furihata

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The discrete variational derivative method is a structure-preserving numerical method for partial differential equations. The obtained schemes mimic some variational structures of the original equations, and they inherit the conservation property or dissipation one. Those are nonlinear when the original equations are nonlinear, and this nonlinearity may be a computational difficulty. We have developed the linearization technique to overcome this difficulty, but the obtained linear schemes tend to be unstable. Furthermore, the technique is applicable to only lower order polynomial equations.
In such a situation, we extended the technique to be applicable to nonpolynomial problems. This means that we are able to obtain fast schemes for every equation, but we do not improve the unstable tendency of the obtained schemes. We, therefore, attempt a breakthrough based on the classical predictor–corrector iteration method to avoid this tendency.

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Energy-preserving compact difference schemes for nonlinear wave equations

T. Matsuo

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For the nonlinear wave equations such as the KdV equation, energy-preserving schemes are preferable whenever that is possible, and there are several systematic ways for constructing such schemes. On the other hand, mainly

in numerical fluid dynamics, it is quite common to employ special difference operators, called compact difference operators, which replicate the original dispersion relation as good as possible for better wave propagations. In this talk, we first show that these two techniques can be combined to construct energy-preserving compact difference schemes. Then we point out that such combination becomes quite nontrivial, when we seek for better compact difference schemes with narrow stencils.
This is a joint work with T. Yaguchi and H. Kanazawa.

Collective integrators for point vortex dynamics on the sphere

K. Modin[a], *R. McLachlan*[b] *and O. Verdier*[c]

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[b] Massey University, New Zealand

[c] Umeå University, Sweden

The dynamics of point vortices have a long history, going back to a seminal 1858 paper by Helmholtz. Point vortices occur as special solutions to 2D incompressible fluid equations. On the sphere, point vortices provide important approximations of certain geophysical flows.
In this talk we present efficient Lie-Poisson integrators for point vortices on the sphere. The approach is based on *collective integrators*: a novel technique to construct structure preserving integrators for general Hamiltonian systems on a Lie-Poisson manifold.

Local discontinuous Galerkin methods for Hamiltonian PDEs

Y. Sun[a], *W. Cai*[b] *and W. Tang*[a]

[a] Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China

[b] School of Mathematical Sciences, Nanjing Normal University, China

In this talk, we present the time-space local discontinuous Galerkin methods [1] for Hamiltonian PDEs in the multisymplectic formulation. With the appropriate quadrature formula, the resulting discretizations are equivalent to the multisymplectic partitioned Runge-Kutta methods [2] whose implementation has not been fully understood besides for a class of multisymplectic Hamiltonian systems in special forms [3]. We use the new discretization strategy to simulate the soliton solutions of nonlinear Schrödinger equation, and observe the errors of numerical solutions and the global charge.

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Discretization of Nonholonomic Dynamics

F. Jimenez and J. Scheurle

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Nonholonomic dynamics can be understood in some cases as a set of Differential Algebraic Equations (DAEs). We explore some techniques to discretize these equations and wonder how this discretization can be reinterpreted as a deformation of the continuous dynamics.

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The Construction and Analysis of Variational Integrators

M. Leok and J. Hall

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Variational integrators are geometric integrators that are based on a discrete Hamilton's variational principle. We will review the role of Jacobi's solution of the Hamilton–Jacobi equation in the variational error analysis of variational integrators. Jacobi's solution can be characterized either in terms of a boundary-value problem or variationally, and these lead to shooting-based variational integrators and Galerkin variational integrators, respectively.
Computable discrete Lagrangians can be obtained by choosing a numerical quadrature formula, and either a finite-dimensional function space or an underlying one-step method. We prove that the resulting variational integrator is order-optimal, and when spectral basis elements are used in the Galerkin formulation, one obtains geometrically convergent variational integrators.
We will also discuss generalizations of variational integrators to Lie groups, homogeneous spaces and Lagrangian PDEs.

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An energy-preserving exponentially-fitted continuous stage Runge–Kutta method for Hamiltonian systems

Y. Miyatake and T. Matsuo

University of Tokyo, Japan

Recently, the construction of symplectic exponentially-fitted Runge–Kutta (EFRK) methods for the numerical integration of Hamiltonian systems with periodic or oscillatory solutions have been attracting a lot of interest (see [1, 3], for example). In this talk, from the standpoint of geometric integration, we consider a derivation of energy-preserving exponentially-fitted methods. For this aim, we show sufficient conditions for energy-preservation in terms of the coefficients of continuous stage RK methods (continuous stage RK methods were introduced by Hairer [2]), and extend the theory of EFRK methods to the context of continuous stage RK methods. In this talk, by combining these two theories, we derive second and fourth order energy-preserving exponentially-fitted schemes.

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Variational Integrators and Discrete Lagrangian Mechanics for Interconnected Systems

H. Yoshimura and S. Hanawa

Applied Mechanics and Aerospace Engineering, Waseda University, Japan

It has been focused upon developing stable and efficient numerical integrators for large scale systems such as electric networks and multibody space structures. In particular, it is no doubt that the structure-preserving or variational integrators must be an essential tool for design and analysis of nonconservative as well as conservative interconnected systems, where the interconnection may be given by constraints (see [1, 2]). In this talk, we explore variational integrators for interconnected systems with degenerate Lagrangians, where the degeneracy may induce the primary constraints in the sense of Dirac in addition to holonomic constraints. We show the discrete variational structures for holonomic Lagrangian systems for electric transmission lines by interconnecting modular electric circuits. We also show numerical validity of our theory in comparison with conventional integrators for constrained Lagrangian systems.

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MS21 – Modelling and numerical methods in financial mathematics

Organized by: Carlos Vázquez

Numerical approaches for the evaluation of derivative securities

M. Breton

GERAD and HEC Montréal, Canada

The evaluation of financial derivatives or of regulatory adjustments regularly requires the use of numerical procedures. In practice, these procedures are used repeatedly and are required to provide precise values in a few seconds. In the last few years, dynamic programming coupled with interpolation has been shown to be an efficient and flexible approach for the evaluation of complex products.
After an overview of classical numerical methods, we present the basic concepts of recursive modeling. Application examples are used to illustrate the flexibility and applicability of recursive models. We finally compare the efficiency of various interpolation and integration approaches.

A General Approach for Stochastic Correlation using Hyperbolic Functions

M. Ehrhardt, L. Teng and M. Günther

University of Wuppertal, Germany

It is well known that the correlation between financial products, financial institutions, e.g., plays an essential role in pricing and evaluation of financial derivatives. Using simply a constant correlation may lead to correlation risk, since market observations give evidence that the correlation is not a deterministic quantity.

In this talk, we suggest a new approach to model the correlation as a hyperbolic function of a stochastic process. Our approach provides a stochastic correlation which is much more realistic to model real world phenomena and could be applied in many financial fields.

As an example, we compute the price of quanto applying our new approach. Using our numerical results we investigate the effect of considering stochastic correlation on pricing the quanto.

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Algorithms and Numerical Methods for High Dimensional Financial Market Models

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A major challenge in Computational Finance is the pricing of options that depend on a large number of risk factors. Prominent examples are basket or index options where dozens or even hundreds of stocks constitute the underlying asset and determine the dimensionality of the corresponding parabolic equation. A number of problems in high-dimensional spaces have been addressed by the usual technique of separation of variables. In order to use the separated representation for numerical analysis applications, many algorithms and operations need to be translated into this framework. The aim of this talk is present and review some of these techniques in the context of High Dimensional Financial Markets Models.

Accurate and Efficient Techniques for Pricing Derivatives and for Computing Risk Measures

C. Oosterlee

CWI - Center for Mathematics & Computer Science, Netherlands

When Fourier techniques are employed to specific option pricing cases from computational finance with non-smooth functions, the so-called Gibbs phenomenon may become apparent. This seriously impacts the efficiency and accuracy of the pricing. For example, the Variance Gamma asset price process gives rise to algebraically decaying Fourier coefficients, resulting in a slowly converging Fourier series. We apply spectral filters to achieve faster convergence. Filtering is carried out in Fourier space; the series coefficients are pre-multiplied by a decreasing filter, which does not add significant computational cost. Tests with different filters show how the algebraic index of convergence is improved.

Robust pricing of European options with wavelets

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We present a novel method for pricing European options based on the wavelet approximation (WA) method and the characteristic function. We focus on the discounted expected payoff pricing formula, and compute it by means of wavelets. We approximate the density function associated to the underlying asset price process by a finite combination of B-splines, and recover the coefficients of the approximation from the characteristic function. Two variants for wavelet approximation will be presented, where the second variant adaptively determines the range of integration. The compact support of a B-splines basis enables us to price options in a robust way, even in cases where Fourier-based pricing methods may show weaknesses. The method appears to be particularly robust for pricing long-maturity options and fat tailed distributions.

Efficient numerical methods for option pricing in time-inhomogeneous models

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Lévy processes have, since their initial use in the early 1990ies by D. Madan and his collaborators, become a standard tool in financial modeling. Time-inhomogeneity severely hampers their efficient performance in pricing derivatives across multiple strikes and maturities in markets which are intrinsically time inhomogeneous.
We present a class of processes beyond Lévy whose time-inhomogeneous parabolic partial integrodifferential equations (PIDEs) exhibit strong degeneracies in time. The arising PIDE reads as follows:

$$\partial_t u - t^\gamma \mathcal{A}(t) u = f \text{ on } I \times D, \tag{2}$$

$$u(0) = g, \tag{3}$$

where $(\mathcal{A}(t))_{t\geq 0}$ is an appropriate family of operators, g the sufficiently smooth initial data, γ a constant with $\gamma \in (-1, 1)$, $I = (0, T)$ and a Lipschitz domain $D \subset \mathbb{R}^d$ for $d \geq 1$. Note that negative exponents γ lead to an explosion at $t = 0$.

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Pricing Derivatives in High-Dimensional Settings via PDE Expansions

C. Reisinger and R. Wissmann

University of Oxford, United Kingdom

We propose a new numerical approach to high-dimensional partial differential equations (PDEs) arising in the valuation of exotic derivatives on the LIBOR curve. The proposed method uses principal component analysis (PCA) of the underlying process in combination with a Taylor expansion of the value function into solutions to low-dimensional PDEs. The approximation is related to anchored analysis of variance (ANOVA) decompositions and is expected to be accurate whenever the covariance matrix has one or few dominating eigenvalues. On the example of Bermudan swaptions and Ratchet floors, which are considered difficult benchmark problems, we are able to demonstrate that for problems with medium to high dimensionality and moderate time horizons the presented PDE method delivers results comparable in accuracy to the MC methods considered here in similar or (often significantly) faster runtime.

Numerical methods for pricing companies with PDE models and GPUs

C. Vázquez, D. Castillo, A. Ferreiro and J.A. García-Rodríguez

Universidade da Coruña, Spain

We propose appropriate numerical methods for companies valuation models proposed in [1]. The models are formulated in terms of final-boundary value problems associated to Kolmogorov type equations, sometimes including an additional unilateral constraint. We also analyze the required boundary conditions so that the final-boundary value problem is well posed, thus allowing to remove unnecessary boundary conditions proposed in [1]. Numerical methods are mainly semilagrangian schemes in the direction without diffusion combined with implicit second order finite differences schemes in the direction where diffusion is present. This choice of numerical methods allows to develop an original parallelization strategy, which results to be specially efficient when using GPUs technologies [2]. This methodology can be applied to problems in mining industry or Asian options pricing [3].

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MS22 – Numerical solution of stochastic differential equations

Organized by: Andreas Rößler and Kristian Debrabant

Post-transcriptional regulation in the nucleus and cytoplasm: a study of mean time to threshold and the narrow escape problem

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[a] CS Oxford, United Kingdom

[b] ENS Paris, France

mRNA can be regulated and degraded by small non-coding RNA molecules: siRNAs and microRNAs. We study the process of RNA interference in mammals by examining the survival condition for mRNAs to escape from the nucleus before being degraded. We develop a model of mRNA interacting with siRNAs. As the number of binding sites is small, many events are stochastic in nature, we compute the probability that mRNA escapes degradation using a stochastic approach. We obtain explicit expressions when the siRNA can bind irreversibly to the mRNA. We also investigate the case of post-transcriptional regulation of the tumour suppressor gene, PTEN. PTEN mRNA are localized to the cytoplasm, and PTEN mRNA can be degraded by microRNAs or protected from degradation by complementary small regulatory RNAs that block the binding sites on the mRNA. We compute the probability of PTEN mRNA translocating to the endoplasmic reticulum before being degraded by microRNAs.

Mean-Square Stability of Stochastic Linear Two-step methods for SDEs

E. Buckwar and T. Sickenberger

Johannes Kepler University Linz, Austria

In this talk we present a linear stability analysis of two-step Maruyama-type methods, for simplicity of notation applied to a scalar stochastic differential equation (SDE), although the analysis also works for a system of SDEs. The main issue is that we obtain a stability matrix, which reflects the asymptotic mean-square stability behaviour of the approximations, and that can be analysed by deterministic methods. We also provide stability plots.

Weak order exponential Runge-Kutta methods for stiff stochastic differential equations

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[c] University of Oxford and Queensland University of Technology

We are concerned with numerical methods which give weak approximations for stiff Itô SDEs. It is well known that the numerical solution of stiff SDEs leads to a stepsize reduction when explicit methods are used. However, there are some classes of explicit methods that are well suited to solving some types of stiff SDEs. One such class is the class of stochastic orthogonal Runge-Kutta Chebyshev methods [1]. Another suitable class of methods is the class of Local Linearization (LL) methods that reduce to some exponential Runge-Kutta (RK) methods when applied to semilinear ODEs. Mora [3] and Carbonell et al. [2] have proposed weak second order LL methods for SDEs with additive noise.
In this talk, we will propose new exponential RK methods which give weak approximations for multi-dimensional, non-commutative SDEs with a semilinear drift term. Their convergence order and stability properties will be confirmed in numerical examples.

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Structure-preserving Runge-Kutta methods for stochastic Hamiltonian equations with additive noise

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[b] University of Oxford and Queensland University of Technology

There has been considerable recent work on the development of energy conserving one-step methods that are not symplectic. Here we extend these ideas to stochastic Hamiltonian problems with additive noise and show that there are classes of Runge-Kutta methods that are very effective in preserving the expectation of the Hamiltonian,

but care has to be taken in how the Wiener increments are sampled at each timestep. Some numerical simulations illustrate the performance of these methods.

Solving Stiff Stochastic Differential Equations with a Stabilized Multilevel Monte Carlo Method

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We introduce a new stabilized multilevel Monte Carlo (MLMC) method for mean square stable stochastic differential equations with multiple scales, problems that we call stiff. Due to time stepsize restriction on the fastest scales, not all levels of the standard MLMC approach based on classical explicit methods can be exploited, and thus, the performance of such MLMC methods deteriorates. Turning to explicit stabilized numerical integrators [1] and balancing the stabilization procedure simultaneously with the hierarchical sampling strategy of MLMC methods, we show that the computational complexity for stiff systems is significantly reduced. The computational algorithm of this new stabilized MLMC method remains fully explicit and easy to implement [2].

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A review on numerical schemes for solving a linear stochastic oscillator

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In recent years several numerical methods to solve a linear stochastic oscillator with one additive noise have been proposed. The usual aim of these approaches was to preserve different long time properties of the oscillator solution, namely, symplecticity, linear growth of its second moment and asymptotic oscillation around zero, among others. In this work we show that these features can be studied in terms of the coefficients of the matrices that appear in the linear recurrence obtained when the schemes are applied to the oscillator.

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Monotone approximation schemes for linear parabolic PDEs by weak SDE approximation methods

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In this talk we consider equations of the form

$$u_t = \frac{1}{2}\mathrm{tr}[\sigma(t,x)\sigma^\top(t,x)D^2u(t,x)] + b(t,x)Du(t,x) + c(t,x)u + f(t,x) \text{ in } \quad (0,T]\times\mathbb{R}^N,$$
$$u(0,x) = g(x) \text{ in } \quad \mathbb{R}^N,$$

containing e. g. the Black–Scholes PDE.
We show how weak approximation schemes for the solution of stochastic differential equations can be used to obtain new higher order monotone PDE approximation methods. Some stability and convergence results are given, including convergence for coefficients which are only bounded and Lipschitz continuous, and the methods are applied to some examples.

Computing deterministic quadrature rules for marginals of SDEs.

L. Yaroslavsteva and T. Müller-Gronbach

University of Passau, Germany

We consider the problem of approximating the marginal distribution of the solution of an SDE by probability measures with finite support. We study deterministic algorithms in a worst case analysis w.r.t. classes of SDEs, defined in terms of smoothness constraints on their coefficients. The cost of an approximation is given by the

sum of the size of its support and the number of evaluations of the coefficients used to compute the corresponding nodes and weights. The error is defined as the worst case quadrature error of the resulting quadrature rule over a class of test functions. We present sharp asymptotic lower and upper bounds on the respective N-th minimal errors in terms of the smoothness of the coefficients and the test functions. Moreover, we present an algorithm, which is based on a space discretization of a weak Taylor scheme and a support reduction strategy. It is easy to implement and it performs asymptotically optimal in many cases. We also show numerical examples.

MS23 – Geometric Numerical Integration for PDEs

Organized by: Erwan Faou

Hamiltonian splitting methods for Vlasov equations and Landau damping

E. Faou

INRIA & ENS Cachan Bretagne & ENS Paris, France

We will consider Hamiltonian splitting methods applied to Vlasov-like equations in the context of semi-Lagrangian methods. We will show how the algebraic structure of the Vlasov-Poisson equation arising in Plasma Physics allows to derive efficient high order methods possessing strong geometrical properties. We will then analyze the long time behavior of these methods, that is the numerical reproduction of the Landau damping phenomenon over long times.
These are joint works with Fernando Casas, Nicolas Crouseilles, Michel Mehrenberger and Frédéric Rousset.

Stability in the presence of transport terms

A. Iserles

University of Cambridge, United Kingdom

Numerous PDEs are of the form $u_t + V(x) \cdot \nabla u = \mathcal{L}(u, x, t)$, where $\mathcal{L}$ is an operator, e.g. convection–diffusion, the forward Kolmogorov equation, the Fokker–Planck equation and the Bolzmann equation. Once this equation, on an arbitrary grid, is discretised using finite differences, in tandem with splitting (e.g. the Strang splitting), the discretisation of transport terms $-V \cdot \nabla u$ is typically unstable. In this talk we prove that such a discretisation is always stable as long as differentiation is approximated with a skew-symmetric matrix but that skew-symmetry on an arbitrary grid is generically consistent with just first-order approximation. We derive conditions that guarantee high-order skew-symmetric approximation of the first derivative and present a method to construct matrices of this kind which are, in addition, banded.

Composition methods based on an almost symmetric Strang splitting

A. Ostermann and L. Einkemmer

Department of Mathematics, University of Innsbruck, Austria

Compared to standard integrators, splitting methods often have superior geometric properties. Moreover, high-order schemes can easily be obtained by composition of Strang splitting, whenever the exact partial flows (or semi-flows) are employed. In certain applications, however, only numerical approximations to these flows are available. This is particularly true for many non-linear problems. In such a situation, Strang splitting looses symmetry, and consequently the related composition schemes exhibit severe order reductions.

In this talk, it will be shown how high order composition schemes can be recovered. The procedure is illustrated with typical examples from ordinary and time dependent partial differential equations that arise in applications. This talk is based on the recent paper [1].

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Implicit-Explicit Runge-Kutta schemes for optimal control problems and applications to PDEs

L. Pareschi

Department of Mathematics and Computer Science, Università di Ferrara, Italy

Implicit-explicit (IMEX) Runge-Kutta methods play a major rule in the numerical treatment of differential systems governed by stiff and non-stiff terms. In this talk we discuss order conditions and symplecticity properties of a class of IMEX Runge-Kutta methods in the context of optimal control problems. Using suitable transformations of the adjoint equation, order conditions up to order three are proven as well as the relation between adjoint schemes obtained through different transformations is investigated. Conditions for the IMEX Runge-Kutta methods to be symplectic are also derived. Applications to some partial differential equations are finally presented.

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MS24 – Fast direct linear solvers for elliptic partial differential equations

Organized by: Eric Darve, Mario Bebendorf, Xiaoye Sherry Li, Luc Giraud and Esmond Ng

Robust LU factorization with logarithmic-linear complexity

M. Bebendorf

University of Bonn, Germany

The factors of the LU factorization of discrete elliptic boundary value problems can be approximated with logarithmic-linear complexity using the methodology of hierarchical matrices. While it is known that the smoothness of the differential operator's coefficients does not enter the complexity, only empirical results on the influence of the coefficient's contrast are available. In this talk, we present a recent analysis of this influence.

A task-based H-matrix solver for acoustic and electromagnetic problems on multicore architectures

B. Lize[a], *G. Sylvand*[a], *E. Agullo*[b] *and S. Thibault*[b]

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$\mathcal{H}$-Matrix [1, 2] is a hierarchical, data-sparse approximate representation of matrices that allows the fast approximate computation of matrix products, LU and LDL^T decompositions, inversion and more. This representation is suitable for the direct solution of large dense linear systems arising from the Boundary Element Method in $O(N \log_2^\alpha(N))$ operations. However, the recursive and irregular nature of these algorithms makes an efficient parallel implementation more challenging, especially when relying on a "Bulk Synchronous Parallel" paradigm [3]. We consider an alternative parallelization for multicore architectures using a task-based approach on top of a runtime system [4]. We show that our method leads to a highly efficient, fully pipelined computation on large real-world industrial test cases in acoustics and electromagnetism.

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A direct solver with O(N) complexity for a spectral multidomain method

P.G. Martinsson

University of Colorado at Boulder, United States

The talk describes a highly accurate technique for solving elliptic PDEs with variable coefficients and smooth solutions. The domain is tessellated into squares (or cubes), and the differential operator is discretized via high order (p=10 or 20) spectral differentiation on each square. A hierarchical direct solver is used to solve the resulting discrete system. The method is very efficient; e.g., a Helmholtz problem on a domain of size 200x200 wavelengths is solved to ten digits of accuracy in ten minutes on a standard laptop (using 6M degrees of freedom).

Conditioning of incomplete Cholesky factorizations with orthogonal approximations

A. Napov

Universite Libre de Bruxelles, Belgium

We consider incomplete Cholesky factorizations based on orthogonal approximations for the iterative solution of symmetric positive definite linear systems. Such factorizations correspond, for instance, to some existing fast direct solvers based on low-rank approximations and which are used with large approximation threshold. Large threshold enables a cheaper factorization, but the resulting solution is less accurate and additional solution steps may be required to refine it, yielding an iterative solver. The number of iterations then depends on the condition number of the preconditioned system, and we show that this latter may be bounded depending only on the accuracy of the individual approximations. The resulting bound is illustrated with some existing factorization algorithms in the context of discretized elliptic partial differential equations.

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MS25 – Numerical solution of integral and integral-algebraic equations of Volterra type

Organized by: Mikhail Bulatov and Pedro Lima

Numerical solution of integro-algebraic equations by multistep methods

M. Bulatov[a] *and O. Budnikova*[b]

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[b] East Siberian State Academy of Education, Russian Federation

Multistep methods are proposed for numerical solution of linear integro-algebraic equations of index one. The algorithms are based on explicit Adams's quadrature formulas and extrapolation formulas. Conditions for the convergence of such algorithms to the exact solution are given. Stability regions have been built.
The work was supported RFBR Grants 11-01-00639-a and 13-01-93002 Viet-a.

On Properties of Integral Algebraic Equations with Rectangular Coefficient Matrices

V. Chistyakov

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In this talk we consider systems of Volterra integral equations

$$(\Lambda_0 + \mathcal{V})x = A(t)y + \int_\alpha^t p(t,s)K(t,s)x(s)ds = \psi(t),\ t \in T = [\alpha, \beta], \tag{1}$$

where $A(t),\ K(t,s)$ are $(m \times n)$ matrices, $p(t,s) = 1$ or $p(t,s) = (t-s)^{-\gamma}, \gamma \in (0,1)$, $x \equiv x(t),\ \psi(t)$ are the desirable and given vector-functions, correspondingly. It is assumed that the following condition holds

$$\mathrm{rank}A(t) < \min\{m,\ n\}\ \forall t \in T. \tag{2}$$

If $m = n$, then (2) is equivalent to $\det A(t) = 0\ \forall t \in T$. Such systems are commonly called integral algebraic equations (IAEs). They appear when modeling developing dynamical systems (based on the Glushkov model) and analyzing game problems. We give sufficient conditions for solvability of (1) satisfying (2). The methods of investigation are based on the results from [1, 2].
This work has been supported by RFBR, Projects No. 11-01-00639 and No. 13-01-93002.

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Solving delay differential equations with diagonally implicit Runge–Kutta methods

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[b] McGill University, Canada

In case of so-called overlapping, when in delay differential equations a delay becomes smaller than the step-size, the standard implementation of continuous Runge–Kutta methods (CRKs) makes the methods fully implicit. Pioneering works by L. Tavernini and recent comprehensive papers by a group of Italian authors show how explicit methods can be applied explicitly even with overlapping. In search of better stability properties we adapt the same technique for Diagonally Implicit CRKs preserving their diagonal structure in the case of overlapping. Methods of different orders are constructed. Problems of practical implementation are also studied: error estimation, automatic step-size control, interpolant overshoot, combining methods for better efficiency etc.

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Analysis and Numerical Approximation of the Generalized Density Profile Equation

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We are concerned with a generalization of the Cahn-Hilliard continuum model for multiphase fluids [1] where the classical Laplacian has been replaced by a degenerate one (so-called p-Laplacian). Using spherical symmetry, the model can be reduced to a boundary value problem for a second order nonlinear ordinary differential equation. One searches for a monotone solution of this equation which satisfies certain boundary conditions. The case of the classical Laplacian was studied in detail in [2] and [3]. In the present work, it is proved that the arising boundary value problem possesses a unique strictly monotone solution The asymptotic behavior of the solution is also analyzed at two singular points; namely, at the origin and at infinity. An efficient numerical technique for treating such singular boundary value problems is presented, based on the shooting method and on nested implicit Runge-Kutta formulas with global error control.

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Sinc-collocation methods for Volterra integro-differential equations

T. Okayama

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In this talk, numerical schemes by means of Sinc methods for Volterra integro-differential equations

$$u'(t) = g(t) + \mu(t)u(t) + \mathcal{V}[u](t), \quad a \le t \le b,$$
$$u(a) = u_a$$

are considered. Here, g and μ are known functions, u is the solution to be determined, and $\mathcal{V}$ is the Volterra integral operator defined by $\mathcal{V}[f](t) = \int_a^t k(t,r)f(r)\,\mathrm{d}r$, where $k(t,r)$ is a known function. As a related study, Zarebnia [1] reduced the given equations to Volterra integral equations, and applied the Sinc-Nyström method developed by Muhammad et al. [2]. However, the computational cost of the method is relatively high, because the

approximate solution includes double summation. Instead, a Sinc-collocation method is developed in this study, where only single summation is included. This study further improves the method by replacing the standard variable transformation with the trending one [3].

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Contributed Talks

Session CS01 – Stochastic partial differential equations

Mean-square convergence order of a stochastic symplectic semi-discrete scheme for the stochastic Schrödinger equation

Ch. Chen and J. Hong

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A stochastic symplectic semi-discrete scheme in temporal direction is proposed for the stochastic Schrödinger equation in Stratonovich sense. To study its convergence order, a convergence theorem is presented. It establishes the relationship between the mean-square convergence order of a semi-discrete scheme and its local error. Based on it, we show that the semi-discrete scheme has mean-square order 1 under appropriate assumptions.

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Sobolev Type Nonlocal Fractional Stochastic Control Systems in Hilbert Spaces

A. Debbouche

Department of Mathematics, Guelma University, Guelma, Algeria

In this talk, we study a class of Sobolev type fractional control nonlocal functional differential equations in a Hilbert space. The results are obtained by using fractional calculus, semigroup theory, fixed point technique and optimal control. An appropriate set of sufficient conditions for the main results of the considered system is constructed and proved. As an application that illustrates the abstract results, provided examples are given.

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Effective computer simulation of the stochastic transport equation

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In this work we propose a new computational scheme for the effective simulation of the stochastic transport equation. For constructing the method, a suitable exponential-based approximation to the solution of an associated auxiliary random integral equation, together with an adapted Padé method with scaling and squaring strategy are conveniently combined. Results on the convergence of the suggested method and details on its efficient implementation are presented. The performance of the introduced method is illustrated through computer simulations

Stochastic Multi-symplectic Preissman Scheme for Stochastic Maxwell Equations

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Based on the stochastic multi-symplectic form of stochastic Maxwell's equations proposed by Hong et al. recently, we give a stochastic multi-symplectic Preissman scheme for 3D stochastic Maxwell equations. We show that the numerical scheme satisfies discrete stochastic multi-symplectic conservation law. And it preserves the discrete local and global evolving energy conservation law exactly.

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Session CS02 – Time integration of partial differential equations

Geometric Time Integration and absorbing boundary conditions. A case study

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We are concerned about the confluence of two subjects of the numerical solution of time evolution PDEs: numerical methods that preserve geometric properties of the flow and absorbing boundary conditions used to reduce the computation to a finite domain. We pay attention to the time stability. The stability regions of time integrators are revisited. Since geometric methods are not always A-stable, it is necessary a suitable behavior of the real part of the eigenvalues of the spatially discretized problem to avoid in practice any time instability. The study is carried out for the one dimensional wave equation discretized with finite differences. Some numerical experiments confirm our results.

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Laplace-finite element methods for integro-differential equations of Volterra type

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In this talk we consider numerical methods for integro-differential problems based on time discretization via Laplace transformation. We focus our attention in models arising in the context of non Fickian solute transport phenomena in porous media. The mathematical models which describe the evolution of the solute concentrations

are characterized by Volterra equations. We present and analyze hybrid methods which combines the Laplace transformation with respect to the time variable with the finite element discretizations in the spatial variables. Numerical results illustrating the performance of the methods are included.

Delay-dependent stability of high order time discretizations for delay partial differential equations

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This talk is concerned with the stability of difference methods for partial differential equations (PDEs) with time-delay. By using a variant of the classical second-order central differences to discretize the spatial derivatives, we first obtain a semi-discrete system, which is a set of ordinary differential equations in the time variable. Then, the time discretizations based on Runge-Kutta methods with a non-constrained mesh are applied, where an equi-stage interpolation procedure is employed to approximate the delay argument. We establish a general stability criterion which can guarantee that the fully discrete system completely preserves the delay-dependent stability of the PDE test problem under consideration. Some high order methods with certain linear or parabolic interpolation are proved to satisfy this criterion. Finally, numerical experiments are presented to confirm the theoretical results.

Geometric integration of two coupled wave equations with absorbing boundary conditions

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Initial value problems with two coupled wave equations are considered. The problem is discretized in space using fourth order implicit finite differences. In order to reduce the computation to a bounded domain, absorbing boundary conditions are deduced. Well posed systems with fifth order of absorption for the diagonalizable case, and third order of absorption for the non diagonalizable one, are obtained. When a part of the solution reaches the boundary and it is absorbed, another part of the solution is still inside the computational interval, where it is important to preserve its geometric properties. This fact supports the simultaneous use of absorbing boundary conditions and symplectic integrators. Numerical experiments are displayed.

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Session CS03 – DAEs and PDAEs

Index Reduction for Semi-explicit Operator DAE's

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The talk is devoted to semi-explicit operator differential equations of the form

$$\begin{aligned} \dot{u}(t) + Ku(t) + B^*\lambda(t) &= F(t), \\ Bu(t) &= G(t) \end{aligned}$$

with given initial value. Because of the saddle point structure, standard semi-discretization schemes in space such as finite elements lead to a differential-algebraic equation (DAE) of index 2. Thus, we call the above equation an operator DAE. An example of a system with this structure is given by the Navier-Stokes equations, where B equals the divergence operator and λ stands for the pressure.
For a certain class of constraint operators B, we present a reformulation of the above system, which can be seen as an index reduction procedure on operator level. By this we mean that a semi-discretization of the reformulated system gives a DAE of index 1. The presented method is based on the index reduction technique of minimal extension [1].

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Stable and efficient simulation of PDAEs describing flow networks

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We are interested in partial differential algebraic equations (PDAEs) describing flow networks. These PDAEs consist of hyperbolic PDEs of the type

$$\begin{aligned} p_t + Am_x &= 0 \\ m_t + Bp_x + H + G(m)m &= 0 \end{aligned}$$

which are coupled with algebraic boundary conditions. For our simulation approach we use the method of lines, yielding a differential algebraic equation (DAE) which is adaptively discretized in time.
We present a perturbation analysis for a simplified prototype motivated by the system above for different types of space discretizations. In particular we will show that the index of the resulting DAEs may depend on the chosen space discretization.
Additionally, we present a network topologically dependent space discretization guaranteeing DAEs of index 1. Furthermore we study a network topological procedure to reduce the resulting DAEs into semi-explicit systems of the form

$$x' = f(x,t)$$
$$y = Mx + r(t).$$

On solution of differential-algebraic equations by collocation-variation splines

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Numerical methods for solving initial value problems for differential-algebraic equations are proposed. The approximate solution is represented as a continuous vector spline whose coefficients are found using the collocation conditions stated for a subgrid with the number of collocation points less than the degree of the spline and the minimality condition for the norm of this spline in the corresponding spaces. Numerical results for some model problems are presented.
The work was supported RFBR Grants 11-01-00639-a and 13-01-93002 Viet-a.

Numerical stability of Runge-Kutta methods for neutral delay differential-algebraic equations

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This talk is concerned with asymptotic stability of linear neutral delay differential-algebraic equations and Runge-Kutta methods. First, we give a new equivalent sufficient condition for the neutral delay differential-algebraic equations to be delay-independently asymptotically stable. Then we investigate the asymptotic stability of the numerical solutions generated by the Runge-Kutta methods combined with Lagrange interpolation. Some results on the asymptotic stability of Runge-Kutta methods of high order are given. Finally, numerical examples of index-1 and index-2 are conducted to confirm our numerical stability result.

Session CS04 – Delay differential equations

Solvability analysis and reformulation of general Linear Delay Differential-Algebraic Equations

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Delay differential equations (DDEs) arise in a variety of applications, including physical systems, biological systems and electronic networks. If the states of the physical system are constrained, e.g., by conservation laws or interface conditions, or some economical interest are involved in the biological model, then algebraic equations have to be included and one has to analyze delay differential-algebraic equations (Delay-DAEs).
In this talk, we present our recent result on the solvability analysis of general linear Delay-DAEs, i.e., systems with linear time variable coefficients. We propose the method to reformulate a Delay-DAE into its underlying delay system, which can be used to address structural properties of the system like existence and uniqueness of a solution, consistency and smoothness requirements. We also consider some spectral properties of Linear Delay-DAEs and their relations to the solvability analysis of the system.

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A delay differential equation describing the evolution of a Herpes virus

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We study a model describing the evolution of a Herpes simplex virus type 2. A delay differential equation is used to model the disease spread. Sufficient conditions of Strong monotonicity and global stability are given. Theoretic results are illustrated by numerical simulations for realistic data.

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Polynomial chaos expansion and stability analysis of uncertain DDEs

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Many problems in science and engineering are modeled with systems of delay differential equations (DDEs). Since they are infinite dimensional dynamical systems, the stability analysis requires effective numerical methods. Beside the mathematical model and the numerical method, another relevant aspect is the specification of the data. The uncertainty in the model constants are often modeled as random processes.
The Polynomial Chaos (PC) expansion provides a representation of random variables, vectors and processes with respect to a basis set of functionals, usually orthogonal polynomials. It is based on the original Wiener's theory of homogeneous chaos [2] and it has been successfully applied in different fields for uncertainty quantification e.g. [1].
We propose to apply PC expansion to quantify the resulting uncertainty in the numerical stability analysis of equilibria of DDEs with random parameters. We introduce some basic ideas and we present preliminary results.

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Session CS05 – Molecular Dynamics

Stochastic correction of kinetic energy spectra in fluids

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Both conservative and diffusive truncations of inviscid fluid models fail to capture the correct power law scaling of the kinetic energy spectrum at small scales. This scaling is important both for downscale transport of vorticity and energy, as for small upscale 'backscatter' that influences variance. In this talk we discuss a simple correction using a stochastic thermostat approach from molecular dynamics. Thermostats are used in MD to perturb dynamics such that trajectories are ergodic in the canonical Gibbs measure (constant temperature). To apply these methods to discretized fluids, several challenges must be met: (i) we perturb only the smallest scales, hence controllability must be established; (ii) we are given expectations (kinetic energy spectrum) instead of invariant measure; (iii) we have to deal with forcing at low wave numbers; (iv) experience from heat conduction problems suggests that artifacts may occur. We report recent progress on these fronts [1, 2].

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A Lagrangian method for numerical analysis of distributed vortical dynamics

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The variant of vortex-in-cells method originally presented in [1, 3] is developed. The equations are the geophysical models of the atmosphere in terms of stream function and vorticity. The method is based on vorticity approximation using its values in particles and the velocity finding by Galerkin method. Computed velocity is used for fluid particles trajectories calculation as ODE system solution.

The effectiveness of integrator is important for the solution of similar problems. The set of different integrators is studied on a number of test problems of particles dynamics. As a result the most suitable methods are suggested. The algorithm of adaptive choice of integrator based on fluid particles locations is offered.

The algorithm for studing the topological structure of vortex configurations and their structural stability is suggested. The effectiveness of numerical methods are illustrated by results of fluid dynamics problems investigation [2].

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Molecular dynamics simulation of lubricant adsorption and depletion under heat treatment

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Understanding the surface dynamics of thin oligomeric films under heat treatment is of fundamental importance in maintaining the stability and reliability of interfacial surfaces for micro- and nano-devices. In this work, the coarse-grained molecular dynamics simulation is employed to study the thermal adsorption and depletion instability of thin perfluoropolyether (PFPE) lubricant. The bead number density is examined to quantify the lubricant adsorption on the surface. The lubricant weight and bond losses are calculated to provide a real-time monitoring of lubricant depletion during rapid heating. Moreover, the depletion kinetics shows that lubricant desorption is favored over decomposition under heat treatment to high temperatures and is the major cause of lubricant degradation on the surface. Therefore, a novel PFPE lubricant suitable for heat assisted magnetic recording should be designed and engineered to overcome the prone to desorption for future hard disk drive applications.

Multilevel Summation for Dispersion: A Linear-Time Algorithm for r^{-6} Potentials

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The multilevel summation method (MLS) was introduced to evaluate long-range interactions in molecular dynamics (MD) simulations. Based on a multilevel matrix summation, [3] MLS was initially developed for Coulomb potentials [1, 2]; with this work, we extend MLS to dispersion interactions. While formally short-ranged, for an accurate calculation of forces and energies in cases such as interfacial systems, dispersion potentials require long-range methods. Since long-range solvers tend to dominate the time needed to perform MD calculations, increasing their performance is of vital importance. Compared to other long-range solvers, such as mesh-based Ewald and fast multipole methods, MLS is particularly attractive for its ability to handle all forms of boundary conditions and for its linear performance. We discuss how the implementation of MLS for dispersion potentials differs from the Coulomb case, and present results establishing the accuracy and efficiency of the method.

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Session CS06 – Implementation issues

Inexact Fixed Point Schemes and Applications in Scientific Computing

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We consider fixed point schemes, where the function evaluation corresponds to inexact solves of linear or nonlinear equation systems. This allows to decide how accurate these systems should be solved to obtain a target error in the fixed point iteration, as well as to decide on a good termination criterion.
The first applicaton is the Picard iteration which is widely used for the incompressible Navier-Stokes equations. Here we can show that this iteration converges regardless of how accurate we solve the subsystems, provided a relative termination criterion is employed.
As a second example, we consider thermal fluid structure interaction problems where heat is exchanged via a coupling interface. This appears in many applications, for example in the cooling process in steel forging. A so called partitioned coupling approach naturally leads to a fixed point iteration, which is then analyzed using the derived methodology.

A pre-fetched BiCGSTAB method in the solution of the trapezoidal rule of large ODEs

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We are concerned with an efficient numerical solution of linear equations at each time-stepping of the trapezoidal rule applied to a system of linear ordinary differential equations (ODEs) with a constant coefficient matrix of large dimension. We do not assume that the matrix is symmetric. Hence numerical solutions in the family of BiCG method are sought. We propose a method to reuse Krylov subspaces in the BiCGSTAB process over a number of computational steps [1]. It can suppress increase of the memory usage as well as reduce the total number of BiCGSTAB iterations. An influence of the non-autonomous term of ODEs is analyzed on the efficiency of our algorithm. Numerical examples depict its efficiency.

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An iterative starting method for multistep methods and its impact on Hamiltonian systems

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Starting methods are used to obtain the inputs for multistep methods. For linear multistep methods, inputs are sufficiently accurate solution approximations over several time-steps. For general linear methods, inputs of greater complexity may be required. In either case, a poorly constructed starting method can render the multistep method useless.
In this talk, we introduce an iterative starting method that approximates the ideal starting method to arbitrary accuracy and investigate the impact of such an initialisation on several Hamiltonian problems.

Two-Step Symmetrization with Extrapolation

N. Razali and R.P.K. Chan

The University of Auckland, New Zealand

The use of Richardson extrapolation in accelerating convergence of a sequence is more efficient if the method has the h^2-asymptotic error expansion. Gragg first proved the existence of this property for the explicit midpoint rule in ordinary differential equations. He introduced the concept of smoothing to suppress the oscillatory parasitic component of the numerical solution and showed the advantage of smoothing applied with extrapolation [2]. In [1], this concept is generalized to arbitrary symmetric Runge-Kutta methods and called symmetrization. The two-step symmetrizer for the implicit midpoint and trapezoidal rules was constructed in [3]. In this talk, we discuss the advantages of using a one-step symmetrizer and investigate what other improvements there are in using two-step symmetrizers. We present experimental results that show the two-step symmetrizer can be more accurate and efficient in certain cases.

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Rosenbrock-Krylov time stepping methods

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This talk discusses a new class of Rosenbrock-type integrators based on a Krylov space solution of the linear systems. The new family, called Rosenbrock-Krylov (Rosenbrock-K), is well suited for solving large scale systems of ODEs or semi-discrete PDEs. The time discretization and the Krylov space approximation are treated as a single computational process, and the Krylov space properties are an integral part of the new Rosenbrock-K order condition theory developed herein. Consequently, Rosenbrock-K methods require a small number of basis vectors determined solely by the temporal order of accuracy. The subspace size is independent of the ODE under consideration, and there is no need to monitor the errors in linear system solutions at each stage. Numerical results show favorable properties of Rosenbrock-K methods when compared to current Rosenbrock and Rosenbrock-W schemes.

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Session CS07 – Stochastic differential equations

New adaptive method for variance reduction using approximating martingales

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Approximating martingales method [1] is a variant of control variates method which can be used to reduce the variance of estimators of certain quantities defined for Markov chains, including their expected hitting times of sets. We introduce a new method for choosing adaptively the function u [2] needed to construct the approximating martingale, to reduce the variance. As opposed to the well-known sample variance minimization method [2], the new method can be applied even when the number of performed simulations is lower than the number of basis functions used in the linear parametrization of u. In our numerical experiments we demonstrate that the new method can achieve on average high variance reductions and that it can significantly outperform the sample variance minimization method.

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Convergence and stability analysis of stochastic delay differential equations

Q. Guo, W. Xie, T. Mitsui and X. Tao

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We introduce multistage methods to numerically solving stochastic delay differential equations, for instance stochastic Hopfield neural networks. With additional conditions, the methods are proved to have a strong convergence. Further, mean-square stability and almost surely stability of the proposed methods are investigated. Numerical experiments illustrate the computational efficiency of the methods.

Fundamental Convergence Theorems of Numerical Methods for SDEs

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In this talk we review theoretical results on the mean-square convergence of numerical methods for stochastic ordinary differential equations, stochastic delay differential equations, neutral stochastic delay differential equations, jump-diffusion differential equations, neutral stochastic delay differential equations with jump-diffusion, stochastic partial differential equations and backward stochastic differential equations. These results are called fundamental convergence theorems of numerical methods for stochastic differential equations.

Weak backward error analysis for Langevin process

M. Kopec, A. Debussche and E. Faou

ENS Cachan Bretagne, France

We consider numerical approximations of stochastic Langevin equations by implicit methods. We show a weak backward error analysis result in the sense that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. This implies that every measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, we prove that, up to negligible terms, the dynamic associated with the implicit scheme considered is exponentially mixing.

Session CS08 – Modelization and Simulation

Towards multiscale modelling in neuroscience: Experiences with coupling cellular and subcellular levels of neuronal organisation

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The nervous system encompasses structure and phenomena at different spatial and temporal scales from molecule to behavior. For example, the dynamics of second messenger pathways can be formulated as stochastic reaction-diffusion systems while the electrical dynamics of the neuronal membrane is often described by compartment models and the Hodgkin-Huxley formalism. While there are a few simulators available which aim at bridging this gap, most readily available packages are designed for a given domain.

In the present talk we report about our experiences with coupled systems both in matlab reference implementations and in coupling established software packages (MOOSE and NeuroRD). We analyse the properties of the underlying numerical methods for solving ordinary and stochastic differential equations and propose new methods for their enhancement.

We acknowledge the support of our collaborators Uphinder S Bhalla, Mikael Djurfeldt, Jeanette Hellgren-Kotaleski.

Reduction of chemical reaction networks through delay distributions

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Stochastic simulations of large chemical reaction networks come at significant computational costs. Here, we present a reduction methodology [1] that represents monomolecular reaction systems by much simpler, abridged models. These can be simulated at significantly lower computational costs while retaining accuracy. The abridgement is achieved by generation of model-specific delay distributions, fed into a delay stochastic simulation algorithm. We show how such delay distributions can be analytically described whenever the system is solely composed of consecutive first-order reactions yielding an exact reduction. For models including other types of monomolecular reactions such as constitutive synthesis or degradation, we adopt a numerical approach for its accurate stochastic representation. We anticipate the use of delays in model reduction will greatly alleviate some of the current restrictions in simulating large sets of chemical reactions.

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A nonFickian coupled model for diffusion in porous media

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Diffusion processes in porous media are usually simulated considering the classical diffusion equation coupled with Darcy's law. In certain scenarios, the diffusion equation induces an anomalous behavior and consequently several improvements were introduced in the literature to overcome them. One approach is to replace the classical Fickian law for the mass flux by a differential equation that should be coupled with a mass conservation law. In this talk we consider models for diffusion process in porous media constructed coupling Darcy's law with the previous models. The qualitative behavior and numerical simulation will be addressed.

Session CS09 – General linear methods

The order of G-symplectic methods

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G-symplectic general linear methods with zero parasitism growth factors are able to preserve quadratic invariants and symplectic structure in a similar way to canonical Runge–Kutta methods. To obtain order p for a method (A, U, B, V), it is necessary that ξ exists such that

$$(E\xi)(t) = B(D\eta)(t) + V\xi(t),$$

for all t such that $|t| \leq p$, where

$$\eta = A\eta D + U\xi.$$

If the method is G-symplectic the order conditions are interrelated and can be reduced to a smaller set. The special case of order 4 methods with $V = \mathrm{diag}(1, -1)$ will be considered in detail. Although there are only two order conditions, there are additional constraints on a possible starting method, represented by ξ. This should not be regarded as a serious handicap because, in a constant step size implementation, a complicated starting method does not represent a computational overhead.

On the construction of sequential second derivative general linear methods

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Second derivative diagonally implicit multistage integration methods (SDIMSIMs) as a subclass of SGLMs have been introduced in [1] in four types, together with their intended applications (for nonstiff or stiff ODEs) and architectures (sequential or parallel). Order barriers for parallel SDIMSIMs, of type four and generalized type four and also for sequential SDIMSIMs of type 2 with Runge–Kutta stability (RKS) property have been discussed in [1, 2]. The coefficients of SGLMs are given by six matrices, instead of four matrices for GLMs, which are obtained by solving linear system of order conditions and usually nonlinear system of RKS conditions. In this survey, we introduce a new formula which causes the order conditions and the stability matrix of SGLMs take simpler form and decreases the complexity of finding coefficients matrices. The constructed A-stable methods are also L-stable.

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Runge–Kutta methods satisfying conjugate order conditions

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It is known that it is impossible to find explicit Runge–Kutta methods with only five stages and with order five. While this is true, a slight modification of the meaning of "Order" makes it false. This generalisation is known as "Effective Order" and can be explained in terms of group conjugacy. The derivation of fifth effective order methods involves 10 order conditions but for convenience we can use simplifying assumptions to make derivation easier. In particular, we have found some new effective order five methods using the $C(2)$ assumption; this leads to simpler and more direct derivation of these methods. Also, we have investigated other cases and reached some conclusions.
Other applications of effective order will be briefly surveyed.

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Numerical solution of Hamiltonian problems by G-symplectic integrators

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It is the purpose of this talk to analyze the employ of General Linear Methods (GLMs) for the numerical integration of Hamiltonian problems. Indeed, even if the numerical flow generated by a GLM cannot be symplectic, Butcher recently introduced in [1] a concept of near conservation, denoted as G-symplecticity, for such methods which, properly combined with other desirable features (such as symmetry and boundedness of parasitic components), allows to achieve a very accurate long time conservation of the Hamiltonian. We also focus our attention on the connections between the order of convergence of a GLM and the observable Hamiltonian deviation, by employing the theory of B-series [3]. Moreover, we derive a semi-implicit GLM [2] which results competitive

with respect to symplectic Runge-Kutta methods. Numerical results on a selection of Hamiltonian problems are presented, confirming the structure-preserving capability of G-symplectic integrators.

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Session CS10 – Variational methods and structure preserving schemes

Preserving Taylor's constraint in magnetohydrodynamics

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The Earth's magnetic field is generated in the outer core, whose behaviour is described by a combination of the Navier-Stokes equation and the Maxwell equation. A problem when solving these equation is that a certain number, the Ekman number, is very small (around 10^{-15}). Usually, people use big computers to solve the equations, but even then the Ekman number in the simulations can only be taken to be 10^{-6}. The alternative is to take the Ekman number equal to zero. This corresponds to a singular limit, in which the equations degenerate into a partial differential algebraic system. Taylor's constraint is an infinite number of quadratic conserved quantities in this limit and it is thought that this constraint causes instabilities in earlier attempt to solve the equations. I will describe our on-going efforts to design and implement a numerical method for solving the equations which preserves Taylor's constraint, making it hopefully stable.

On higher order variational schemes for numerical optimal control

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Direct methods for optimal control problems rely on a discretization of the underlying dynamical system. The method DMOC [2] is based on variational integrators [1] such that geometric properties of the system are preserved in the discrete solution. To ensure moderate computational costs, typically first or second order integrators are used. However, many applications demand more accurate discretization schemes.
We derive and analyze higher order variational schemes for the structure-preserving simulation of mechanical systems. This leads to a higher accuracy of the discrete solution and less computational cost, while geometric properties are still preserved. The order of accuracy and stability properties of the integrators are analytically and numerically determined [3]. Furthermore, we investigate the approximation order of the discrete adjoint equations resulting from the necessary optimality conditions of the discretized optimal control problem.

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Effective approximation for the linear time-dependent Schrödinger equation

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The computation of the linear Schrödinger equation presents major challenges because of the presence of a small parameter. Assuming periodic boundary conditions, the standard approach consists of semi-discretisation with a spectral method, followed by an exponential splitting. We follow an alternative strategy: our analysis commences from the investigation of the free Lie algebra generated by the operations of differentiation and multiplication with the interaction potential. It turns out that this algebra possesses structure that renders it amenable to a very effective form of *asymptotic splitting:* exponential splitting where consecutive terms are scaled by increasing powers of the small parameter. The number of terms of the splitting increases linearly with time accuracy. This leads to methods that attain high spatial and temporal accuracy and whose cost scales like $O(N \log N)$, where N is the number of degrees of freedom.

Lagrangian approach of the discrete gradient method based on finite element methods

T. Yaguchi

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In this talk, we propose a finite element framework of the Lagrangian approach of the discrete gradient method to deriving energy-preserving schemes for the Euler–Lagrange partial differential equations.
Recently a framework that derives energy-preserving finite difference schemes for the Euler–Lagrange PDEs is proposed [1]. This approach is based on a combination of the symmetry of time translation of discrete Lagrangians and the discrete gradient method.
In this talk, we show that the same combination is also workable on the finite element framework. Because our method is based on Lagrangian mechanics, this method can be said to be a Lagrangian counterpart of the energy-preserving method for Hamiltonian systems by Matsuo [2]. Some applications will be also provided.

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Session CS11 – Software issues

Numerical Treatment of Two-Point Boundary Value Problems of Fractional Differential Equations

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We consider the numerical treatment of two-point boundary value problems of fractional differential equations with Caputo's derivatives of order γ where $1 < \gamma < 2$. We introduce the fractional Green functions in order to prove the existence and uniqueness of the solutions to the problem. Numerically, we introduce the simple shooting method for linear and nonlinear problems. The results obtained are accurate and competes well with results by other authors using different approaches.

C++ Template Programs for ODE and DAE by Taylor Series

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The arithmetic operations and functions of Taylor series can be defined by C++ language easily. It is shown that Taylor series solutions of the following ordinary differential equations and differential algebraic equations

$$\mathbf{F}(\mathbf{y}, \mathbf{y}', x) = 0 \quad \text{with initial conditions} \quad \mathbf{y}(0) = \mathbf{y}_0$$

can be computed by similar methods as above Taylor series methods. The solutions can be expanded up to arbitrary order, so they can be used instead of higher order Runge-Kutta formula. Taylor series can be used for the evaluations of the errors and the optimal step size within given error allowance easily. We can also transform Taylor series into Padé series, which give A-stable methods for solving differential algebraic equations numerically.

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On Numerical Properties of Accelerated Multiple Precision Fully Implicit Runge-Kutta Methods

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We have implemented a multiple precision ODE solver based on high-order fully implicit Runge-Kutta (IRK) methods. This ODE solver uses any order Gauss type formulas, and can be accelerated by using (1) MPFR [1] as multiple precision floating-point arithmetic library, (2) real tridiagonalization supported in SPARK3 [2], of linear equations to be solved in simplified Newton method as inner iteration, (3) mixed precision iterative refinement method [3], (4) parallelization with OpenMP, and (5) embedded formulas for IRK methods [4]. In this talk, we describe the reason why we adopt such accelerations, and show the efficiency of the ODE solver through numerical experiments such as 1D Kuramoto-Sivashinsky equation.

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Overdetermined Regularization of Modelica based Model Equations for Dynamical Systems and its Efficient Numerical Simulation

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The modeling of dynamical systems often leads to higher index differential-algebraic equations (DAE)

$$E(x,t)\dot{x} = f(x,t)$$

containing hidden constraints leading to several problems in its direct numerical integration. Therefore, a regularization reducing the index but, in particular, preserving the set of solutions is necessary. Classical regularization approaches often are very technical or lead to DAEs which are enlarged in size or still not suitable for numerical integration due to drift.
We discuss an efficient and robust numerical simulation of dynamical systems modeled using the language Modelica. We present an approach combining 1st a derivative array based regularization to obtain an equivalent overdetermined DAE with the same set of solutions and containing no hidden constraints with 2nd the subsequent numerical integration of this overdetermined DAE using adapted methods. Within the Modelica framework, currently there exist no integrator suited for overdetermined systems.

Session CS12 – Spatial discretization of partial differential equations

Stability of finite difference schemes for complex reaction-diffusion processes

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Complex diffusion is a commonly used denoising procedure in image processing [3]. In particular, nonlinear complex diffusion proved to be a numerically well conditioned technique that have been successfully applied in medical imaging despeckling [2]. The stability properties of a class of finite difference schemes for the nonlinear complex diffusion equation, where both explicit and implicit schemes were considered, was studied in [1]. In the present talk we extend those results for nonlinear complex reaction-diffusion equations discretized with both implicit and semi-implicit finite differences schemes. Some numerical results for despeckling optical coherence tomograms from the human retina, obtained in the context of a collaboration with the Institute of Biomedical Research in Light and Image (IBILI), a research institution of the Faculty of Medicine of the University of Coimbra, are also presented.

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Alignment of optimally transported meshes

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Solutions of partial differential equations are often highly anisotropic and have strongly directional features. Examples include PDES which have shocks and interfaces in the solution. When calculating the solutions to these PDEs it is important to use computational meshes which align themselves with features in the solution. In this talk I will describe a mesh redistribution algorithm based on optimal transport methods which is cheap and robust to implement. I will show further (including giving a set of rigorous results) that this method is very effective at aligning elements along solution features including linear shocks and radially symmetric structures. This allows the solutions to be very well approximated and I will give results to prove this.

Two new schemes for the Degasperis-Procesi equation

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Two new numerical schemes are proposed to solve the Degasperis-Procesi equation. One is a symplectic integrator which preserves invariants very well. The other is constructed by the splitting method which can handle with the shockpeakon cases while the first one cannot. Fifth-order WENO scheme and multisymplectic pseudospectral method are involved in the construction of the splitting method. It also shows nice properties in invariant preservation. Various numerical tests are presented to show the advantages of these two schemes with respect to different kind of solutions.

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Spectral Method for the Transport Equation – Fast Expansion into a Suitable Basis

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We wish to solve equations with transport terms and Dirichlet boundary conditions by spectral methods, combined with splitting in time. The condition for stability is that the differentiation matrix is skew-symmetric, but this is unattainable by any polynomial basis. Using a stretched Fourier transformation, I derive an orthogonal basis with a tridiagonal skew-symmetric differentiation matrix together with an algorithm for fast expansion into this basis for analytic functions. This expansion converges geometrically fast and we only need $O(n \log n)$ operations to compute the first n coefficients.

Session CS13 – Stability properties of numerical methods for ODEs

Long-term stability of multi-value methods for ordinary differential equations

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The recent literature regarding geometric numerical integration of ordinary differential equations has given special emphasis to the employ of multi-value methods: in particular, some authors have addressed their efforts to the construction of general linear methods with the aim of achieving an excellent long-time behavior for the integration of Hamiltonian systems. In this talk, a backward error analysis is presented, which permits to get sharp estimates for the parasitic solution components and for the error in the Hamiltonian. For carefully constructed methods (symmetric and zero growth parameters) the error in the parasitic components typically grows like $h^{p+4}\exp(h^2Lt)$, where p is the order of the method, and L depends on the problem and on the coefficients of the method. This is confirmed by numerical experiments.

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Nonlinear stability of generalized additive and partitioned implicit multirate Runge-Kutta schemes

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Multirate schemes are an efficient tool to exploit different time scales in ordinary differential, differential-algebraic and partial differential equations by asigning appropriate step sizes to different components of the solution or the right-hand side.
In this presentation we will generalize the class of additive and partitioned Runge-Kutta schemes [4] to derive multirate schemes that are characterized by excellent nonlinear stability properties. The derivation of order

conditions will be based on a combination of N-trees and P series. The class of generalized Runge-Kutta, Rosenbrock-Wanner and W methods [3, 2, 1] can be embedded into this new approach. The properties of this new class of multirate schemes will be validated by various numerical results.

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Strong stability properties for some classes of nonlinear problems

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Spacial discretization of some partial differential problems (PDEs) give rise to ordinary differential equations (ODEs). Sometimes, the solutions to these PDEs have qualitative properties, e.g., monotonicity, positivity, etc., which are relevant in the context of the problem. In these cases, it is convenient to preserve these properties both in the spatial discretization of the PDE and in the time stepping process of the resulting ODE.

A common class of methods widely used in the literature are Runge-Kutta methods. For these schemes, some of these qualitative properties can be ensured under certain stepsize restrictions given in terms of the Kraaijevanger's coefficient. However, for some problems, several schemes with trivial Kraaijevanger's coefficient also provide good numerical solutions.

In this talk we will explain how, under additional conditions on the problem, some qualitative properties can be obtained for some methods with trivial Kraaijevanger's coefficient.

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Rational functions with maximal radius of absolute monotonicity

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We study the radius of absolute monotonicity R of rational functions with numerator and denominator of degree s that approximate the exponential function to order p. Such functions arise in the application of implicit s-stage, order p Runge–Kutta methods for initial value problems, and the radius of absolute monotonicity governs the numerical preservation of properties like positivity and maximum-norm contractivity. We construct a function with $p = 2$ and $R > 2s$, disproving a conjecture of van de Griend and Kraaijevanger. We determine the maximum attainable radius for functions in several one-parameter families of rational functions, and we prove earlier conjectured optimal radii in some families with 2 or 3 parameters. Our results also prove the optimality of some strong stability preserving implicit and singly diagonally implicit Runge–Kutta methods. Whereas previous results in this area were primarily numerical, we give all constants as exact algebraic numbers.

Session CS14 – Boundary value problems

The numerical solution of a BVP which rises in the prediction of meteorological parameters.

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Using tools of Information Geometry, the minimum distance between two elements of a statistical manifold is defined by the corresponding geodesic, e.g. the minimum length curve that connects them. Such a curve, where the probability distribution functions in the case of our meteorological data are two-parameter Weibull distributions, satisfies a 2^{nd} order quadratic BVP system.

This system can be solved by finite differences employing Newton's method or quasi-Newton methods for the resulting nonlinear system and taking into consideration the special form of the Jacobian matrix. Another approach is to use MIRK formulas to get a solution of the problem. As the problem is quadratic MIRK schemes constructed for such problems can be considered.

This research has been co-funded by the European Union and Greek nat. resources under the framework of the "Archimedes III: Funding of Research Groups in TEI of Athens" project of the "Education and Lifelong Learning" Op. Progr.

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Approximate solutions of fractional differential equations with Riesz fractional derivatives in a finite domain

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This paper states approximate solutions of fractional differential equations with Riesz fractional derivatives (FDE-RFD) in a finite domain. FDE-RFD are used in many fields, especially in the prediction of the diffusion of radioactive materials [1]. FDE-RFD in an infinite domain have already solved by using fractional Fourier transform [2]. In contrast, we consider how to solve FDE-RFD in a finite domain.
In this paper, we assume FDE-RFD in a finite domain can be solved by the method of separation of variables and the analytical solution is constructed by polynomials. As a result, we find the analytical solution can be obtained by solving a linear equation with infinite size, and we get approximate solutions from solving a linear equation which is approximated to finite size. Note that approximate solutions in this paper mean the solutions which are closely related to asymptotic expansions.

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Numerical Solution of Sturm–Liouville Problems via Fer Streamers

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We address the numerical challenge of solving Sturm–Liouville problems in Liouville's normal form with certain boundary conditions. The novelty of our approach, which is based on a non-standard truncation of Fer expansions, which we call Fer streamers, lies in the construction of a numerical method, which does not impose any restriction on the step size, regardless of the size of the eigenvalue. This unique feature paves the way to the initial development of an effective numerical method to compute any eigenvalue, in clear contrast with the state of the art, where it is not feasible to compute large eigenvalues due to restrictions on the step size. Moreover, our theory holds whenever the potential is piecewise analytic and, in each piece, its average is upper bounded by the smallest eigenvalue we seek. We emphasise that our numerical method is at an early stage of development, and comment on our investigation of efficient discretisation schemes for integrals arising in Fer streamers.

Session CS15 – Optimal control

Self-conjugate differential and difference operators arising in the optimal control of descriptor systems

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We analyze the structure of the linear differential and difference operators associated with the necessary optimality conditions of optimal control problems for descriptor systems in continuous- and discrete-time. It has been shown in [2] that in continuous-time the associated optimality system is a self-conjugate operator associated with a self-adjoint pair of coefficient matrices. We show that the necessary optimality conditions for discrete-time linear quadratic control problems with variable coefficients leads to self-conjugate difference operators associated with self-adjoint triples of coefficient functions, thus achieving a similar result as in the continuous time case. We also extend the results to higher order differential or difference equation constraints and shown how first order reductions can be carried out that lead to first order systems with the same structural properties.

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One Approach to Numerical Solution of a Finite-Horizon Linear-Quadratic Optimal Control Problem for Time Delay Systems

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The well known approach to solution of a finite-horizon Linear-Quadratic Control Problem (LQCP) with state delays in dynamics reduces this problem to a set of three Riccati-type matrix functional-differential equations: one ordinary and two partial first-order with two and three independent variables [1]. This set does not allow, in general, an exact solution. Several approaches to approximate solution of the LQCP with state delays are known: 1) an approximation of the original problem [1]; 2) an asymptotic solution [3, 4]; 3) a finite-difference

approximation of the set of Riccati-type equations [2]. In [4], an eliminating the unknown matrix with three arguments from the set of Riccati-type equations, following by a finite-difference approximation of the reduced set, is suggested for a simple example. In this talk, we extend this approach to a much more general case. This approach reduces considerably a computer memory and a computing time, which is illustrated by examples.

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Numerical Solution of Large-Scale Differential Riccati Equations

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The numerical treatment of linear quadratic regulator/gaussian design problems for parabolic partial differential equations requires solving large-scale Riccati equations. In the finite time horizon case, the differential Riccati equation (DRE) arises. Typically, the coefficient matrices of the resulting DRE have a given structure [1] (e.g. sparse, symmetric or low rank). Methods based on a low-rank approximation of the solution and a matrix-valued implementation of the usual ODE methods exploit efficiently this structure [2]. Here, we discuss several variants of the available methods, which allow to have a fast computation. In particular, we discussed the Rosenbrock type methods, BDF methods and different ways for solving the resulting algebraic Riccati equation. The performance of each of these methods is tested in numerical experiments.

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Session CS16 – Inverse problems and Kalman filtering

Adaptive ODE Solvers in the Continuous-Discrete Extended Kalman Filtering Method I: Numerical Tests and Comparison

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This paper elaborates a new approach to nonlinear filtering based on an accurate implementation of the continuous-discrete extended Kalman filter (CD-EKF). It means that the arising moment differential equations for calculating the predicted state mean of the stochastic dynamic system and the corresponding error covariance matrix are solved accurately, i.e. with negligible error. The latter is achieved by using ODE solvers with global error control and allows the total error of the CD-EKF to be reduced, significantly. The new numerical scheme also retains the symmetry and the semi-positivity of the error covariance matrix, that is important for proper work of the CD-EKF. Eventually, our method results in a new *Accurate Continuous-Discrete Extended Kalman Filter*. The designed technique is compared numerically with other known implementations of the CD-EKF to confirm its outstanding performance on test problems.

Adaptive ODE Solvers in the Continuous-Discrete Extended Kalman Filtering Method II: Square-Root Implementation and Application to Target Tracking

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The new *Accurate Continuous-Discrete Extended Kalman Filter* based on the combined use of the embedded Runge-Kutta pair `NIRK4(2)` with the global error control from [1] and Mazzoni's scheme [2] is discussed in detail, here. First, its square-root variant is designed to improve accuracy and robustness for a finite-precision computer arithmetics. Then, it is examined in severe conditions of tackling a seven-dimensional radar tracking problem, where an aircraft executes a coordinated turn. The latter is considered to be a challenging one for testing nonlinear filtering algorithms. Our numerical results confirm that the presented technique is flexible and robust. It treats successfully (and without any additional tuning) the target tracking problem for various initial data and for a range of sampling times.

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Detection of weak inclusions in poroelastic soils using Small Amplitude Homogenization

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This contribution is devoted to the determination of subsurface images for the identification of aquifers, oil and gas reservoirs, which are very important for applications in hydrology, groundwater quality assessment, among many others. To this end, we consider the Biot's model for fully saturated poroelastic soils in time harmonic regime, where it is applied some recent developments for inverse problems as the small amplitude homogenization method. This conceives the construction of a minimizing sequence by assuming that the contrast between the two possible values for the parameters are not very large. Hence, it is performed an asymptotic approximation up to second order with respect to the contrast parameter, which lead us to a new set of simplified equations to solve. In particular, this evaluation involves the computation of the H-measure associated to the Biot's model. Finally, some numerical results will be shown to demonstrate the performance and reliability of this method.

Wavefield simulation and velocity inversion based on the acoustic wave equation

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In geophysical exploration the mathematical model based on the acoustic wave equation is usually adopted. Modelling the wave propagation underground and inversing the media velocity are very helpful in geophysical data processing. Here, we investigate numerical inversion methods for velocity based on the acoustic waveform. Waveform inversion is in fact an optimization problem which minimizes the residuals between the recorded data and the synthesized data. As the data are observed on the partial boundary this problem is the highly ill-posed problem. We use the least-square method to solve the problem. Various iterative methods such as the Gauss-Newton method and the Levenberg-Marquardt method may be used. The performance of the different iterative methods is compared. Considering the computational efficiency the second-order finite-difference method are used to simulate the wavefield. The absorbing boundary conditions in simulation are the Clayton-Engquist conditions.

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Session CS17 – Implicit-explicit methods for ODEs

Nordsieck methods with inherent quadratic stability

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We will discuss general linear methods (GLMs) for the numerical solution of systems of ordinary differential equations. They are characterized by four integers (p, q, r, s), where p is the order of the method, q is the stage order of the method, s is the number of internal stages and r is the number of external approximations.
In order to simplify the analysis of this class, we introduce the inherent quadratic stability property (IQS), i.e., the conditions on method's coefficients that guarantee that the stability function assumes quadratic form

$$p(w, z) = w^{r-1}(w^2 - p_1(z)w + p_0(z)),$$

where $p_1(z)$ and $p_0(z)$ are rational function of z. Then the stability properties are determined by the quadratic part of the stability polynomial.
We assume, that the vector of external stages approximates the Nordsieck vector. After applying order, stage order and IQS conditions we search for methods with desired stability properties.

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Multivalue methods for non-separable Hamiltonian systems

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This talk considers the properties of a new class of multivalue methods designed to integrate non-separable Hamiltonian problems. Computational comparisons are made with Gauss and DIRK methods.

Efficient Implicit-Explicit Runge-Kutta methods with low storage requirements

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Space discretization of some time-dependent PDEs gives rise to systems of ordinary differential equations in additive form

$$y' = f(y) + g(y)\,, \qquad y(t_0) = y_0\,, \tag{4}$$

where $f, g : \mathbb{R}^k \to \mathbb{R}^k$ are sufficiently smooth functions with different stiffness properties. For these problems, implicit methods should be used to treat the stiff terms while efficient explicit methods can still be used for the nonstiff part of the equation.
We consider different implicit-explicit Runge-Kutta methods for additive differential equations of the form (4). In the construction of Runge-Kutta methods, stability and accuracy properties should be taken into account. However, in some contexts, storage requirements of the schemes play an important role.

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A class of implicit-explicit general linear methods

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Implicit-explicit (IMEX) time stepping methods can efficiently solve differential equations with both stiff and nonstiff components. IMEX Runge-Kutta methods and IMEX linear multistep methods have been studied in the literature. In this talk we discuss new implicit-explicit methods of general linear type (IMEX-GLMs). We develop an order conditions theory for high stage order partitioned GLMs that share the same abscissae, and show that no additional coupling order conditions are needed. Consequently, GLMs offer an excellent framework for the construction of multi-method integration algorithms. Next, we propose a family of IMEX schemes based on diagonally-implicit multi-stage integration methods and construct practical schemes of order three. Numerical results confirm the theoretical findings.

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Session CS18 – Dynamical systems

Exponentially long transient oscillations in a class of cooperative cellular networks

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The real-time processing capabilities of CNNs are inherently related to the fast convergence time of the solutions toward the asymptotically stable equilibria. A typical requirement is that the settling time should not exceed a few (or at most ten) cell time constants. We report on a class of completely stable nonsymmetric cooperative CNN rings whose solutions display unexpectedly long transient oscillations for a wide set of initial conditions and interconnection parameters. Numerical simulations show that the oscillations can easily last hundreds of cycles, and thousands of cell time constants, before settling to a steady state, thus possibly impairing their real-time processing capabilities. Laboratory experiments on a discrete-component prototype of the CNN ring shows that the long oscillation phenomenon is physically robust with respect to the non-idealities of the circuit implementation. Finally, asymptotic estimates on the duration of the transients are given.

Modified Trigonometric Integrators

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We study modified trigonometric integrators, which generalize the popular class of trigonometric integrators for highly oscillatory Hamiltonian systems by allowing the fast frequencies to be modified. Among all methods of this class, we show that the IMEX (implicit-explicit) method, which is equivalent to applying the midpoint rule to the fast, linear part of the system and the leapfrog (Störmer/Verlet) method to the slow, nonlinear part, is distinguished by the following properties: (i) it is symplectic; (ii) it is free of artificial resonances; (iii) it is the unique method that correctly captures slow energy exchange to leading order; (iv) it conserves the total energy and a modified oscillatory energy up to second order; (v) it is uniformly second-order accurate in the slow components; and (vi) it has the correct magnitude of deviations of the fast oscillatory energy, which is an adiabatic invariant. These theoretical results are supported by numerical experiments on the Fermi-Pasta-Ulam problem and indicate that the IMEX method, for these six properties, dominates the class of modified trigonometric integrators.

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Multiple convective flows in porous annular domains

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Coexistence of multiple patterns in Lapwood convection (D. Lyubimov) was explained by cosymmetry theory (V. Yudovich). Study of the flows and its bifurcations for this problem requires special numerical methods to preserve cosymmetry in the discrete approximation of underlying system of partial differential equations. We analyze the family of steady convective fluid patterns in annular enclosure filled with a porous medium by the finite-difference method [1]. Results of computation of the families of steady states for two annular domains are given. Non-uniform stability spectra is found for convective patterns belonging to the family of steady states. The continuation of the family up to the appearance of unstable states is done and the scenario with simultaneous instability at three points is detected. So, this bifurcation is being a cosymmetrical effect not a symmetrical one.

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Symplectic simulation of guiding-center motion

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The guiding center motion of charged particles is the physical process that underlies the collective dynamics of magnetized plasmas. In numerical simulation for the guiding-center equation which is a Hamiltonian system with non-canonical symplectic structure, we transform it into canonical Hamiltonian system and use symplectic scheme. Compared with standard integrators, such as the fourth order Runge-Kutta method, the symplectic scheme has superior numerical properties over long integration time. This is important for modern large-scale simulation studies of fusion plasmas where it is critical to use algorithms with long-term accuracy and fidelity.

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