SciCADE 2015

2015 International Conference on Scientific Computation and Differential Equations

September 14–18, 2015

University of Potsdam, Potsdam, Germany

Book of Abstracts

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Plenary Talks

PDE control and numerics: Some recent progress and challenges

E. Zuazua

BCAM - Ikerbasque, Spain

Most applications not only involve modelling and forward resolution of PDE models but also parameter identification, control and observation problems. It turns out that a successful development of the needed computational tools cannot be achieved by simply superposing the state of the art on PDE, Control and Inverse Problem Theory, with classical Numerical Analysis.
The number of interesting and often difficult issues that arise in the interplay of numerics and PDE inversion and control are huge.
In this lecture we shall address some of them, with special focus on the following two ones:

–We first address the problem of inverse design, aiming to identify the initial source leading to a desired final configuration, in the context of hyperbolic or viscous conservation laws. This problem is ill-posed because of the instabilities of backward parabolic problems and, in the inviscid hyperbolic context, because of the lack of uniqueness. We discuss numerical strategies for an efficient inversion, in particular, in the presence of multiple solutions. This leads, in particular, to interesting open problems on the numerical approximation of all possible weak solutions of conservation laws and not only the entropic ones.

–We then analyse the impact of numerical meshes on the propagation properties of numerical solutions. When dealing with transport and wave equations, Fourier analysis allows showing that high frequency wave packets have the tendency of evolving very slowly, ruining the efficiency of inversion procedures. We show how, for a given inversion problem, taking its geometric features into account, an ad hoc computational mesh can be built so to ensure the efficient observation, inversion and control of all numerical waves.

We shall conclude describing some challenging open problems and possible directions for future research.

Low-rank ODEs for matrix nearness problems

N. Guglielmi

Università dell'Aquila and Gran Sasso Science Institute (GSSI), Italy

The topic of this talk is a methodology based on differential equations on low-rank matrix manifolds for the efficient solution of structured matrix nearness problems such as the distance to instability or to passivity of a matrix with a certain structure, or the distance of a given connected weighted graph to a nearest non-connected weighted graph.
In all cases we obtain a characterization of extremal perturbations, which turn out to be of low rank and are attractive stationary points of the low-rank differential equations that we derive.
We use a two-level approach; in the inner level we determine extremizers over the set of perturbations of a given norm, say epsilon, by following the low-rank differential equations up to a stationary point, and in the outer level we optimize with respect to epsilon.
This permits us to obtain fast algorithms - exhibiting quadratic convergence - for solving the considered matrix nearness problems.
The talk is inspired by recent and current works with Paolo Butta', Daniel Kressner, Christian Lubich, Manuela Manetta, Wim Michiels, Silvia Noschese, and Michael Overton.

Word series and mollified methods for highly oscillatory problems

M. Paz Calvo

Universidad de Valladolid, Spain

B-series have played a most important role in the analysis of numerical integrators, particularly so in the context of geometric integration. Word series are a recently introduced alternative. They possess a narrower scope of application but are easier to handle than B-series. In the talk I shall provide some general background on word series and present some applications, including the analysis of mollified methods for highly oscillatory problems.

Hessian-based Implicit Dimension Reduction for Large-scale Bayesian Inverse Problems

O. Ghatthas

The University of Texas, Austin, USA

Bayesian inference provides a systematic framework for quantifying uncertainty in the solution of ill-posed inverse problems. Given uncertainty in observational data, the forward model, and any prior knowledge of the parameters, the solution of the Bayesian inverse problem yields the so-called posterior probability of the model parameters, conditioned on the data. The fundamental challenge is how to explore this posterior density, in particular when the forward model is represented by PDEs and the uncertain parameters are given by (a discretized) infinite dimensional field. To overcome the prohibitive nature of Bayesian inversion for high-dimensional, expensive-to-evaluate models, we exploit the fact that, despite their large size, the observational data typically provide only sparse information on model parameters. This implicit dimension reduction is effected by low rank approximation of the data misfit Hessian, preconditioned by the prior covariance. We also discuss extensions of these ideas to low-rank approximations of higher-order derivative tensors.

The specific inverse problem we address here is the flow of ice from polar ice sheets such as Antarctica and Greenland, which is the primary contributor to projected sea level rise. One of the main difficulties faced in modeling ice sheet flow is the uncertain spatially-varying Robin boundary condition that describes the resistance to sliding at the base of the ice. Satellite observations of the surface ice flow velocity, along with a model of ice as a creeping incompressible shear-thinning fluid, can be used to infer this uncertain basal boundary condition. We cast this ill-posed inverse problem in the framework of Bayesian inference, which allows us to infer not only the basal sliding parameters, but also the associated uncertainty. We show results for Bayesian inversion of the basal sliding parameter field for the full Antarctic continent.

This work is joint with Nick Alger (UT-Austin), Tobin Isaac (UT-Austin), James Martin (UT-Austin), Noemi Petra (UC-Merced), and Georg Stadler (NYU).

Numerical methods in molecular dynamics

T. Lelièvre

École des Ponts ParisTech CERAMICS, Paris, France

Molecular dynamics is now a very widely used tool to study by numerical simulations the matter at the molecular level. It is used in various fields, such as biology, chemistry or materials science in order to relate the macroscopic properties of matter to its atomistic features.
One of the numerical difficulty is related to timescales: the typical timescale of a molecular dynamics simulation is much smaller than the typical timescale at which the crucial events, from a macroscopic viewpoint, occur. This is related to the metastability of a molecular dynamics trajectory.
Many methods have been proposed in the molecular dynamics community to deal with these difficulties, and we will focus on two prototypical ones for which a mathematical analysis gives useful insights. We will first present adaptive importance sampling techniques, which have been proposed to sample efficiently statistical ensembles. Then, we will propose a mathematical analysis of accelerated dynamics methods which have been introduced by A.F. Voter to generate efficiently metastable dynamics.

Well-balanced and scale-dependent time integration and for weakly compressible (atmospheric) flows

R. Klein

Frei Universität Berlin, Germany

Atmospheric flows feature a cascade of characteristic scales induced by the presence of several independent small dimensionless parameters in the governing equations. The most important ones are the Mach, Froude, and Rossby numbers. Depending on the length and time scales considered, different asymptotic limit regimes prevail, leading to very different typical flow behavior, as revealed by single-scale asymptotic analysis. The development of numerical schemes for the full three-dimensional compressible flow equations that properly respect such balances in each individual regime has a considerable history.

Current super-computers allow atmospheric modellers to resolve a broad range of these scales in one and the same simulation. The numericist is thus challenged to devise numerical integrators that simultaneously respect the asymptotic balances across all length and time scale combinations that arise in a particular flow case.

In the first part of this presentation I will introduce the asymptotic characterization of scale-dependent atmospheric flow regimes. In the second part, I discuss recent developments towards related multi-scale time integrators.

Multilevel Monte Carlo in the small noise setting: from jump to diffusion processes

D. Anderson

University of Wisconsin-Madison, USA

Monte Carlo methods are used ubiquitously in the study of stochastic processes. The multilevel Monte Carlo method of Mike Giles (2008), with related earlier work by Stefan Heinrich (1998), can dramatically increase the speed of Monte Carlo estimation by generating multiple samples from coupled pairs of processes (with different discretization parameters) and combining them in an appropriate manner. The computational complexity of multilevel methods depends sensitively upon the size of the variance between the coupled pairs of processes. In order to estimate this variance, at least asymptotically, it is often sufficient to simply analyze the L^2 distance between the pairs.

In this talk, I will consider multilevel Monte Carlo in the small noise setting. Stochastic models with small noise structure arise in a number of settings including biochemistry and cell biology, finance, computational fluid dynamics, ecology, neuroscience, and population dynamics. In this setting, I will show that the L^2 distance between coupled pairs of paths is sometimes asymptotically larger than the variance between the pairs, and, therefore, a direct analysis of the variance is necessary in order to obtain optimal complexity estimates. I will focus on the cases of (i) continuous time Markov chain models, as arise in biochemistry and cellular biology, and (ii) diffusion processes with small noise structure. In the diffusive setting, multilevel Monte Carlo combined with an Euler-Maruyama discretization is shown to work optimally without the need for discretization schemes that are customized to the small noise setting. Perhaps surprisingly, I will show that even though diffusion processes with small noise structure often arise as natural approximations to continuous time Markov chain models under an appropriate scaling, the variance of the coupled diffusion processes can not be inferred from the variance of the analogous coupled jump processes.

Minisymposia Talks

MS01 – Time integration of partial differential equations

Organized by: Marlis Hochbruck, Alexander Ostermann

Convergence of an ADI splitting scheme for the Maxwell system with currents

R. Schnaubelt

Karlsruhe Institute of Technology, Germany

The error analysis of an alternating direction implicit method for the Maxwell system on product domains is investigated. In a recent joint paper with M. Hochbruck and T. Jahnke, we proved second-order convergence of the time-discretization for the homogeneous Maxwell system. In a modified functional analytic framework, we now also treat non-zero resistancy, currents or charges.

Error analysis of the Lee-Fornberg ADI method for Maxwell's equations

T. Jahnke

Karlsruhe Institute of Technology, Germany

The propagation of electromagnetic waves is described by Maxwell's equations, and solving these equations numerically is a crucial task in numerous applications. For problems on a cuboid, alternating-direction implicit (ADI) methods are particularly attractive, and several such methods have been proposed in the literature. The idea is to decompose the operator of the Cauchy problem into two or more parts and to apply a splitting method to compute an approximation. This makes it possible to construct integrators which are unconditionally stable but computationally cheap, because only small (one-dimensional) linear problems have to be solved in each time-step.
In this talk, an ADI splitting method proposed by Lee & Fornberg (2003) and Chen, Li & Liang (2010) will be considered. In their approach, the Maxwell operator is decomposed in such a way that three pairs of one-dimensional wave equations have to be solved in each sub-step. We will present an error bound for the semi-discretization in time, discuss in which sense this improves earlier results, and sketch possible extensions.

Maxwell's Equations and Nano-Plasmonic Systems: A User Perspective

K. Busch

Humboldt University of Berlin, Germany

Discontinuous Galerkin methods represent powerful approaches for computing the optical properties of nano-structured systems. Corresponding time-domain simulations for plasmonic systems require material models that are amenable to auxiliary differential equation techniques. In this work, suitable models for the magneto-optic properties of transition metals as well as for the nonlocal and nonlinear properties of ordinary metals are described and a number of the resulting effects and phenomena are investigated. This includes the analysis of Kerr rotation angles, electron energy loss spectra, and second harmonic generation from nano-plasmonic structures.

Numerical solutions

E. Faou

INRIA, France

In this talk I will summarize some results concerning the numerical computation of ground states. I will first consider the behavior of the imaginary time Schroedinger equation used to compute the shape of solitons, and prove the convergence of this normalized gradient algorithm. I will then address the question of numerical orbital stability for the time evolution of the cubic nonlinear Schroedinger equation discretized by symplectic splitting methods. These are joint works with T. Jézéquel, D. Bambusi and B. Grébert.

Exponential integrators of EPIRK-type: theory and software

M. Tokman

University of California, Merced, United States of America

In this talk we will provide an overview of the latest advances in development of the exponential propagation iterative methods of Runge-Kutta (EPIRK) type. We explain the similarities between the EPIRK methods and other exponential integrators as well as the differences that enable construction of EPIRK schemes with desirable properties. We will discuss how the stiff order conditions and convergence theory can be extended to EPIRK methods and how the structural flexibility of EPIRK framework is utilized to construct efficient schemes. In addition, the new software package that implements the most efficient EPIRK schemes for serial and parallel platforms will be presented. Performance of the methods will be illustrated using problems from several applications.

Numerical treatment of reaction-diffusion problems by trigonometrically fitted methods

B. Paternoster and Raffaele D'Ambrosio

Department of Mathematics, University of Salerno, Italy

We deal with the numerical solution of partial differential equations, mainly focusing on systems of coupled reaction-diffusion equations, which are known to generate traveling waves as fundamental solutions. Such problems have been typically used as models for life science phenomena exhibiting the generation of periodic waves

along their dynamics, e.g. cell cycles, frequently behaving if they are driven by an autonomous biochemical oscillator, or intracellular calcium signalling, since calcium shows many differrent types of oscillations in time and space, in response to various extracellular signals.
The periodic character of the problem suggests to propose a numerical solution which takes into account this oscillatory behavior, i.e. by tuning the numerical solver to accurately and efficiently follow the oscillations appearing in the solution, since classical numerical methods would require the employ of a very small stepsize to accurately reproduce the dynamics. For this reason, we propose an adaptation of classical numerical schemes based on finite difference schemes which will take into account the qualitative nature of the solutions. Such schemes provide a twofold level of adaptation to the problem: along space, by means of finite differences based on nonpolynomial fitting techniques? along time, by means of special purpose numerical time solvers.The coefficients of the resulting methods will depend on the unknown values of parameters related to the problem (e.g. the values of the frequencies of the oscillations): suitable techniques leading to estimates of the parameters will be discussed. Practical constructive aspects and accuracy issues will be treated, as well as numerical experiments showing the effectiveness of the approach will be provided.

Numerical analysis of parabolic problems with dynamic boundary conditions

B. Kovács and C. Lubich

University of Tübingen, Germany

Space and time discretisations of parabolic differential equations with dynamic boundary conditions are studied in a weak formulation that fits into the standard abstract formulation of parabolic problems, just that the usual $L_2(\Omega)$ inner product is replaced by an $L_2(\Omega) \oplus L_2(\partial\Omega)$ inner product. The class of parabolic equations considered includes linear problems with time- and space-dependent coefficients and semi-linear problems such as reaction-diffusion on a surface coupled to diffusion in the bulk.
The spatial discretisation by finite elements is studied in the proposed framework, with particular attention to the error analysis of the Ritz map for the elliptic bilinear form in relation to the inner product, both of which contain boundary integrals. The error analysis is done for both polygonal and smooth domains. We further consider mass lumping, which enables us to use exponential integrators and bulk-surface splitting for time integration.

Numerical methods for KdV and related equations

N.H. Risebro

University of Oslo, Norway

We consider numerical, mainly finite difference, methods to approximate solutions of KdV like equations. The main focus is on proving the convergence of these methods as the discretization parameters vanish.

MS02 – Geometric integration of differential equations

Organized by: Elena Celledoni, Brynjulf Owren

Unconventional exponential methods for non-autonomous linear equations

F. Casas

Universitat Jaume I, Spain

In this talk we consider an initial value problem of the form $u'(t) = A(t)u(t)$, where $A(t)$ is a time-dependent matrix resulting from a spatial semi-discretization of some (unbounded) linear operator. Particular examples are the Schrödinger equation with a time-dependent potential and parabolic initial-boundary value problems.
Although exponential methods based on the Magnus expansion constitute a useful option in this context, they present nevertheless certain unfavorable features, derived from the presence of matrix commutators in the algorithm. For this reason, other commutator-free alternatives have been considered in the literature for solving different physical problems involving the Schrödinger equation. The resulting schemes, however, involve backward time integrations at intermediate stages when applied to autonomous problems and consequently suffer from poor stability properties for evolution equations of parabolic type. This limitation motivates the design and analysis of new (optimized) unconventional high-order schemes that are appropriate for the time integration of parabolic problems, such as those involving complex coefficients, as well as analyzing their corresponding stability and error behavior.
This talk is based on work done in collaboration with Mechthild Thalhammer and Sergio Blanes.

Explicit symplectic RKN methods for perturbed non-autonomous oscillators: splitting, extended and exponentially fitting methods

S. Blanes

Universitat Politècnica de València, Spain

We consider the numerical integration of perturbed non-autonomous oscillatory systems using high order methods. The autonomous case has been efficiently integrated using explicit and symplectic Runge-Kutta-Nyström (RKN) methods like extended RKN methods, exponentially fitting RKN methods and splitting methods for perturbed systems. Recently, it has been shown that explicit and symplectic extended RKN methods and exponentially fitting RKN methods are equivalent (Wu et al. BIT, 52 (2012), pp. 773–795) and in this work we show that these methods are also equivalent to splitting methods for perturbed oscillators. We provide a constructive proof which at the same time allows us to build for the first time new explicit and symplectic extended RKN methods for the non-autonomous problem (for multidimensional time dependent frequencies). The new methods obtained, while built from splitting methods, are different in the treatment of the time-dependent terms and can be superior in

some cases. We build some new methods and show their performance on numerical examples. More details can be found in [1].

[1] S. Blanes, Explicit symplectic RKN methods for perturbed non-autonomous oscillators: splitting, extended and exponentially fitting methods. Comput. Phys.Comm., 195 (2015), pp. 10-18.

Structure preserving methods for port-Hamiltonian systems

E. Calledoni and Hoel Høiseth

Norwegian University of Science and Technology, Norway

Port-Hamiltonian systems are a generalization of Hamiltonian systems allowing to include inputs and outputs. Port-Hamiltonian systems offer a simple paradigm for modelling complex physical systems by the energy-consistent interconnection of a (possibly large) number of simple subsystems. This approach can also be viewed as a technique for control design [1, 2, 3]. The structure-preserving (in particular passivity-preserving) integration of this generalisation of Hamiltonian systems is of interest both from a theoretical perspective and in engineering applications.

We present some preliminary results in the structure preserving discretization of port-Hamiltonian systems. We analyse these methods, focusing in particular on discrete energy-preserving and passivity-preserving interconnection of simpler systems.

[1] R. Ortega, A. van der Schaft, B.M. Maschke, Stabilization of port-controlled Hamiltonian systems via energy balancing Stability and stabilization of Nonlinear systems, Lecture Notes in Control and Information Sciences, vol 246, pp. 239-260.

[2] A. van der Schaft, Port-Hamiltonian systems: an introductory survey, Proceedings of the International Congress of Mathematics, 2006.

[3] H. Yoshimura and J.E. Marsden, Dirac structures in Lagrangian mechanics, Journal of Geometry and Physics, 2006.

Geometric Integration for Multi-Conformal-Symplectic PDEs

B. Moore

University of Central Florida, United States of America

Conformal Hamiltonian systems are generalized to PDEs where there is conformal symplectic structure in both space and time. The conformal symplectic structure in time generally takes the form of weak linear damping, but the conformal symplectic structure in space, could take many forms including nonlinear, diffusion, and convection terms. Though a multi-conformal-symplectic structure is very special, there are several PDEs that arise in applications which have this structure. In addition, a multi-conformal-symplectic conservation law has a concise form for these equations and has a straightforward interpretation in a discrete setting, paving the way for construction of discretizations that preserve the property. Presentation of methods of this type will be followed by a brief exploration of the benefits of using such discretizations.

Adaptive Energy Preserving Methods for Partial Differential Equations

S. Eignes, B. Owren and T. Ringholm

Norwegian University of Science and Technology, Norway

A method for constructing first integral preserving numerical schemes for time-dependent partial differential equations on non-uniform grids is presented. The method can be used with both finite difference and partition of unity approaches, thereby also including finite element approaches. The schemes may be extended to accommodate different kinds of adaptivity, while still preserving an approximated first integral. The method is applied to two test cases and results from numerical experiments are presented.

The construction of parallel energy-preserving methods for Hamiltonian systems

Y. Miyatake[a] *and J.C. Butcher*[b]

[a] Nagoya University, Japan

[b] The University of Auckland, New Zealand

Energy-preserving methods for Hamiltonian systems have been attracting attention in the last decades. In particular, one can construct high order integrators based on recently proposed the average vector field collocation method or Hamiltonian boundary value method. However, the computational costs of such integrators increase as the order of accuracy increases.
In this talk, we propose high order and parallel energy-preserving methods. For this aim, focusing on a matrix which characterizes continuous stage Runge–Kutta methods, we consider (i) an energy-preserving condition, (ii) order conditions and (iii) criteria for parallel implementation using real arithmetic. We then put together these perspectives to construct energy-preserving methods which can be computed in parallel. We derive concrete integrators up to order six.

Discrete variational derivative methods for the EPDiff equation

S. Larsson[a]*, T. Matsuo*[b]*, K. Modin*[a] *and M. Molteni*[a]

[a] Chalmers University of Technology, Sweden

[b] The University of Tokyo, Japan

We construct structure preserving schemes for the solution of the EPdiff equation, with particular emphasis on the two dimensional case. Three known schemes for the one-dimensional version of such an equation, based on the Discrete Variational Derivative Method (DVDM), are adapted to the 2-dimensional case, for a rectangular

domain discretized with a regular, structured, orthogonal grid. A predictor-corrector routine based on these schemes, and a new original scheme are also constructed. The numerical solutions we obtain have properties consistent with the nature of the equation, since the DVDM is known to preserve the Hamiltonian structure of the problem and to respect certain conservation laws. Numerical experiments are presented for the two-dimensional equation, in the case of interest, investigated also in several other recent papers, of interaction of singular wave fronts. An empirical convergence study is reported, together with an analysis of performance, preservation of energy and reversibility of the schemes. Although all the tests and schemes are only considered on a 2-dimensional domain, the generalization to a 3-dimensional domain follows straight-forward from our analysis.

Structure preserving model reduction on Lie groups

E. Calledoni[a], *B. Owren*[a] *and H. Parks*[b]

[a] NTNU, Norway

[b] UCSD, USA

Model reduction via Principal Orthogonal Decomposition (POD) is widely used in fluid dynamics, but it has also been applied in other areas, including control. POD, also known as the Karhunen-Loewe expansion and Principal Component analysis, produces a least-squares optimally ordered basis for a given set of data. In model reduction applications, POD is used to identify an ordered basis of (linear) phase space from a set of data points called snapshots. Truncating the POD basis and projecting the dynamics onto that subspace provides a lower-dimensional model of the system.
In this work we shall seek to adapt this approach to mechanical systems on Lie groups. It is of essence to find a reduced model which inherits the geometric features of the original problem, either in the Lagrangian or Hamiltonian setting. The fact that the phase space in question is a manifold poses additional difficulties. Lall, Krysl and Marsden (2003) proposed to accomplish this by first embedding the manifold into a larger Euclidean space, perform standard model reduction there and finally intersecting the reduced (linear) model space by the original manifold. We have not been able to develop this strategy in a way such that efficient methods can be obtained, but have instead opted for an approach where local coordinates is applied. This causes however other difficulties, in particular related to the switching of coordinate charts. There are various ways to address the problem and we shall present one way that seems promising in terms of numerical results.

MS03 – Geometric numerical integration of PDEs

Organized by: Erwan Faou

Locally implicit time integration for linear Maxwell's equations

M. Hochbruck and A. Sturm

Karlsruhe Institute of Technology, Germany

An attractive feature of discontinuous Galerkin (DG) spatial discretizations of the Maxwell equations is their ability to handle complex geometries by using unstructured, possibly locally-refined meshes. Furthermore, DG methods lead to block diagonal mass matrices which in combination with an explicit time integration method allow for a fully explicit scheme. However, such explicit approaches require a constraint on the time step size related to the smallest mesh element to ensure stability. This makes the simulation inefficient if the number of tiny elements is small compared to the total number of elements. A natural way to overcome this restriction is obtained by using implicit time integrators but at the expense of having to solve a large linear system each time step.

A more suitable approach consists in treating only the tiny mesh elements implicitly while retaining an explicit time integration for the remaining elements. This results in so called locally implicit methods.

In this talk we will present an error analysis for the full discretization of locally implicit methods based on a variational formulation and energy techniques.

On numerical Landau damping for the Vlasov-HMF model

R. Horsin

Inria Rennes, France

We consider solutions of the Vlasov-HMF model starting in a small Sobolev neighborhood of a spatially homogeneous stationary state satisfying a stability criterion (Penrose criterion), and time discretizations of these solutions based on splitting methods (Lie & Strang) between the linear and non-linear part of the equation. We prove that the numerical solutions converge weakly to a modified state (Landau damping) which is close to the continuous one. We also prove that our numerical scheme is convergent, with a convergence rate of order one for Lie splittings, and two for Strang splittings.

Numerical computation of travelling waves for the Nonlinear Schrödinger equation in dimension 2.

D. Chiron[b] *and C. Scheid*[a]

[a] University of Nice & INRIA Sophia Antipolis, France

[b] University of Nice, France

We are interested in the numerical study of the two dimensional travelling waves of the Nonlinear Schrödinger Equation for a general nonlinearity and with nonzero condition at infinity. The equation has a variational structure that we propose to exploit to design a numerical method. We characterize certain saddle points of the action as minimizers of another functional, allowing us to use a gradient flow. Combining this approach with a continuation method in the speed of the wave, we obtain the numerical solution for the full range of velocities. We plot the energy-momentum diagrams for different type of non-linearities. Through various examples, we show that even though the nonlinearity has the same behaviour as the well-known Gross-Pitaevskii (GP) nonlinearity, the qualitative properties of the travelling waves may be extremely different. For instance, we observe cusps, a modified Kadomtsev-Petviashvili I (KP-I) asymptotic in the transonic limit (as the speed of the wave approaches the speed of sound), various multiplicity results. Excited states are also of interest. Even though we do not have at our disposal the same minimization structures, we managed to compute new branches of solutions with the continuation method.

Multisymplectic integrators for geometrically exact beam dynamics

F. Gay-Balmaz

CNRS / Ecole Normale Superieure de Paris, France

Multisymplectic variational integrators are structure preserving numerical schemes especially designed for PDEs derived from covariant spacetime Hamilton principles. In this talk I will present a class of multisymplectic variational integrators for mechanical systems on Lie groups. The multisymplectic scheme is derived by applying a discrete version of the spacetime covariant Hamilton principle. The Lie group structure is used to rewrite the discrete variational principle in a trivialized formulation which allows us to make use of the vector space structure of the Lie algebra, via the use of the Cayley map. In presence of symmetries, we derive a discrete version of the covariant Noether theorem. This approach is used to construct a multisymplectic integrator for geometrically exact beams.

A conservative discontinuous Galerkin scheme for the two-dimensional Navier-Stokes equations

L. Einkemmer and M. Wiesenberger

University of Innsbruck, Austria

In this talk we consider a conservative discretization of the two-dimensional incompressible Navier-Stokes equations. It is well known that the continuous model conserves vorticity, kinetic energy, and enstrophy. If long time scale phenomena (such as zonal flows and mean equilibrium shear flows in the edge of fusion plasmas) are of interest, conservation of these invariants is of paramount importance for a successful numerical method.
Arakawa's classical finite difference scheme for fluid flow in the vorticity-stream function formulation succeeds in preserving the linear (vorticity) and the two quadratic invariants (kinetic energy and enstrophy) for the semi-discrete problem (i.e. where space is discretized but time is left continuous).
In this talk we propose an extension of Arakawa's classical finite difference scheme to a high order discontinuous Galerkin approximation. In this context we reinterpret Arakawa's finite difference scheme as a consequence of the product rule which is not necessarily satisfied for a given space discretization. This allows us to obtain discontinuous Galerkin methods of arbitrary order which conserve the three invariants considered above.
In addition, we show numerical simulations that demonstrate the accuracy of the scheme and verify the conservation properties. Furthermore, we discuss the massively parallel implementation on graphic processing units, where a speedup of up to a factor of six is observed as compared to a similar parallel implementation on the CPU.

Multiscale methods and analysis for the nonlinear Klein-Gordon equation in the nonrelativistic limit regime

W. Bao

National University of Singapore, Singapore

In this talk, I will review our recent works on numerical methods and analysis for solving the nonlinear Klein-Gordon (KG) equation in the nonrelativistic limit regime, involving a small dimensionless parameter which is inversely proportional to the speed of light. In this regime, the solution is highly oscillating in time and the energy becomes unbounded, which bring significant difficulty in analysis and heavy burden in numerical computation. We begin with four frequently used finite difference time domain (FDTD) methods and obtain their rigorous error estimates in the nonrelativistic limit regime by paying particularly attention to how error bounds depend explicitly on mesh size and time step as well as the small parameter. Then we consider a numerical method by using spectral method for spatial derivatives combined with an exponential wave integrator (EWI) in the Gautschi-type for temporal derivatives to discretize the KG equation. Rigorious error estimates show that the EWI spectral method show much better temporal resolution than the FDTD methods for the KG equation in the nonrelativistic limit regime. In order to design a multiscale method for the KG equation, we establish error estimates of FDTD and EWI spectral methods for the nonlinear Schrodinger equation perturbed with a wave operator. Based on a large-small amplitude wave decompostion to the solution of the KG equation, a multiscale method is presented for discretizing the nonlinear KG equation in the nonrelativistic limit. Rigorous error estimates show that this multiscale method converges uniformly in spatial/temporal discretization with respect to the small parameter for the nonlinear KG equation in the nonrelativistic limite regime. Finally, applications to several high oscillatory dispersive partial differential equations will be discussed.

Plane wave stability of numerical discretizations for the NLS under perturbations of low order

L. Gauckler

Technische Universität Berlin, Germany

The cubic nonlinear Schrödinger equation on a torus has solutions that are plane waves. In the talk, the stability of these solutions under small perturbations after a numerical discretization by the split-step Fourier method will be discussed. In contrast to previous work, the focus will be on perturbations that are small in a low-order Sobolev space, which requires different techniques of proof.

Structure-preserving integration of the Benjamin type equations

T. Matsuo[a], *Kimiaki Kinugasa*[a] *and Yuto Miyatake*[b]

[a] The University of Tokyo, Japan

[b] Nagoya University, Japan

The Benjamin equation (Benjamin, 1992) and Benjamin–Ono equation (Benjamin, 1967; Ono, 1975) describe one-dimensional internal waves in fluids. They are non-local partial differential equations involving the Hilbert transform, and have several geometric structures with associated invariants. Although for the Benjamin–Ono equation there have been some numerical challenges, there seems quite few for the Benjamin equation, and no structure-preserving integrators in the literature for both equations. In this talk, we discuss some structure-preserving discretizations of the Benjamin type equations.

MS04 – Advanced time-stepping methods for wave propagation

Organized by: Marcus Grote, Stéphane Lanteri

Efficient multiple time-stepping algorithms of higher order

A. Demirel[a], *J. Niegemann*[b], *K. Busch*[c] *and* *M. Hochbruck*[a]

[a] Karlsruhe Institute of Technology, Germany

[b] ETH Zürich, Switzerland

[c] Humboldt-University Berlin, Germany

Multiple time-stepping (MTS) algorithms allow to efficiently integrate large systems of ordinary differential equations, where a few stiff terms restrict the timestep of an otherwise non-stiff system. In this talk, we discuss a flexible class of MTS techniques, based on multistep methods. Our approach contains several popular methods as special cases and it allows for the easy construction of novel and efficient higher-order MTS schemes. In addition, we demonstrate how to adapt the stability contour of the non-stiff time-integration to the physical system at hand. This allows significantly larger timesteps when compared to previously known multistep MTS approaches. As an example, we derive novel predictor-corrector (PCMTS) schemes specifically optimized for the time-integration of damped wave equations on locally refined meshes. In a set of numerical experiments, we demonstrate the performance of our scheme on discontinuous Galerkin time-domain (DGTD) simulations of Maxwell's equations.

Asynchronous numerical scheme for modeling hyperbolic systems

A. Toumi[a], *G. Dufour*[a], *R. Perrussel*[b], *T. Unfer*[b]

[a] ONERA, France

[b] Université de Toulouse, LAPLACE, CNRS/UPS/INPT, Toulouse, France

Numerical simulation has become a central tool for the modeling of many physical systems such as atmospheric plasmas or wave propagation. Multi-scale phenomena make the integration of these models very difficult in terms of accuracy and computation time. We developed an asynchronous method for the explicit integration of multi-scale partial differential equations. The asynchronous algorithm permits the selection of independent time steps in each mesh element so that the local time steps do not bear an integral relation to each other. The time advance is done by organizing computational elements into a priority queue based on their precomputed update times. First, we developed an asynchronous forward Euler scheme for modeling hyperbolic systems. We proved that this method converges faster than the classical first order scheme. Moreover, we noted good numerically properties of this scheme : it reduces numerical diffusion and computational cost. To improve the convergence rate of the asynchronous scheme, we derived an asynchronous Runge-Kutta 2 scheme (ARK2) from a standard explicit Runge-Kutta method. We assessed via numerical simulations, that the ARK2 scheme is second order

convergent and it is effective in term of computation time for a fixed error in comparison with the classical integration.

Runge-Kutta type explicit local time-stepping methods for wave propagation

M. Grote and M. Mehlin

University of Basel, Switzerland

Locally refined meshes severely impede the efficiency of explicit Runge-Kutta (RK) methods for the simulation of time-dependent wave phenomena. By taking smaller time-steps precisely where the smallest elements are located, local time-stepping (LTS) methods overcome the bottleneck caused by the stringent stability constraint of but a few small elements in the mesh. Starting from classical or low-storage explicit RK methods, explicit LTS methods of arbitrarily high accuracy are derived. When combined with an essentially diagonal
finite element mass matrix, the resulting time-marching schemes retain the high accuracy, stability and efficiency of the original RK methods while circumventing the geometry-induced stiffness. Numerical experiments with continuous and discontinuous Galerkin
finite element discretizations corroborate the expected rates of convergence and illustrate the usefulness of these LTS-RK methods.

Implicit hybridizable discontinuous Galerkin method for time-domain electromagnetics

A. Christophe Argenvillier[a], S. Descombes[b] and S. Lanteri[a]

[a] INRIA, France

[b] University of Nice - Sophia Antipiolis, France

Discontinuous Galerkin (DG) methods have been the subject of numerous research activities in the last 15 years and have been successfully developed for various physical contexts modeled by elliptic, mixed hyperbolic-parabolic and hyperbolic systems of PDEs. One major drawback of high order DG methods is their intrinsic cost due to the very large number of globally coupled degrees of freedom as compared to classical high order conforming finite element methods. Different attempts have been made in the recent past to improve this situation and one promising strategy has been recently proposed by Cockburn et al. in the form of so-called hybridizable DG formulations. The distinctive feature of these methods is that the only globally coupled degrees of freedom are those of an approximation of the solution defined only on the boundaries of the elements of the discretization mesh. The present work is concerned with the study of such a hybridizable DG method for the three-dimensional time-domain Maxwell equations time integrated by an implicit scheme.

MS05 – Multiscale and splitting methods: Theory and Applications

Organized by: Jürgen Geiser

Recent advanced in Iterative Splitting Methods for Multicomponent and Multiscale: Theory and Applications

J. Geiser

Ruhr University of Bochum, Germany

Since recent years, decomposition methods for multicomponent and multiscale problems have become an increasingly important role in the numerical solution for spatial-and time-dependent partial differential equations. Decomposition strategies are important to reduce computational time of large scale and multicomponent and multiscale problems and are nowadays applied to physical and engineering problems. Since recent years, decomposition methods for multicomponent and multiscale problems have become an increasingly important role in the numerical solution for spatial-and time-dependent partial differential equations. Decomposition strategies are important to reduce computational time of large scale and multicomponent and multiscale problems and are nowadays applied to physical and engineering problems. Based on the ideas of the physical conservations of the problems, the methods have taken into account the numerical and physical errors of the problems. The talk will present the latest research results in iterative splitting methods of high accuracy, efficiency and effectiveness in the field of multiscale and multicomponent problems. Iterative Splitting schemes use relaxation and linearization methods to overcome nonlinear problems in space and time of the partial differential equations. We investigate the following topics for important engineering and physics applications and discuss:
1.) Theory of iterative splitting and multi-splitting methods, see [1].
2.) Iterative Splitting methods as Multiscale solvers, see [2].
3.) Stability and convergence of iterative splitting methods, see [1].
4.) Engineering applications in computational fluid-dynamics (CFD) problems based on deterministic and stochastic differential equations, see [3] and [4].
At the end of the talk, we summarize our results.

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A new generation of symplectic integrators for perturbed systems

F. Casas

Universitat Jaume I, Spain

We present new families of symplectic splitting methods designed for the long time numerical integration of Hamiltonian systems which are perturbations of integrable ones. Based on a previous derivation of an independent set of necessary and sufficient conditions to be satisfied by splitting methods to achieve a prescribed order, we identify the relevant equations for the class of problems at hand and construct several sets of coefficients. In addition, we apply the processing technique to get splitting methods involving a reduced number of stages. The resulting integrators are appropriate for dealing with different problems in dynamical astronomy, and in particular for the numerical simulation of the Solar System described in both Jacobi and Heliocentric coordinates.
This talk is based on work done in collaboration with Sergio Blanes, Ariadna Farrès, Jacques Laskar, Ander Murua and Joseba Makazaga.

Pathwise analysis for split-step methods and multiscale variable splitting in spatial stochastic kinetics

S. Engblom

Uppsala University, Sweden

I this talk I will review recent progress in spatial stochastic modeling within the reaction-diffusion framework. In particular, I will present some analysis of split-step methods and certain multiscale approximations, all performed in a pathwise, or "strong" sense. These analytical techniques hint at how effective (i.e. parallel) numerical implementations can be designed. Some fairly large-scale simulations will serve as illustrations of the inherent flexibility of the modeling framework. While much of the initial motivation for this work came from problems in cell biology, I will highlight examples from epidemics and neuroscience.

Modelling turbulent time series by Ambit Stochastics

J.R. Schmiegel

University of Aarhus, Denmark

We review some recent developments in the field of Ambit Stochastics with focus on the special case of Brownian semistationary processes. As an application, the modelling of time series of the energy dissipation in a turbulent flow by continuous cascade processes and the modelling of time series of the turbulent velocity are discussed.

Asynchronous Multi-Splitting Waveform Relaxation Methods for Differential Equations: Theory and Applications

J. Geiser

Ruhr University of Bochum, Germany

Based on the motivation of systematic studying transport networks, in order to improve the stability, the robustness, and the sustainability of these systems, we study delicate models of differential-algebraic equation (DAE) systems, which are nonlinear and stiff. To solve such delicate large DAE systems, we have take into account parallel time-integration methods and also fast solvers for the nonlinear and stiff equations. In the talk, we concentrate on novel algorithms, that based on so called Multi-splitting Waveform relaxation methods, that can be coupled by Parareal methods, to obtain efficient solver of differential equations and differential algebraic equations. We discuss the super-linear convergence theory of the novel algorithms. We extend the convergence to Multi-splitting Waveform-relaxation (MSWR) methods coupled with Parareal algorithms. Further, we present some first experiments of the transient stability analysis of large power systems.
This talk is based on work done in collaboration with Frederic Magoules, CentraleSupelec Paris, France.

Planar finite element modeling of hollow and locked-coil helical constructions

N. Karathanasopoulos

ETH Zurich, Switzerland

The current work addresses the mechanical response of helical structures with non-circular cross sections. To that extent, a planar finite element model for the analysis of the helix axial, torsional and thermal loading mechanical response is explicated. Thereupon, the impact of the cross section shape on the construction?s stiffness properties is elaborated, while the applicability limits of analytical, closed-form expressions are demarcated. Finally, the computational cost of the numerical scheme is analyzed, highlighting its merits.

Differential-Algebraic Equations: an Overview

R. McKenzie[a], *J. Pryce*[a], *N. Nedialkov*[b] *and G. Tan*[b]

[a] Cardiff University, United Kingdom

[b] McMaster University, Canada

Differential-Algebraic Equations frequently occur in different application areas, such as control problems, electronic circuits and the solution of discretized PDEs. This talk aims to present an overview of how DAEs arise in such areas and presents ways of solving them, specifically focusing on index reduction and a new approach by the authors that eliminates some issues found in the commonly used Dummy Derivative index reduction technique.

The locally extrapolated exponential time differencing LOD scheme for multidimensional reaction-diffusion-advection systems

A.Q.M. Khaliq

Middle Tennessee State University, United States of America

We introduce the local extrapolation of first order locally one-dimensional exponential time differencing scheme for numerical solution of multidimensional nonlinear reaction?diffusion-advection systems. This novel scheme has the benefit of solving multidimensional problems in locally one dimensional fashion by implementing sequences of tridiagonal matrix solvers instead of solving a banded system. The storage size needed for solving systems in higher dimensions with this scheme is similar to that needed for one spatial dimension systems. The stability, monotonicity, and convergence of the locally extrapolated exponential time differencing scheme have been examined. Stability analysis shows that the scheme is strongly stable (L-stable) and is particularly beneficial to nonlinear partial differential equations with irregular initial data or discontinuity involving initial and boundary conditions due to its ability to damp spurious oscillations caused by high frequency components in the solution. The performance of the novel scheme has been investigated by testing it on a two-dimensional Schnakenberg model, two and three-dimensional Brusselator models, and a three-dimensional enzyme kinetics of Michaelis-Menten type reaction-diffusion model. Numerical experiments demonstrate the efficiency, accuracy, and reliability of the scheme.

MS06 – Modelling, theory and numerical approximation of nonlinear waves

Organized by: V.A. Dougalis, A. Duran

Toward a justification of variational asymptotics for multiscale systems with strong gyroscopic forcing

M. Oliver

Jacobs University, Germany

In systems with strong gyroscopic forces, approximate equations for the dynamics on a slow manifold can be found via variational asymptotics. The results generally differ from those obtained by classical Hamiltonian normal form theory. We explain the method, using the non-relativistic limit of the nonlinear Klein-Gordon equation as an example, and prove a shadowing result for this particular case.

A modified Galerkin / Finite Element Method for the Serre-Green-Naghdi system

D. Mitsotakis

Victoria University of Wellington, New Zealand

We solve numerically the Serre-Green-Naghdi (SGN) system using a stable, accurate and efficient fully discrete numerical scheme based on a modified Galerkin/finite element method. Although the SGN equations contain third-order derivatives, the modified Galerkin/finite element method allows the use of Lagrange finite elements and combined with explicit Runge-Kutta schemes for the discretization in time approximate solutions of the SGN system with variable bottom efficaciously. Compared to other methods, such as finite volume and discontinuous Galerkin methods, that have been applied for the same system, finite element methods appeared to have certain advantages since they are not dissipative and also can approximate the high order nonlinear terms very accurately. After reviewing the properties of the proposed numerical scheme, a detailed study of the dynamics of the solitary waves of the SGN system over variable bottom topographies is presented. A numerical study of the various collisions of solitary waves with wall boundaries is being performed while in some cases a comparison with experimental data is presented.

Aposteriori error control and adaptivity for Schrodinger equations

T. Katsounis[a] *and I. Kyza*[b]

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

[b] University of Dundee, Dundee, UK

We derive optimal order a posteriori error estimates for fully discrete approximations of linear Schrodinger-type equations. For the discretization in time we use the Crank-Nicolson method, while for the space discretization we use finite element spaces that are allowed to change in time. The derivation of the estimators is based on a novel elliptic reconstruction that leads to estimates which reflect the physical properties of Schrodinger equations. The final estimates are obtained using energy techniques and residual-type estimators. Various numerical experiments for the one-dimensional linear Schrodinger equation in the semiclassical regime, verify and complement our theoretical results. The numerical implementations are performed with both uniform partitions and adaptivity in time and space. For adaptivity, we further develop and analyze an existing time-space adaptive algorithm to the cases of Schrodinger equations. The adaptive algorithm reduces the computational cost substantially and provides efficient error control for the solution and the observables of the problem, especially for small values of the Planck constant.

The analysis is extended also for the nonlinear Schrodinger eq.

Mathematical modeling of large amplitude internal waves

R. Barros

MACSI, University of Limerick, Ireland

Large amplitude internal solitary waves excited typically by the interaction of tidal currents with bottom topography have been observed frequently in coastal oceans through in-situ measurements and satellite images. The simplest physical setup supporting internal wave motion is that of a two-layer incompressible Euler fluid in a channel. Weakly nonlinear models have been extensively used to study internal waves and, among them, the (uni-directional) KdV model have played a crucial role in the early investigations of these waves. However, internal solitary waves often have amplitudes comparable to the thickness of the well-mixed upper layer, which limits considerably the validity of these models. Hence, the need for more elaborate higher-order nonlinear models allowing a more accurate description of internal waves. We will describe in this talk our recent attempts to develop new mathematical models for the time evolution of these highly nonlinear features and present some remaining challenges.

A hybrid finite volume-finite difference scheme for weakly dispersive shallow water flows

C. Escalante[a], *T. Morales de Luna*[b] *and M.J. Castro Díaz*[a]

[a] UMA, Spain

[b] UCO, Spain

Shallow water equations are not appropriate for deep or moderate waters simulations where frequency dispersion effects may become more important that nonlinearity. In this framework, Boussinesq type models are commonly used.

Boussinesq [1] described a system of equations when the vertical velocity component is included in the integrated motion equations. Both Madsen-Sorensen [5] and Nwogu [6] improved Boussinesq equations to cover a wide range of the coastal area (i.e. from intermediate to shallow waters). These models were extended to cover the dynamics of the surf zone, by considering some mechanisms of wave breaking ([4], [8]). Both models could be split into two parts: one corresponding to the non-linear shallow water system in conservative form and the other corresponding to the high order dispersive terms. Following [4] and [7] we have developed an efficient second-order well-balanced numerical method, which combines finite-volume and finite-difference schemes. The hyperbolic part of the system is discretized using a PVM path-conservative finite-volume method [2], and the dispersive terms with compact finite differences. The resulting ODE system is discretized using a TVD Runge-Kutta method [3]. Although the scheme implies solving a big linear system, we present an efficient way to solve it and easy to parallelize.

A breaking mechanism similar to [4] is adopted, exploiting the fact that in very shallow flows, dispersive terms become negligible, so the models collapses onto Shallow Water equations, matching from a dispersive model to the nonlinear shallow water discretized by means of a finite volume method.

Finally, some numerical tests including comparisons with laboratory data will be presented.

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On shallow capillary-gravity waves

D. Dutykh[a], *A. Galligo*[b] *and D.Clamond*[b]

[a] CNRS - University Savoie Mont Blanc, France

[b] University of Nice Sophia Antipolis

In this talk we are going to discuss the problem of travelling capillary-gravity waves in the shallow water regime. The governing equations are provided by the fully nonlinear Serre-Green-Naghdi system completed with the surface tension term. In the first time we will discuss the formulation for travelling waves based on the conservation laws. Then, we will show that these solutions will belong to a family of algebraic curves parametrized by the Froude and Bond numbers. Finally, we will employ some methods of the algebraic geometry in order to classify the possible topologies of these curves depending on the values of physical parameters.

Galerkin - finite element methods for the Shallow Water equations with characteristic outflow boundary conditions *

V. Dougalis and D. Antonopoulos

Institute of Applied and Computational Mathematics-FORTH, Greece

We consider the Shallow Water equations (SW) in one space dimension, posed on a finite interval, in the subcritical or supercritical flow regime. At the endpoints of the interval we impose outflow characteristic boundary conditions, that, as is well known, are transparent for the SW. The initial-boundary value problems (ibvp's) for the SW with these boundary conditions are known to possess smooth solutions, locally in time. We discretize the ibvp's in space using the standard Galerkin - finite element method with continuous, piecewise polynomial functions of degree $r-1$, $r \geq 2$, on a quasiuniform mesh with maximum meshlength h, and prove, in the case of smooth solutions, error estimates in L^2 for the resulting semidiscretizations with error bounds of $O(h^{r-1})$, when $r \geq 3$.
We consider in particular the spatial discretization with piecewise linear continuous functions, which are $O(h^2)$ accurate in L^2 in the case of uniform mesh, and discretize the resulting semidiscrete problem in time using the classical, explicit, fourth-order accurate Runge-Kutta method. The fully discrete problem can be implemented in a straightforward way for both flow regimes considered, and it is stable under a Courant-number restriction. We test the method in several numerical experiments involving subcritical and supercritical flows, and conclude that the numerical characteristic boundary conditions are highly absorbing. We also compare the (nonlinear) characteristic boundary conditions in the subcritical case with their linearized analogs and show, by means of numerical experiment, that the latter are less accurate, i.e. less absorbing.

* This work was performed at IACM/FORTH in the framework of the PEFYKA project within the KRIPIS Action of the GSRT. The project is funded by Greece and the European Regional Development Fund of the European Union under the NSRF and the O.P. Competitiveness and Entrepreneurship

On Benjamin type equations for internal wave propagation. A numerical study

A. Duran

University of Valladolid, Spain

The talk is focused on Benjamin type equations as models for the evolution of waves on the interface of a two-layer fluid system under gravity and surface tension effects. A numerical study of the models is introduced. It is focused on the numerical generation and stability of solitary wave solutions and explores some cases of singularity formation.

MS07 – Discontinuous dynamical systems: Theory and numerical methods

Organized by: Luciano Lopez, Cinzia Elia

Classification of hidden dynamics in discontinuous dynamical systems

E. Hairer

University of Geneva, Switzerland

This talk considers ordinary differential equations with discontinuous right-hand side, where the discontinuity of the vector field takes place on smooth hyper-surfaces of the phase space. Solutions may traverse a hyper-surface, but they can also stick in them (Filippov's sliding mode).

A complete classification of possible transitions of solutions close to the intersection of two discontinuity surfaces is given. The result is sometimes counterintuitive. In the presence of high oscillations in solutions of the regularized differential equation, the new insight permits to propose a simple modification that suppresses these high oscillations and makes the numerical treatment much more efficient.

This is joint work with Nicola Guglielmi from the University of L'Aquila.

Discontinuous dynamical systems in the neighborhood of a co-dimension 2 discontinuity manifold: can one say what should happen?

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

[a] University of Bari, Italy

[b] Georgia Institute of Technology

In this talk we consider non smooth dynamical systems of Filippov's type in the neighborhood of a co-dimension 2 discontinuity manifold Σ. We are concerned with the behavior of solutions both when Σ is attractive and when Σ ceases to be attractive. This loss of attractivity will be characterized through the definition of generic potential exit points. We consider a "typical" trajectory of the non smooth dynamical system together with solutions of space regularizations in a neighborhood of Σ.

Most stable trajectories of linear switched systems

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

[a] University of Trieste, Italy

[b] University of L'Aquila, Italy

We deal with discrete-time *linear switched system* of the form

$$x(n+1) = A_{\sigma(n)}\, x(n), \quad \sigma : \mathbf{N} \longrightarrow \{1, 2, \ldots, m\},$$

where $x(0) \in \mathbf{R}^k$ and $A_{\sigma(n)} \in \mathbf{R}^{k\times k}$ is an element of a finite family of matrices $\mathcal{F} = \{A_i\}_{1\le i\le m}$ associated to the system and σ denotes the *switching law*.
It is known that the *most stable switching laws* are associated to the so-called *spectrum-minimizing products* of the family $\mathcal{F}$. Moreover, for a family $\mathcal{F}$ of matrices which share an invariant convex cone K and is normalized (i.e., its *lower spectral radius* $\check{\rho}(\mathcal{F})$ is equal to 1), for any initial value $x(0)$ in the interior of K the *most stable trajectories* lie on the boundary of the *unit antiball* of a so-called *invariant Barabanov antinorm*.
So far no general constructive method was proposed to determine such invariant Barabanov antinorms. In this talk (see also Guglielmi & Zennaro [2]) we show how, parallel to the constructive procedure for polytope extremal antinorms recently introduced by Guglielmi & Protasov [1], a canonical constructive procedure for invariant polytope Barabanov antinorms can be automatically provided as well.
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Numerical simulation of discontinuous reactions in diagenesis

A. Scotti, A. Agosti, B. Giovanardi and L. Formaggia

Politecnico di Milano, Italy

The process by which rocks are formed from an initial sediment, due to a burial process, consists of the coupled effects of mechanical compaction and geochemical reactions, that can significantly alter the porosity and permeability of the rock because of dissolution and precipitation processes. Such processes often present discontinuous behaviours that can be effectively modelled by differential ODEs with discontinuous right
hand side, where the discontinuity depends on the solution itself. We present a numerical model to simulate the coupled problem of flow, compaction and reaction treating the discontinuous right hand side by means of specially tailored event-driven numerical schemes. We show their performances in terms of positivity, mass conservation and accuracy also with comparison with more traditional approaches that rely on a regularization of the discontinuous terms.

A Runge-Kutta code for the solution of non-smooth Filippov IVPs

J.I. Montijano, M. Calvo and L. Rández

Universidad de Zaragoza, Spain

In this talk an adaptive Runge-Kutta code, based on the DOPRI5(4) pair for solving discontinuous Initial Value Problems for differential systems is presented. A remarkable feature of this code is its automatic detection and accurate location of the discontinuity points of the numerical solution and the restarting of the integration after them. The code requires from the user only a well defined description of the vector field of the system and the functions defining the hypersurfaces where the discontinuities are located. Further, in the case of Filippov systems, algorithms to handle properly sliding regions in an automatic way are included. Several numerical experiments are presented to illustrate the reliability and efficiency of the code.

Numerical treatment of discontinuous dynamical systems generating periodic orbits

R. D'Ambrosio [a], *L. Dieci*[b] *and F. Difonzo*[b]

[a] University of Salerno, Italy

[b] Georgia Institute of Technology, Atlanta, USA

It is the purpose of this talk to present recent advances in the numerical solution of piecewise smooth dynamics systems, described by systems of ordinary differential equations with discontinuous right-hand side. It is well known that such systems generate complex dynamics (e.g., crossing the discontinuity surfaces, sliding motion on surfaces of several co-dimensions, exiting from the discontinuity surfaces, etc.), which have to be accurately and efficiently handled by a reliable numerical scheme.

With special emphasis on problems generating periodic orbits, and on sliding motion on the intersection of two discontinuity surfaces, we present a numerical approach based on an event-driven numerical scheme. The approach is based on a combination of a classical step-by-step strategy for the time integration with the detection of event points for the specification of the occurring dynamics. The main novelty of our approach is the systematic use of the "moments regularization" to select a sliding vector field on the (intersection of) discontinuity surfaces. A dynamical study of the periodic behavior will also be provided, by means of the Floquet multipliers of the monodromy matrix.

Numerical experiments will be presented, in order to confirm the effectiveness of the approach.

Numerical approximation of the Turing-Hopf spatio-temporal dynamics in reaction-diffusion models

I. Sgura

University of Salento, Italy

This talk concerns numerical approximations of reaction-diffusion systems in the neighbourhood of a Turing-Hopf bifurcation point where inhomogeneous Turing patterns that are oscillatory in time (weak case) or both in space and time (strong case) arise.
Stability analysis on a test reaction-diffusion system with oscillating solution allows comparisons of a selection time integrators in terms of stability regions and stepsize restrictions: the well known IMEX Euler method, the explicit and semi-implicit ADI methods and two new methods, symplectic in absence of diffusion, named IMSP and IMSP_IE. For the space discretization, Extended Central Difference Formulas (ECDFs) of order p=2,4 are applied.
We report numerical simulations for the Schnackenberg model, prototype of reaction-diffusion system with Turing-Hopf patterns, and for the morphochemical DIB model for metal growth described in Sgura (2012), supported by comparisons with electrodepostion experiments.
We show that both IMSP and IMSP_IE methods require smaller timesteps, nevertheless the explicit ADI method reaches good accuracy with lower computational cost.
Current research concerning the Turing-Hopf pattern formation on the sphere and other 3D surfaces will be also presented.

Time-transformations for the event location

S. Maset

Università di Trieste, Italy

We consider numerical methods for the location of events of ordinary differential equations. These methods are based on particular changes of the independent variable, called time-transformations. Such a transformation reduces the integration of an equation up to the unknown point where an event occours to the integration of another equation up to a known point, which corresponds to the unknown point by means of the transformation.

MS08 – Frontiers in numerical continuation methods

Organized by: Christian Kühn, Daniele Avitabile, Hannes Ücker

Continuation of invariant pairs for nonlinear eigenvalue problems

W.-J. Beyn

Bielefeld University, Germany

Invariant pairs are the proper generalizations of invariant subspaces from linear to nonlinear eigenvalue problems. We consider large parameterized nonlinear eigenvalue problems and aim at the continuation of a low-dimensional invariant pair that belongs to a small spectral subset inside a prescribed contour. The approach is based on two methodologies: a locally fast process for fixing initial approximations and performing the corrector step, and a global method for obtaining initial approximations and observing eigenvalues crossing the prescribed contour during continuation. For the first task we use a Newton-type method while for the second task we employ a rather recent algorithm based on contour integration of projected resolvents. The underlying idea of the contour algorithm is the theorem of Keldysh for holomorphic eigenvalue problems with Fredholm operators. We present applications to the stability analysis of fronts and pulses where the nonlinearity is caused by projection boundary conditions. The talk is based on joint work with D.Kressner, C. Effenberger (EPFL Lausanne), J. Rottmann-Matthes (Karlruhe) and Y. Latushkin (Columbia).

Depinning transitions in driven soft-matter systems - a users perspective on continuation

U. Thiele

Universität Münster, Germany

When changing a control parameter past a depinning transition, a steady structure starts moving. Such behaviour occurs when heterogeneities that pin a structure compete with a 'lateral' driving force: One example examples are drops pinned by wettability patterns that only move for a driving larger than a critical one [1]. Further examples include drops on a rotating cylinder [2], driven clusters of colloidal particles in corrugated nano-channels [3], and the deposition of lines in dip-coating processes [4].
First, we introduce a number of experimental systems, review the developed models and give an overview of the solution structure of selected models - that are often forth order, nonlinear PDEs or nonlinear IDEs. Thereby, we emphasise the employed numerical path-following techniques and packages, their strengths and shortcomings. We conclude this part with a summary of the various encountered depinning transitions via local and global bifurcations that are encountered when employing the driving strength as main control parameter.
Then we pose the question how the entire rich bifurcation structure emerges when changing another control parameter that corresponds to a 'distance' to the critical point of an underlying phase transition and show that the process of emergence is more involved than one would expect. As examples we use the line deposition via Langmuir-Blodgett transfer [5] and the depinning of drops on the rotating cylinder [6].

We conclude with a brief summary, a user's wishlist for the development of future contnuation tools and an ad for the "Muensteranian Torturials" - a growing set of hands-on tutorials on nonlinear science [7].

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[2] U. Thiele, J. Fluid Mech 671, 121-136 (2011).

[3] A. Pototsky et al., Phys. Rev. E 83, 061401 (2011).

[4] M. H. Kopf, S. V. Gurevich, R. Friedrich and U. Thiele New J. Phys. 14, 023016 (2012).

[5] M.H. Kopf and U. Thiele, Nonlinearity 27, 2711-2734 (2014).

[6] T.-S. Lin, D. Tseluiko, U. Thiele (in preparation)

[7] http://www.uni-muenster.de/CeNoS/Lehre/Tutorials/auto.html

Complete titles/links can be found under www.uwethiele.de/publ.html

Equation-free analysis of agent-based models and systematic parameter determination: A NetLogo Implementation

D. Lloyd, S. Thomas and A. Skeldon

University of Surrey, United Kingdom

The snowballing of computational modelling (in particular agent-based modelling) outside the natural sciences has led to an unprecedented growth in applications, leading to a step change in these subjects. Unravelling the complex relationships and their consequences in these models by simulation alone is a major challenge. The emergence of equation-free (EF) methods provides us with an exciting tool to efficiently explore the highly intricate behaviour of these models.

To date, EF methods have been applied to a few specific examples. For each case, choices have to be made for algorithmic parameters, such as: the number of micro-simulations carried out at each parameter point; the time window for each micro-simulation and the size of the steps in parameter space. These parameters have been chosen largely by trial-and-error and often a large number of micro-simulations are needed. As a result the EF analysis is currently limited to users with knowledge of EF continuation and there is a significant over-head in configuring the EF method to the specific problem.

Here we develop a generic framework for the EF continuation of agent-based models (ABM)s that does not require any knowledge of the mathematics or programming implementation involved, enabling numerical continuation to be performed by any ABM user. By embracing the uncertainty of the sampling errors, we show that one can construct an efficient and robust algorithm. Our framework includes a systematic method for the automatic configuration of EF computational parameters to a specific ABM. Our implementation is coded in Java as it can interface with the NetLogo programming language which is a popular tool for coding ABMs.

We demonstrate our method with application to several ABM models revealing parameter dependence, bifurcation and stability analysis of these complex systems that are not otherwise easily obtainable.

The partial support of the UK Engineering and Physical Sciences Research Council for programme grant EP/H021779/1 (Evolution and Resilience of Industrial Ecosystems (ERIE)) is gratefully acknowledged.

PDEpath

D. Wetzel

University of Oldenburg, Germany

One can use the software tool AUTO to treat continuation and bifurcation problems for elliptic PDEs over 1D domains. pde2path is developed to treat such problems over 2D domains. It is based on MATLAB. Implemented are continuation and bifurcation methods, while it uses MATLAB's PDE Toolbox for finite element methods. OOPDE is an open source FEM-package, which is also based on MATLAB and works over 1D, 2D, and 3D domains.

PDEpath uses the FEM routines of OOPDE and the continuation and bifurcation routines of pde2path. Thus it is independent of MATLAB's PDE Toolbox and can be used for PDEs over 1D, 2D, and 3D domains. In my talk I explain the main routines of PDEpath and show some examples combined with new results for 3D Turing patterns.

Data-Driven Reduction for a Class of Multiscale Fast-Slow Stochastic Dynamical Systems

Y. Kevrekidis

Princeton University, United States of America

Multiple time scale stochastic dynamical systems are ubiquitous in science and engineering, and the reduction of such systems and their models to only their slow components is often essential for scientific computation and further analysis. Rather than being available in the form of an explicit analytical model, often such systems can only be observed as a data set which exhibits dynamics on several time scales. We will focus on applying and adapting data mining and manifold learning techniques to detect the slow components in such multiscale data.

Traditional data mining methods are based on metrics (and thus, geometries) which are not informed of the multiscale nature of the underlying system dynamics; such methods cannot successfully recover the slow variables. Here, we present an approach which utilizes both the local geometry and the *local dynamics* within the data set through a metric which is both insensitive to the fast variables and more general than simple statistical averaging. Our analysis of the approach provides conditions for successfully recovering the underlying slow variables, as well as an empirical protocol guiding the selection of the method parameters.

Noise reduction in coarse bifurcation analysis of stochastic agent-based models: an example of consumer lock-in

D. Avitabile[a] , *R. Hoyle*[b] *and G. Samaey*[c]

[a] University of Nottingham, United Kingdom

[b] University of Surrey, United Kingdom

[c] KU Leuven, Belgium

We investigate coarse equilibrium states of a fine-scale, stochastic, agent-based model of consumer lock-in in a duopolistic market. In the model, agents decide on their next purchase based on a combination of their personal preference and their neighbors' opinions. For agents with independent identically distributed (i.i.d.) parameters and all-to-all coupling, we derive an analytic approximate coarse evolution-map for the expected average purchase. We then study the emergence of coarse fronts when the agents are split into two factions with opposite preferences. We develop a novel Newton–Krylov method that is able to compute accurately and efficiently coarse fixed points when the underlying fine-scale dynamics is stochastic. The main novelty of the algorithm is in the elimination of the noise that is generated when estimating Jacobian-vector products using time-integration of perturbed initial conditions. We present numerical results that demonstrate the convergence properties of the numerical method and use the method to show that macroscopic fronts in this model destabilize at a coarse symmetry-breaking bifurcation.

Using control for for bifurcation analysis in multi-particle systems

J. Sieber

University of Exeter, United Kingdom

Usually feedback control is applied only when one wants to track unstable equilibria or periodic orbits in experiments since setting initial conditions at will is often infeasible there. We show that applying feedback control can be a viable alternative to the more commonly used equation-free methodology when tracking emerging equilibria, periodic orbits and their bifurcations in multi-particle systems.

Spatial patterns in distributed optimal control problems

H. Uecker[a] *and D. Grass*[b]

[a] Universität Oldenburg, Germany

[b] TU Wien, Austria

Spatial patterns in distributed optimal control problems We consider infinite time-horizon optimal control problems where the state variables fulfill a parabolic systems of PDEs. The associated canonical system (CS) for the

states and co-states then consists of a forward-backward diffusion system. We study these CS numerically in two steps. First we compute (branches and bifurcations) of canonical steady states (CSS) using the continuation and bifurcation software pde2path. Then we use the add-on module p2pOC to pde2path to compute time dependent canonical paths and their values, which requires a second continuation algorithm in the initial states. We illustrate the approach by some ecological and economical examples, yielding interesting optimal patterned steady states.

MS09 – Numerical time integration strategies for highly oscillatory systems of hyperbolic PDEs

Organized by: Tommaso Benacchio, Luca Bonaventura, Rupert Klein

Magnetic Cycles in Global Large-Eddy Simulation of Solar Convection

P.K. Smolarkiewicz[a] *and P. Charbonneau*[b]

[a] European Centre for Medium-Range Weather Forecasts, United Kingdom

[b] Universitè de Montreal, France

The works of Ghizaru et al. (2010, ApJL 715, L133), Racine et al. (2011, ApJ 735, 46) and several others that followed produced unprecedented, and still unmatched, regular solar-like magnetic cycles and dynamo action in global large-eddy simulations of solar magneto-convection. All these calculations used the EULAG-MHD code of Smolarkiewicz & Charbonneau (2013, JCP 236, 608), a spin-off of the numerical model EULAG (Prusa et al., 2008, Comput. Fluids 37, 1193) predominantly used in atmospheric and climate research. Because of its meteorological heritage, EULAG-MHD incorporates some features non-standard in anelastic solar codes, which clearly proved beneficial for simulation of the global dynamo. Among these the most emphasized is the Implicit Large Eddy Simulation (ILES) approach, becoming now widely appreciated in the solar physics community. Most certainly the work of Racine et al. (2011) demonstrated that numerical treatment of small scales may be critical for the production of cyclic behaviour and regular polarity reversals in this type of global simulations. However, there are other aspects of our numerical design (e.g., particular formulation of the governing equations and the unique semi-implicit time integration scheme) that appear equally important. Because the period of simulated solar cycles is O(10) years, computing a number of regular cycles requires millions of time steps. Consequently, extensive numerical sensitivity studies are hardly affordable, and defining the minimal set of the EULAG properties that make this clock tick still eludes us. This talk will identify, and reflect on, the modifications of solar MHD model adopted from the atmospheric experience.

Space-time adaptive ADER discontinuous Galerkin finite element schemes with a posteriori sub-cell finite volume limiting

M. Dumbser

University of Trento, Italy

The purpose of this work is to propose a novel a posteriori finite volume subcell limiter technique for the Discontinuous Galerkin finite element method for nonlinear systems of hyperbolic conservation laws in multiple space dimensions that works well for arbitrary high order of accuracy in space and time and that does not destroy the natural subcell resolution properties of the DG method. High order time discretization is achieved

via a one-step ADER approach that uses a local space-time discontinuous Galerkin predictor method to evolve the data locally in time within each cell.
Our new limiting strategy is based on the so-called MOOD paradigm, which a posteriori verifies the validity of a discrete candidate solution against physical and numerical detection criteria after each time step. Here, we employ a relaxed discrete maximum principle in the sense of piecewise polynomials and the positivity of the numerical solution as detection criteria. Within the DG scheme on the main grid, the discrete solution is represented by piecewise polynomials of degree N. For those troubled cells that need limiting, our new limiter approach recomputes the discrete solution by scattering the DG polynomials at the previous time step onto a set of Ns=2N+1 finite volume subcells per space dimension. A robust but accurate ADER-WENO finite volume scheme then updates the subcell averages of the conservative variables within the detected troubled cells. The recomputed subcell averages are subsequently gathered back into high order cell-centered DG polynomials on the main grid via a subgrid reconstruction operator. The choice of Ns=2N+1subcells is optimal since it allows to match the maximum admissible time step of the finite volume scheme on the subgrid with the maximum admissible time step of the DG scheme on the main grid, minimizing at the same time also the local truncation error of the subcell finite volume scheme. It furthermore provides an excellent subcell resolution of discontinuities. Our new approach is therefore radically different from classical DG limiters, where the limiter is using TVB or (H)WENO reconstruction based on the discrete solution of the DG scheme on the main grid at the new time level. In our case, the discrete solution is recomputed within the troubled cells from the old time level using a different and more robust numerical scheme on a subgrid level. In this way, the new DG limiters are using the governing PDE system itself in the process of limiting, while standard limiters are usually only based on some measure of smoothness of the discrete solution, without using the PDE inside the limiter.
We illustrate the performance of the new a posteriori subcell ADER-WENO finite volume limiter approach for very high order DG methods via the simulation of numerous test cases run on Cartesian grids in two and three space dimensions, using DG schemes of up to tenth order of accuracy in space and time (N=9). The method is also able to run on massively parallel large scale supercomputing infrastructure, which is shown via one 3D test problem that uses 10 billion space?time degrees of freedom per time step.
We finally show possible extensions of our approach to space-time adaptive Cartesian grids with time-accurate local time stepping (LTS), leading to an unprecedented level of resolution of discontinuities.

A discontinuous Galerkin approach for the integration of ordinary differential equations

P.F. Antonietti[a], *N. Dal Santo*[a], *I. Mazzieri*[a] *and A. Quarteroni*[b]

[a] Politecnico di Milano, Italy

[b] CMCS-MATHICSE, École Polytechnique Fédérale de Lausanne, Switzerland

We introduce a new DG spectral element method for the approximation of a system of second order ordinary differential equations

$$u'' + cLu' + Ku = f,$$

where L and K are symmetric and positive definite matrices and c can be either one or zero. The above system arises after the discretization in space of a general wave propagation problem with arbitrary (continuous or discontinuous) polynomials. Using the energy of the system, we prove the stability of the resulting DG scheme and we derive the a-priori error analysis of the method. After validating these results on some test cases, we present computations obtained on two dimensional seismic wave propagation problems.

A semi-implicit, semi-Lagrangian DG framework for adaptive numerical weather prediction

G. Tumolo[a] *and L. Bonaventura*[b]

[a] The Abdus Salam ICTP, Italy

[b] Politecnico di Milano, Italy

We present an adaptive discretization approach for model equations typical of Numerical Weather Prediction, which combines the semi-Lagrangian technique with a TR-BDF2 based semi-implicit time discretization and with a Discontinuous Galerkin spatial discretization with (arbitrarily high) variable and dynamically adaptive element degree. The resulting method has full second order accuracy in time, is unconditionally stable and can effectively adapt at runtime the number of degrees of freedom employed in each element, in order to balance accuracy and computational cost. Numerical results of classical 2D benchmarks for shallow water equations on the sphere and Euler equations on a vertical slice with topography confirm the potential of the proposed formulation.

Split-explicit methods and their connections to exponential integrators

O. Knoth

Institute of Troposspheric Research, Germany

Split-explicit methods are a common integration method in numerical weather prediction. They combine two explicit methods to integrate different parts of the right hand side with different time steps. Common combinations are for the slow part Leap-Frog, Runge-Kutta, or Adams-method and for the fast part a Verlet-type integration method. For Runge-Kutta methods as the slow integrator Wensch et.al give a generalization (MIS-method) and analyzed this new method in case of an exact integration of the fast part. An outcome of their analysis is that the methods of Wicker and Skamarock can have at least order two. In the talk we will apply this new methods to a splitting of the right hand side where the fast part is linear and is made of a partial Jacobian of the right hand side representing the fast acoustic waves. The method can be implemented by providing subroutines for computing the right hand side and a solver of choice for the linear differential equation. From the construction exponential integrators can also be implemented in this framework.

For numerical weather prediction special stability requirements are necessary. The eigenvalues of the slow and fast operator lie near the imaginary axes or are purely imaginary. For this case many exponential integration methods have a reduced stability area. We will explain this phenomena for the linear acoustic equation.

Finally we will compare our new integrators and known methods for the two-dimensional compressible Euler-equations for examples with different Mach-numbers and grid configurations.

Spectral deferred corrections with fast wave - slow wave splitting

D. Ruprecht[a] *and R. Speck*[b]

[a] University of Leeds, United Kingdom

[b] Juelich Supercomputing Centre, Forschungszentrum Juelich GmbH, Germany

Spectral deferred corrections (SDC) are an easy way to construct higher order methods from simple base integrators, e.g. backward Euler. In general, performing k SDC-sweeps (i.e. iterations) with a first-order base integrator results in a method with formal order k. This allows for the easy construction of high-order splitting methods: A split implicit-explicit Euler can be used as base method while still increasing the order of the resulting SDC method by one per sweep. Mostly, such semi-implicit SDC methods (SISDC), introduced by M. Minion in 2003, have been studied for advection-diffusion problems, where the fast, stiff process comes from a diffusive term in the PDE.

Here, we present an adoption to problems with two oscillatory components, a fast and a slow one: The fast part is integrated implicitly to maintain stability while the slow part is treated explicitly to reduce computational cost. Typically, the slow mode will correspond to advection while the fast mode corresponds to acoustic waves. We present a theoretical analysis confirming that fast wave-slow wave SDC (FWSW-SDC) still increases the order by one in every sweep as well as a stability analysis for the scalar fast wave-slow wave test equation. Additionally, we show how FWSW-SDC can be introduced as a preconditioned fixed point iteration to solve the collocation equation and present an estimate for the norm of the error propagation matrix. Using a combination of the Python codes pySDC and ClawPack, numerical results for different PDEs are presented to illustrate performance of the method.

Asymptotic Parallel-in-Time for highly oscillatory PDEs in weather and climate

B.A. Wingate

University of Exeter, United Kingdom

In this talk I will present an algorithm for parallel-in-time for highly oscillatory PDEs and show results with the shallow water equations, a model used as a benchmark for weather and climate models. This algorithm is inspired by a mathematically rigorous understanding of the method of multiple time scales by Schochet (1994), Embid and Majda (1998), and others. I will describe the relationship of this theory to the new algorithm and show that the parallel speed-up increases as the time scale separation increases which results in an arbitrarily greater efficiency gain relative to standard numerical integrators. I will also present numerical experiments that demonstrate the parallel speed up is more than 100 relative to exponential integrators such as ETDRK4 and more than 10 relative to the standard parareal method with a linearly exact coarse solver. Finally I will show that the method also works in the absence of time scale separation, allowing for the method to work in different model regimes.

Stability properties of two HE-VI discretizations

M. Baldauf and G. Zängl

Deutscher Wetterdienst, Germany

The currently used numerical weather prediction models at the Deutscher Wetterdienst (DWD), COSMO and ICON, both use the so called HE-VI approach (horizontally explicit-vertically implicit) to integrate the compressible, non-hydrostatic Euler equations. This approach circumvents the strong time step restriction induced by the fast sound wave expansion in the vertical. Additionally very good scalability on massively parallel machines can be achieved by a horizontal domain decomposition that is easily possible due to the horizontally explicit time integration.
However, there are differences in the detailed formulation of the time integration. In the regional model COSMO the multi-scale aspect of the flow, indicated by in general (but not always) low Mach numbers, is taken into account by using the time-splitting procedure of Wicker and Skamarock (2002), embedded into a 3-stage Runge-Kutta method. In contrast, the global model ICON, which is used with much higher model domains, where higher wind speeds occur, the time-splitting was given up and a predictor-corrector-method is used instead with the small sound time step.
In the presentation, stability properties of these two HE-VI approaches are compared. Limitations for high model tops are explored since the models in future will take into account also the middle atmosphere until z 100 km. The stability properties are investigated by a von-Neumann- and a mixed von-Neumann-normal-mode-analysis.

MS10 – Anisotropic mesh adaptation

Organized by: Weizhang Huang, Lennard Kamenski

Anisotropic mesh refinement in polyhedral domains

T. Apel[a], *A. Lombardi*[b,c] *and M. Winkler*[a]

[a] Universität der Bundeswehr München, Germany

[b] Universidad de Buenos Aires, Argentina

[c] Universidad Nacional de General Sarmiento, Buenos Aires, Argentina

The presentation is concerned with the finite element solution of the Poisson equation with homogeneous Dirichlet boundary condition in a three-dimensional domain. Anisotropic, graded meshes are used for dealing with the singular behaviour of the solution in the vicinity of the non-smooth parts of the boundary. The discretization error is analyzed for the piecewise linear approximation in the $H^1(\Omega)$- and $L^2(\Omega)$-norms by using a new quasi-interpolation operator. This new interpolant is introduced in order to prove the estimates for $L^2(\Omega)$-data in the differential equation which is not possible for the standard nodal interpolant. These new estimates allow for the extension of certain error estimates for optimal control problems with elliptic partial differential equation and for a simpler proof of the discrete compactness property for edge elements of any order on this kind of finite element meshes.

Image segmentation with anisotropic mesh adaptation

J. Wang[a] *and W. Huang*[b]

[a] Fuzhou University, People's Republic of China

[b] University of Kansas, United States of America

We propose using the eigenfunctions of an anisotropic diffusion operator in the problem of image segmentation, where the diffusion coefficient is defined by the input image. We show that our PDE model is indeed the continuous form of popular discrete spectral clustering models, such as the Normalized-Cuts image segmentation model. The eigenfunctions capture key features of the input image. We develop a highly efficient numerical algorithm based on finite element method with an anisotropic mesh adaptation strategy to solve the segmentation problem. We show that our algorithm can be faster by orders of magnitude than traditional approaches when input image is of high resolution. We also discuss several interesting features of the model with numerical examples and possible applications.

Higher Dimensional Embedding Mesh Adaptation

F. Dassi[a], *H. Si*[a], *S. Perotto*[b] *and T. Streckenbach*[a]

[a] WIAS, Germany

[b] Politecnico di Milano, Italy

We propose a novel anisotropic mesh adaptation technique for adaptive finite element analysis. It is based on the concept of higher dimensional embedding and it does not need the computation of an error estimator nor a metric field. This strategy was already exploited to get an anisotropic curvature adapted mesh that fits a complex input geometry. We extend this idea to adaptive finite element analysis for both two and three dimensional problem, i.e., when we are dealing with two-dimensional flat domain or a volume. The proposed embedding contains informations related to the gradient and the function itself, in this way the elements in the adapted mesh will be stretched and aligned according to the features of the solution of the Partial Differential Equation. To validate the proposed approach, we provide a series of numerical tests for a piecewise linear interpolation of a known functions, then we move to the adaptive finite element framework. We compare these results with the ones obtained by the software BAMG and MMG3d, which are metric-based adaptive mesh generators.

On the conditioning of the linear finite element equations with arbitrary anisotropic grids

L. Kamenski

WIAS, Germany

Anisotropic mesh adaption proved to be an indispensable tool for adaptive finite elements. However, there is a concern that elements of high aspect ratio may dramatically increase the conditioning of the arising equations. Classic results for isotropic adaption are not directly applicable for anisotropic grids since they lead to an excessive overestimation of the real condition number of the stiffness matrix. A new analysis was necessary. In this talk an overview of the available results as well as recent achievements will be presented, which show that the conditioning of the finite elements is not necessarily as bad as it is sometimes assumed.

A sharp error estimator for the transport equation with anisotropic, stabilized finite elements and the Crank-Nicolson scheme

M. Picasso and S. Dubuis

EPFL, Switzerland

The transport equation in two space dimensions is considered. Stabilized finite elements are used for the space discretization, as in Burman CMAME 2010, the Crank Nicolson scheme is used for the time discretization. The mesh triangles may have large aspect ratio whenever needed.
Following Lozinsky Picasso Prachittham SISC 2009, a space/time error estimator is derived, order two in time. An adaptive space/time algorithm is presented and numerical results confirm the sharpness of the error estimator.

Maximum principle preservation in adaptive finite element solution of heterogeneous anisotropic diffusion problems

W. Huang[a] *and X. Li*[b]

[a] University of Kansas, United States of America

[b] University of Missouri at Kansas City, United States of America

Heterogeneous anisotropic diffusion problems arise in various areas of science and engineering including plasma physics, petroleum engineering, and image processing. Standard numerical methods can produce spurious oscillations when they are used to solve those problems. A common approach to avoid this difficulty is to design a proper numerical scheme and/or a proper mesh so that the numerical solution preserves the maximum principle satisfied by the continuous solution. A well known mesh condition for preserving the maximum principle by the linear finite element solution of isotropic diffusion problems is the non-obtuse angle condition that requires the dihedral angles of mesh elements to be non-obtuse. In this talk a generalization of the condition, the so-called anisotropic non-obtuse angle condition is presented for the finite element solution of heterogeneous anisotropic diffusion problems. The new condition is essentially the same as the existing one except that the dihedral angles are now measured in a metric depending on the diffusion matrix of the underlying problem. Metric tensors for use in anisotropic mesh generation and adaptation are developed to account for maximum principle preservation and the combination of maximum principle preservation and mesh adaptivity. Two and three dimensional numerical examples are presented to demonstrate the features of the linear finite element method for anisotropic meshes generated with the metric tensors.

MS11 – Simulation and control of constrained dynamical systems

Organized by: Andreas Steinbrecher, Volker Mehrmann

Generalized-α methods for a class of singularly perturbed systems

M. Köbis and M. Arnold

Martin Luther University Halle-Wittenberg, Germany

It has recently been shown that the generalized-α time integration method, a very popular second order Newmark-type integrator, suffers from order reduction in the context of index-three DAEs for nonlinear mechanical systems. An index reduction may, however, be used to circumvent this problem. Nonlinear systems that are subject to stiff potential forces approach those index-three systems in the limit case and order reduction can be observed in this singularly perturbed (ODE-) setting as well.
In this talk we present a convergence result for generalized-α time integration methods for strongly damped mechanical systems, i.e. singularly perturbed systems that are subject to very large nonlinear damping terms. Methods from the analysis in the DAE case will be exploited to show that the order reduction does not occur in this situation where the limit forms an index-two system.

Numerical Integration of DAEs Based on the Structural Analysis

A. Steinbrecher

TU Berlin, Germany

The complete virtual design of dynamical systems, e.g., mechanical systems, electrical circuits, flow problems, or whole production processes, plays a key role in our technological progress. The modeling of dynamical processes often leads to systems of differential-algebraic equations (DAEs) of the form

$$(1) E(x(t), t)x'(t) = k(t, x(t))$$

where x are the unknown variables.
In general, the direct numerical integration leads to instabilities, non-convergence, or an order reduction of the numerical methods. These difficulties in the numerical integration occur due to so-called hidden constraints which are contained in the DAE but not explicitly stated as equations. Therefore, a regularization or remodeling of the model equations is required which preserves the set of solutions and explicitly contains all formerly hidden constraints. In modern simulation environments often a structural analysis is used to obtain required information for a suitable regularization.
In this talk we discuss the efficient and robust numerical integration of DAEs (1) of high index. First, we present an approach for the regularization of DAEs that is based on the Signature method of Pryce. Such a regularization may be valid only locally since the state selection can vary with the dynamical behavior of the system. The obtained regularization can then be solved piecewisely using stiff ODE-solvers.
To avoid this varying state selection, secondly, we will propose an approach which also uses the information obtained from the Signature method to construct a regularized overdetermined formulation.

Based on that regularization approaches we present the software package QUALIDAES which is suited for the direct numerical integration of both of the proposed regularizations.

On the Rothe Method for Constrained PDEs

R. Altmann

TU Berlin, Germany

The application of the Rothe method to time-dependent PDEs, i.e., to discretize in time first, is popular in the finite element community. With this approach, adaptive FEM schemes may be applied to the resulting stationary PDEs in each time step. For constrained systems, which may be seen as differential-algebraic equations in an abstract setting, instabilities occur. This lack of robustness already appears in the finite-dimensional case in which regularization techniques are well-established. In this talk, we introduce an extension of such a regularization to the PDE case which eliminates the stability issues.

Pro-active chassis control

M. Gerdts and J. Michael

University of the Federal Armed Forces at Munich, Germany

The talk addresses the problem of controlling the damper properties in a chassis in a pro-active way taking into account future road disturbances. The goal is to maximize comfort and/or handling properties. This task can be modeled as an optimal control problem subject to the equations of motion of a mechanical multibody system. Assuming permanent tyre-road contact leads to a differential-algebraic equation while the loss of tyre-road contact requires to take into account contact conditions and contact forces. Numerical methods for the simulation and optimization of such problems will be discussed and numerical results will be presented. For realtime calculations a simple quarter car model with senstivity updates will be used.

Controlled invariance for DAEs

T. Berger

Universität Hamburg, Germany

We study the concept of locally controlled invariant submanifolds for nonlinear descriptor systems. In contrast to classical approaches, we define controlled invariance as the property of solution trajectories to evolve in a given submanifold whenever they start in it. It is then shown that this concept is equivalent to the existence of a feedback which renders the closed-loop vector field invariant in the descriptor sense. This result is motivated by a preliminary consideration of the linear case.
Local controlled invariance leads to the concept of output zeroing submanifolds. We show that the outcome of the differential-algebraic version of the zero dynamics algorithm yields a maximal output zeroing submanifold.

The latter is then used to characterize the zero dynamics of the system. In order to guarantee that the zero dynamics are locally autonomous (i.e., locally resemble the behavior of an autonomous dynamical system), sufficient conditions involving the locally maximal output zeroing submanifold are presented.

Output regulation for DAE-systems

A. Ilchmann

Ilmenau technical University, Germany

We consider the class of linear multi variable DAE systems which are right-invertible and have stable zero dynamics. It is shown that for this class funnel control is feasible: i.e. a simply proportional output error feedback controller achieves tracking of a reference signal within a prespecified funnel.

Controllability and observability are not dual for switched DAEs

F. Küsters[b] *and S. Trenn*[a]

[a] TU Kaiserslautern, Germany

[b] Fraunhofer ITWM, Kaiserslautern, Germany

Duality of controllability and observability is a classical property of linear time-invariant ODE- and DAE-systems and also plays an important role for optimal control. For discontinuously time-varying DAEs (switched DAEs) such a duality result was not available until recently. In fact, even the characterizations of observability and controllability have only been established for switched DAEs a few years ago. With simple examples it can be shown that a naive definition of the dual for a switched DAEs does not work. Indeed, it turns out that the dual of a switched DAE is not a switched DAE anymore because additional "impacts" must be added. Furthermore, a time-inversion is necessary to obtain causal systems. Because of the time-inversion the duality of controllability and observability does NOT hold, instead it can be shown that there are the two new duality pairs: reachability/observability and controllability/determinability.

DAE-Formulation for Optimal Solutions of a Multirate Model in Radio Frequency Applications

R. Pulch and B. Kugelmann

Ernst-Moritz-Arndt-Universität Greifswald, Germany

In radio frequency applications, electric circuits produce high-frequency signals, whose amplitude as well as frequency changes slowly in time. A multivariate signal model is able to decouple the time scales. The mathematical

model of the circuit, which consists of differential algebraic equations (DAEs), is transformed into multirate partial differential algebraic equations (MPDAEs). A local frequency function appears as a degree of freedom in the multivariate modelling. The determination of appropriate solutions of the MPDAEs can be seen as a problem from optimal control. We apply a method of lines to discretise the MPDAEs into a larger system of DAEs, where a necessary condition for an optimal solution is included. We consider the local frequency function as a part of the unknown solution in this DAE system. Consequently, the index of the DAE-formulation is analysed. Moreover, the determination of consistent initial values for the local frequency function is investigated. We present results of numerical simulations for an example of an electric circuit.

MS12 – Simulation and control of delay differential-algebraic equations

Organized by: Benjamin Unger, Volker Mehrmann

Perturbation theory, stability and control for classes of delay differential-algebraic equations

S.M. Verduyn Lunel

Utrecht University, The Netherlands

A neutral delay differential equation can be written as a system of a retarded delay differential equation coupled with a difference equation and such a system can be considered as a delay differential-algebraic equation. In contrast to the case for retarded delay equations, there is not yet an effective perturbation theory for difference equations and more general for delay differential-algebraic equations available.

For a given neutral delay differential equation, one defines a semigroup of operators by shifting along the solution. The need to develop a perturbation theory for such solution semigroups arises in the context of stability and control problems. The answer employs the variation-of-constants formula, which involves integration in a Banach space. The reason that there does not yet exist a perturbation theory for delay differential-algebraic equation is related to the fact that in general the solution of a delay differential-algebraic equation lacks smoothness properties.

Already in 1953 Feller [1] emphasized that one might use the Lebesgue integral for scalar valued functions of time obtained by pairing a linear semigroup acting on an element of the primal space with an element of the dual space and that there is no need to require strong continuity. More recently this point of view was elaborated by Kunze [2] who defined a Pettis type integral in the framework of a norming dual pair of spaces.

The aim of the lecture, which is based on joint work with O. Diekmann, is to show that a combination of the Feller/Kunze ideas and the idea of describing a perturbation at the generator level by a cumulative output map [3], leads to a powerful version of the variation-of-constants formula for general classes of delay differential-algebraic equations.

We illustrate our perturbation theory with some results about stability and control of difference equations with applications to boundary control of partial differential equations.

[1] W. Feller , Semi-groups of transformations in general weak topologies, Ann. of Math. 57 (1953) 287-308.

[2] M. Kunze , A Pettis-type integral and applications to transition semigroups, Czech. Math. J. 61 (2011) 437-459.

[3] O. Diekmann, M. Gyllenberg & H.R. Thieme , Perturbing semigroups by solving Stieltjes Renewal Equations, Diff. Int. Equa. 6 (1993) 155-181.

Weak solutions of neutral problems with state dependent delays

N. Guglielmi[a] *and E. Hairer*[b]

[a] Università dell'Aquila, Italy

[b] Université de Genève, Switzerland

In this talk state-dependent neutral delay differential equations, which are equivalent to differential algebraic delay differential equations will be considered. These equations are often characterized by discontinuities which are due to breaking points at which the solution derivative may have jumps. When the vector field points from both sides towards the discontinuity manifold, it is common to consider so-called weak solutions which evolve in the manifold. A standard approach consists in assuming that in the discontinuity manifold the function is replaced by an element in the convex hull of the one-sided limits (Fillippov or Utkin solution). This is certainly an excellent choice in one dimension. In higher dimension, however, there is no evidence that the line segment connecting the one-sided limits is the best choice. This talk discusses weak solutions associated to an arbitrary path connecting the one-sided limits. It is shown that the particular choice of a path may introduce new weak solutions or avoid weak solutions that are present for the Utkin path. It may also change the stability of codimension-2 weak solutions. Moreover, a regularization of the problem is considered that transforms weak solutions into classical ones, so that standard software can be applied. The choice of the path connecting the one-sided limits strongly influences the numerical approximation.

Direct Transcription Solution of Optimal Control Problems with State Constraints and Delays

S.L. Campbell[a]*, J.T. Betts*[b] *and K. Thompson*[a]

[a] North Carolina State University, United States of America

[b] Applied Mathematical Analysis, United States of America

The numerical solution of optimal control problems is important in many areas. Often the models for these problems have delays. Direct transcription is a popular approach for the numerical solution of optimal control problems.

Much less work has been done on the direct transcription solution of optimal control problems with delays. This talk will describe progress and challenges in developing a general purpose industrial grade direct transcription code that can handle problems with delays. Of special interest will be the more challenging case of control delays. The algorithms and software formulate the problem as a differential algebraic equation independent of whether the original system model was a differential algebraic equation or an ordinary differential equation. This talk is a followup to one given at the 2013 SIAM Control Conference in San Diego and provides additional more general analysis helping to resolve some of the questions posed in 2013.

Optimal Control of Delay Differantial-Algebraic Equations

M. Burger[a] *and M. Gerdts*[b]

[a] Fraunhofer Institute for Industrial Mathematics (ITWM), Germany

[b] Universität der Bundeswehr München

In this contribution, we motivate the treatment of Delay Differential-Algebraic Equations from the perspective of mechanical engineering. Here, the considered dynamical systems are typically multibody systems, mathematically described as index-3 DAE. We consider a problem scenario for input load generation for such mechanicl systems, in which the (unknown) control has to be evaluated at delayed time points. We discuss an optimal control formulation to solve the problem. Moreover, we present and discuss results on necessary optimality conditions for optimal control problems with Delay DAEs.

MS13 – Functional analytic aspects of DAEs

Organized by: Roswitha März, Caren Tischendorf

Sobolev gradients for differential algebraic equations

M. Sauter

Ulm University, Germany

We apply steepest descent methods based on Sobolev gradients and weighted Sobolev gradients to DAEs. As usual these methods aim to minimise an error functional on a suitable function space by following a gradient flow. However, we employ gradients that are tailored to the geometry of the DAE. This approach is motivated by theoretical results and greatly improves numerical performance for DAEs compared to using conventional gradient descent.

In order to illustrate that there are a variety of gradients, note that by definition a gradient represents the Frechét derivative in terms of an inner product. So the gradient depends on the chosen inner product. For a nonlinear DAE it is natural to choose an appropriate inner product that varies depending on the position in the function space.

In this talk we first introduce Sobolev gradients and the required theoretical background. Then we discuss their application to DAEs. Based on our implementation we discuss both strengths and shortcomings of this method. The presented results are joint work with Robin Nittka.

Optimality conditions for linear-quadratic control problems with differential-algebraic constraints

S. Zhuk

IBM Research - Ireland

The talk will present LQ control problems from the operator standpoint, namely a linear unbounded closed operator, induced by a linear DAE of arbitrary index, will be introduced together with its adjoint. It will be shown that classical optimality conditions (in the form of Pontryagin maximum principle) may be too restrictive for a class of LQ problems for DAEs which induce a linear operator with non-closed range. Efficient methods of constructing optimal solutions for such problems will be presented and maximum principle on a manifold will be derived.

Boundary value problems in DAEs and their numerical treatment by standard collocation

E.B. Weinmüller[a], *R. Lamour*[b] *and R. März*[b]

[a] Vienna University of Technology, Austria

[b] Humboldt University Berlin, Germany

We consider nonlinear BVPs in DAEs with properly stated leading term. We introduce and discuss the following notions describing the problem: well-posed BVP, accurately stated boundary conditions, locally unique, and isolated solution. Moreover, we describe the relations between those notions.
Then, the convergence behavior of the collocation method applied to an index 1 DAE system in its original form is studied. While for the index 1 problems collocation turns out to be a robust and fast convergent method, it can fail for higher index case. By means of examples, we illustrate the limits of applicability of the collocation in this case.

Least-squares collocation for higher index differential algebraic equations

M. Hanke[a], *R. März*[b], *C. Tischendorf*[b], *E. Weinmüller*[c] *and S. Wurm*[c]

[a] KTH Royal Institute of Technology Stockholm, Sweden

[b] Humboldt University Berlin, Germany

[c] Technical University Vienna, Austria

Collocation methods are well-established methods for the solution of boundary value problems in ordinary differential equations and index-1 differential-algebraic equations (DAEs). Higher index DAEs are ill-posed in naturally chosen topologies. A possible regularization method for solving them is the least-squares collocation. While the classical collocation methods break down for higher index DAEs the latter one has a rather low order of convergence.
In the present talk we report on preliminary results for a method combining least-squares collocation and projection onto spaces of piecewise polynomials. Computational experiments indicate its excellent convergence properties.

Differential-algebraic operators are extraordinary

R. März

Humboldt University Berlin, Germany

Aiming for a favorable treatment of DAEs as operator equations and least-squares problems one has to provide suitable function spaces and basic functional-analytic properties of differential-algebraic operators acting in these spaces. Astonishingly, till now, this issue has been considered on rare occasions only.
We investigate operators associated with linear and nonlinear DAEs. We ask for boundedness, closedness, and, if applicable, for possible representations of the closures. In the nonlinear case we also pay attention to smoothness. When figuring out appropriate function spaces, we consider both, continuous and measurable functions, indicating classical and generalized solutions of the DAEs, respectively.
The differential-algebraic operators featuring a properly involved derivative appear to be the closures of the operators associated with standard form DAEs.
The class of differential-algebraic operators showing a closed range and the class of operators being fredholm will be specified.
Furthermore, we establish the class of regular differential-algebraic operators associated with regular DAEs. We describe a characteristic operator splitting and specify the ranges of the linear operators.
Regarding appropriate additional boundary conditions leads to an injective composed operator associated with the boundary value problem. In contrast to the case of ordinary differential operators where an integral operator serves as the inverse, it may well happen that, in case of DAEs, a certain component of the inverse is again a differential-algebraic operator. This makes differential-algebraic operators extraordinary and challenging.
Reference:
R. März: Differential-Algebraic Equations from a Functional-Analytic Viewpoint: A Survey.
Surveys in Differential-Algebraic Equations II, Springer DAE-F, 2015, 163-285

Formulation of Constrained PDEs as Operator DAEs

R. Altmann

TU Berlin, Germany

We consider dynamical systems from fluid dynamics, which are constrained by the incompressibility condition, and flexible multibody dynamics, which are constrained through boundary conditions. With the help of suitable Sobolev-Bochner spaces we may formulate these systems as DAEs in an abstract setting, also called operator DAEs. This corresponds to the weak formulation of the underlying PDE systems. In particular, we discuss the well-posedness of initial conditions as well as their consistency.

Perturbation Analysis of hyperbolic PDAEs

C. Huck and C. Tischendorf

Humboldt-University of Berlin, Germany

We consider hyperbolic partial differential-algebraic equations describing flow transport networks. First we discuss the modeling of water transport networks. We show that such network can be described by a combination of hyperbolic partial differential equations for each pipe and linear constrained equations for junctions. We study the PDAE system as an operator DAE and derive perturbation estimations for perturbed PDAE systems including perturbations of the equations, of the initial values as well as of the boundary values.

On Adjoint Discrete Descriptor Systems with Properly Stated Leading Terms

G. Kurina

Voronezh State University, Russian Federation

In memoriam Katalin Balla
We consider two discrete descriptor systems
A(i+1)B(i+1)x(i+1) = C(i)x(i)
and
B(i)*A(i)*z(i) = C(i)*z(i+1),
where i = 0, 1, 2,..., superscript * means an adjoint operator, x(i) belongs to X, z(i) belongs to Z, A(i), B(i) and C(i) are linear bounded operators, acting in corresponding spaces, the operators A(i), B(i) are normally solvable, ImB(i) is the orthogonal complement to KerA(i) in Y; X, Y, Z are real Hilbert spaces.
Considered systems are called as adjoint systems. For solutions of such systems the inner product (A(i)B(i)x(i), z(i)) is constant.
Properties of explicit systems, following from given systems, are studied. In particular, under some condition, we obtain from the first system an explicit system of the same form with respect to B(i)x(i) and from the second system we have an explicit system of the same form with respect to A(i)*z(i). These systems are adjoint. Illustrative examples are presented.

MS14 – Numerical methods for gradient flows

Organized by: Bertram Düring, Daniel Matthes

Discretization of functionals involving the Monge-Ampère operator

Q. Mérigot

CNRS / Université Paris Dauphine, France

Gradient flows in the Wasserstein space have become a powerful tool in the analysis of diffusion equations, following the seminal work of Jordan, Kinderlehrer and Otto (JKO). The numerical applications of this formulation have been limited by the difficulty to compute the Wasserstein distance in dimension two or more. One step of the JKO scheme is equivalent to a variational problem on the space of convex functions, which involves the Monge-Ampère operator. Convexity constraints are notably difficult to handle numerically, but in our setting the internal energy plays the role of a barrier for these constraints. This enables us to introduce a consistent discretization, which inherits convexity properties of the continuous variational problem. We show the effectiveness of our approach on nonlinear diffusion and crowd-motion models. Joint work with J.D Benamou, G. Carlier and É. Oudet.

On the computation of long time Hamiltonian trajectories for molecular systems

H.R. Schwetlick, J. Zimmer and D. Sutton

University of Bath, United Kingdom

We present the Maupertuis principle as an effective method to compute Hamiltonian trajectories linking two given configurations. Via this principle; these trajectories are described as (global) geodesics in a corresponding Riemannian manifold.

As such the problem is converted into a length minimisation. This approach can be viewed as a so-called string method.

We showed convergence of an algorithm based on Birkhoff's method for local (short) geodesics.

We demonstrate how to extend this approach to global geodesics and thus arbitrary boundary values of the corresponding Hamiltonian problem.

Further, we analyse the effectiveness of the numerical minimisation algorithm from the background of gradient flow as well as Gauss-Newton type methods.

Two-phase mean curvature flow via a vector-valued phase field model

O. Vantzos

University of Bonn, Germany

We present a model for the mean curvature-like flow of a hypersurface, where every point on the hypersurface can be in two distinct states with different surface tension constants. The geometry of the hypersurface and the distribution of the two states on it are described simultaneously via a single vector-valued phase field, and its evolution is driven by the L2 gradient flow of a modified Ginzburg-Landau functional. We discuss formal asymptotics and numerics in two and three spatial dimensions. Joint work with Martin Rumpf.

A gradient flow approach to quantization of measures

M. Iacobelli

University of Rome Sapienza & École Polytechnique Paris, France

The problem of quantization of a d-dimension probability distribution by discrete probabilities with a given number of points can be stated as follows: Given a probability density ρ, approximate it in the Wasserstein metric by a convex combination of a finite number N of Dirac masses.
In a recent paper we studied a gradient flow approach to this problem in one dimension.
By embedding the problem in L^2, we find a continuous version of it that corresponds to the limit as the number of particles tends to infinity. Under some suitable regularity assumptions on the density, we prove uniform stability and quantitative convergence result for the discrete and continuous dynamics.

MS15 – Piecewise smooth dynamic simulations via algorithmic piecewise differentation

Organized by: Andreas Griewank, Todd Munson

Piecewise linearizations of nonsmooth equations and their numerical solution

T. Streubel

Humboldt-Universität zu Berlin, Germany

Piecewise smooth functions (PS) can be approximated locally by piecewise linear models (PL) with a second order error in the distance to the reference point. Those models are locally Lipschitz continuous w.r.t. to the reference point and can be obtained by a slight modification of common AD-Tools as a structured Block matrix called the abs-normal Form. It will be shown under which conditions successive piecewise linearization will lead to a convergent sequence of approximations, whose limit is a root of the underlying PS function.

Generalized midpoint and trapezoidal rules for Lipschitzian RHS

R. Hasenfelder

Humboldt-Universität zu Berlin, Germany

Based on algorithmic piecewise linearization we generalize the implicit midpoint and trapezoidal rule to ODEs with Lipschitz-continuous RHS. These generalized methods maintain a local truncation error of order 3 without event location. On general problems one obtains globally second order of convergence compared to the classical methods, whose order drops to 1. Assuming transversality of the analytical trajectory for kink surfaces one obtains by Richardson extrapolation a convergence of order 3 compared to 2 for the classical schemes. We demonstrate these properties both theoretically and by numerical experiments.

Implementation and Application of the Generalized Midpoint Rule for Lipschitzean ODEs

P. Boeck

Humboldt Universität zu Berlin, Germany

PLAN-C is the implementation of numerical integrators for ODEs with Lipschitz continuous right hand sides. It's aim is to have an easy to use solver for these problems that maintains a high order of convergence in the presence of discontinuous derivatives. It is written in C++ and uses ADOL-C to perform automatic derivation.

Is piecewise linear based implicit midpoint rule symplectic?

F. Fonseca Kerkhoff

Humboldt-Universität zu Berlin, Germany

In this talk I will present two results on numerical one-step integrators, applied to ODEs in hamiltonian form.

(i) The classic implicit midpoint rule is symplectic for $C^{1,1}$ hamiltonians.

(ii) The implict midpoint rule based on piecewise linearisation[1] of the hamiltonian gradient is *not* necessarily symplectic for $C^{1,1}$ hamiltonians.

The notion of symplectic Lipschitz-functions follows the 2008 paper *Volume-energy preserving integrators for piecewise smooth approximations of Hamiltonian systems.*[2]

[1] Cf. previous talks and A. Griewank: *On Stable Piecewise Linearization and Generalized Algorithmic Differentiation*, 2012

[2] P. Chartier, E. Faou: *Volume-energy preserving integrators for piecewise smooth approximations of Hamiltonian systems*, M2AN, Vol. 42, No. 2, 2008

MS16 – Multiscale methods for atmosphere-ocean modeling

Organized by: Daan Crommelin, Onno Bokhoven

A simple model for abrupt millennial climate change

G. Gottwald

University of Sydney, Australia

We first confirm that the time series of Calcium concentrations in GRIP ice-core data exhibits a significant alpha-stable noise component as previously found by Ditlevsen (GRL 1999). Building on recent theoretical results from homogenisation theory for deterministic systems, we propose a simple conceptual entirely deterministic multi-scale model of the ocean-atmosphere-ice system which exhibits alpha-stable behaviour. Unlike in most models employing homogenisation theory we employ here chaotic dynamics exhibiting intermittency. The intermittency is associated with the atmospheric dynamics interacting with sea-ice dynamics.

A climate-sensitive closure for low-order atmospheric models

S. Dolaptchiev, M. Pieroth, M. Zacharuk and U. Achatz

Goethe University Frankfurt, Germany

Low-order atmospheric models utilize parameterizations to represent unresolved scales. Such closures can be objectively tuned using first and second statistical moments from a simulation with a "high-order" model (which resolves the scales to be parameterized) or from observations. However, the resulting parameterizations fail to reproduce the correct response of the system, if some anomalous forcing is applied. We use the fluctuation-dissipation theorem to predict the changes in the statistical moments due to the anomalous forcing. This information is then used to correct the closure parameters of the low-order model. The approach is applied within the framework of one- and three-layer quasigeostrophic model on the sphere with stochastic parameterization.

Data-driven stochastic representations of mesoscale ocean eddies

N. Verheul[a] *and D. Crommelin*[a,b]

[a] Centrum Wiskunde & Informatica, Amsterdam

[b] University of Amsterdam, KdV Institute for Mathematics

We investigate how to use sample data, generated by a fully resolved multiscale model, to construct stochastic representations of unresolved processes in a reduced model. These representations are formulated as stochastic processes, conditioned on a covariate (the resolved model state). We demonstrate that the tested strategies

significantly reduce the degrees of freedom of the respective model, while retaining the essential driving force of the unresolved processes. We will discuss how we use this methodology to find parameterizations of mesoscale ocean eddies.

Direct control of the small-scale energy balance in 2D fluid dynamics

J. Frank[a], *B. Leimkuhler*[b] *and K. Myerscough*[c]

[a] Utrecht University, The Netherlands

[b] University of Edinburgh, UK

[c] K.U. Leuven, Belgium

We explore the direct modification of the pseudo-spectral truncation of 2D, incompressible fluid dynamics to maintain a prescribed kinetic energy spectrum. The method provides a means of simulating fluid states with defined spectral properties, for the purpose of matching simulation statistics to given information, arising from observations, theoretical prediction or high fidelity simulation. In the scheme outlined here, Nosé-Hoover thermostats, commonly used in molecular dynamics, are introduced as feedback controls applied to energy shells of the Fourier-discretized Navier-Stokes equations. As we demonstrate in numerical experiments, the dynamical properties (quantified using autocorrelation functions) are only modestly perturbed by our device, while ensemble dispersion is significantly enhanced compared to simulations of a corresponding truncation incorporating hyperviscosity.

Variational modelling of nonlinear water waves

A. Kalogirou and O. Bokhove

University of Leeds, United Kingdom

Mathematical modelling of water waves is demonstrated by investigating variational methods asymptotically and numerically. A reduced potential flow water wave model is derived using variational techniques, which is based on the assumptions of waves with small amplitude and large wavelength. This model consists of a set of modified Benney-Luke equations describing the deviation from the still water surface and the bottom potential. A novel feature in our model is that the dynamics are non-autonomous due to the explicit dependence of the equations on time.

As a first example, we consider the problem of a soliton splash in a long water channel with a contraction at its end, resulting after a sluice gate is removed at a finite time. The removal of the sluice gate is included in the variational principle through a time-dependent gravitational potential. A second example involving non-autonomous dynamics concerns the motion of a free surface in a vertical Hele-Shaw cell. Explicit time-dependence now enters the model through a linear damping term due to the effect of wall friction, and a term representing the motion of an artificially driven wave pump. In both cases, the asymptotic model is solved numerically using a Continuous Galerkin Finite Element Method and the numerical results are compared to wave structures observed in experiments.

The Benney-Luke approximation for water waves is also adapted to accommodate nonlinear ship dynamics. The novelty is this case is the coupling between the water wave dynamics, the ship dynamics and water line dynamics on the ship. For simplicity, we consider a simple ship structure consisting of V-shaped cross-sections.

Hamiltonian Discontinuous Galerkin Finite Element Method for Internal Gravity Waves

A.M. van Oers

NIOZ Royal Netherlands Institute for Sea Research, The Netherlands

The equations governing internal gravity waves in a stratified ideal fluid posses a Hamiltonian structure. A discontinuous Galerkin finite element method has been developed in which this Hamiltonian structure is discretized, resulting in conservation of phase space and of a discrete analog of energy. This required (1) the discretization of the Hamiltonians structure using alternating flux functions and symplectic time integration, (2) the discretization of a divergence-free velocity field using Dirac's theory of constraints and (3) the handling of the large-scale computational demands due to the three-dimensional nature of internal gravity waves and possibly its narrow zones of attraction.

MS17 – Set-oriented numerics: coherent structures and invariant sets

Organized by: Kathrin Padberg-Gehle, Christof Schuette

Towards tensor-based methods for the numerical approximation of the Perron-Frobenius and Koopman operator

S. Klus

Freie Universität Berlin, Germany

Information about the behavior of dynamical systems can often be obtained by analyzing the eigenvalues and corresponding eigenfunctions of linear operators associated with a dynamical system. Examples of such operators are the Perron-Frobenius and the Koopman operator. Although these two operators are adjoint to each other in appropriately defined function spaces and it should therefore theoretically not matter which one is used to study the system's behavior, there are, from a practical point of view, considerable differences. In this talk, we will review different methods to compute finite-dimensional approximations of these infinite-dimensional operators – e.g. Ulam's method and Extended Dynamic Mode Decomposition – and highlight the similarities and differences between these approaches. Furthermore, we will present tensor-based extensions of these methods which might facilitate the computation of eigenfunctions associated with high-dimensional dynamical systems. The results will be illustrated using simple molecular dynamics examples.

Coherent Families: Spectral Theory for Transfer Operators in Continuous Time

P. Koltai[a] *and G. Froyland*[b]

[a] Freie Universität Berlin, Germany

[b] University of New South Wales, Australia

The decomposition of the state space of a dynamical sys- tem into metastable or almost-invariant sets is important for understanding macroscopic behavior. This concept is quite well understood for autonomous dynamical systems, and has recently been generalized to non-autonomous systems via the notion of coherent sets. We elaborate here on the theory of coherent sets in continuous time for periodically driven flows and describe a numerical method to find periodic families of coherent sets without trajectory integration.

Computing coherent sets using time-continuous diffusion

A. Denner

Technische Universität München, Germany

In time dependent dynamics, it is often possible to divide phase space into sets which are seperated by transport barriers. Finding these sets helps to understand the global dynamical behavior of systems arising in, e.g. atmospheric flows, plasma physics and biological models. In this talk we present a new approach for the computation of coherent sets by incorporating time-continuous diffusion into the model. This leads to an advection-diffusion equation (the Fokker-Planck equation) whose solution we approximate using spectral collocation. The approach does not need any particle trajectories and is therefore suited for systems where these are hard to obtain, e.g. turbulent systems.

Cluster-based extraction of finite-time coherent sets from sparse and incomplete trajectory data

K. Padberg-Gehle[a] *and G. Froyland*[b]

[a] Technische Universität Dresden, Germany

[b] University of New South Wales, Sydney, Australia

Coherent features in time-dependent dynamical systems are difficult to identify. Most identification algorithms require knowledge of the dynamical system or high-resolution trajectory information, which in applications may not be available. We present a fast and simple method that is based on spatio-temporal clustering of trajectory data. It provides a rough and rapid coherent structure analysis and is particularly aimed at situations where the available information is poor: there are few trajectories, the available trajectories do not span the full time duration under consideration, and there are missing observations within trajectories.

On the Computation of Attractors for Delay Differential Equations

M. Dellnitz

University of Paderborn, Germany

In this talk we will introduce a numerical method which allows to approximate (low dimensional) invariant sets for infinite dimensional dynamical systems. We will particularly apply these techniques to the computation of attractors for delay differential equations. The numerical approach is inherently set oriented - that is, the invariant sets are computed by a sequence of nested, increasingly refined approximations -, and does not rely on long term simulations of the underlying system.

Pseudo Generators of Spatial Transfer Operators

A. Bittracher[a], *P. Koltai*[b] *and O. Junge*[a]

[a] Technische Universität München, Germany

[b] Freie Universität Berlin, Germany

Metastable behavior in dynamical systems may be a significant challenge for a simulation based analysis. In recent years, transfer operator based approaches to problems exhibiting metastability have matured, but in order to make these approaches computationally feasible for larger systems, various reduction techniques had to be proposed. For example, Schütte introduced a spatial transfer operator which acts on densities on configuration space, instead of the full phase space.
In this talk, we show that even though the family of spatial transfer operators is not a semigroup, it possesses a well defined generating structure. What is more, the underlying "pseudo generators" up to order 4 in the Taylor expansion of this family have particularly simple, explicit expressions involving no momentum averaging. This makes collocation methods particularly easy to implement and computationally efficient, which in turn may open the door for further efficiency improvements in, e.g., the computational treatment of conformation dynamics.

Robust boundary tracking for reachable sets of nonlinear differential inclusions

J. Rieger

Imperial College London, United Kingdom

The Euler scheme is, up to date, the most important numerical method for general ordinary differential inclusions, because the use of the available higher-order methods is prohibited by their enormous complexity after spatial discretization of the right-hand side. Therefore, it makes sense to reassess the Euler scheme and optimize its performance. A considerable reduction of the computational cost can be achieved by setting up a numerical method that computes the boundaries instead of the complete reachable sets of the fully discretized Euler scheme from lower-dimensional data only. I will discuss the surprisingly difficult rigorous proof for the propriety of this method and give numerical examples which illustrate the gain of computational efficiency as well as the robustness of the scheme against changes in the topology of the reachable sets.

Set-oriented numerics for stochastic processes with multiple scales

C. Schütte[a,b]

[a] Zuse Institute Berlin (ZIB), Germany

[b] Freie Universität Berlin, Germany

This talk addresses set-oriented numerics for stochastic processes with high dimension state space exhibiting rare events on very long timescales. Such processes appear in different application areas such as molecular dynamics or materials science. Typically the processes has a rather small number of collective variables with slow dynamics while most variables show very fast dynamics. However, in most real-life applications the information on which variables are fast or slow is not known and algorithms for their computational identification are not available. We will present new transfer operator based approaches to the simultaneous identification of collective variables and almost invariant sets.

MS18 – Numerical treatment of stochastic differential equations

Organized by: Kristian Debrabant, Andreas Rößler

Discretizing the Heston model: an analysis of the weak convergence rate

A. Neuenkirch and M. Altmayer

Universität Mannheim, Germany

We analyze the weak convergence rate of a discretization scheme for the Heston model. Under mild assumptions on the smoothness of the payoff and on the Feller index of the volatility process, respectively, we establish a weak convergence rate of order one. This result is accompanied by several numerical examples. Our error analysis relies on a classical technique from Talay and Tubaro (1990), a recent regularity estimate for the Heston PDE from Feehan and Pop (2013) and Malliavin calculus.

Stability Issues in the Numerical Treatment of Stochastic Differential Equations

E. Buckwar[a] *and C. Kelly*[b]

[a] Johannes Kepler Universität Linz, Austria

[b] University of the West Indies, Kingston, Jamaica

We consider numerical methods for the simulation of stochastic ordinary differential equations and discuss stability issues arising in the application of available methods. In particular we present recent results concerning the determination of almost sure stability properties for several test systems of stochastic ordinary differential equations.

Fully discrete approximation of one-dimensional stochastic wave equations

D. Cohen[a] *and L. Quer-Sardanyons*[b]

[a] Umeå University, Sweden

[b] Universitat Autònoma de Barcelona, Spain

A fully discrete approximation of one-dimensional nonlinear stochastic wave equations driven by multiplicative noise is presented. A standard finite difference approximation is used in space and a stochastic trigonometric

method for the temporal approximation. This explicit time integrator allows for error bounds uniformly in time and space. Moreover, uniform almost sure convergence of the numerical solution is proved.

Postprocessed integrators for the high order sampling of the invariant distribution of stiff SDEs and SPDEs

G. Vilmart[a] *and E.-C. Bréhier*[b]

[a] University of Neuchatel, Switzerland

[b] University of Geneva, Switzerland

J.C. Butcher's effective order is a popular methodology in the deterministic literature for the construction of efficient and accurate integrators for differential equations over long times. The idea is to enhance the accuracy of a numerical method by using an appropriate change of variables called the processor. We show that this technique can be extended to the stochastic context for the construction of efficient high order integrators for the sampling of the invariant measure of ergodic stiff systems. The approach is illustrated with a high-order modification with negligible overhead of the standard implicit Euler-Maruyama method for a class of parabolic SPDEs with additive space-time noise.
Publications and preprints available at: http://www.unige.ch/ vilmart/publications.html

MS19 – Numerical methods for stochastic differential equations

Organized by: Evelyn Buckwar, David Cohen

Structure preserving splitting integrators for stochastic differential equations

M. Ableidinger, E. Buckwar and H. Hinterleitner

Johannes Kepler University, Austria

In this talk we will discuss stochastic differential equations, where the solution trajectories are governed by geometric structures as, e.g., energy preservation or dissipation. An efficient strategy for constructing structure preserving integrators is to split the SDE into subsystems which inherit the geometric structure and build a numerical integrator by composition of the exact flows of the subsystems. We apply this approach on SDEs arising in micromagnetism (stochastic Landau-Lifshitz-Gilbert equation) and neuroscience (stochastic Jansen and Rit Neural Mass Model).

On partial differential equations with random coefficients

A. Mugler

Brandenburg University of Technology Cottbus - Senftenberg, Germany

Besides stochastic partial differential equations driven by some kind of white noise also partial differential equations with random data especially random coefficients play an important role in a number of applications in engineering. Therefore uncertainty quantification in such a context has been of growing interest in the last years. For example the modelling of complex systems like subsurface flows with random permeability can be mentioned here.

In this talk we focus on the question of existence of a unique weak solution to an illustrative model problem where the random coefficient can be strictly bounded away from zero and above by random variables only. This is an important issue from the application point of view but the classical deterministic approach to solve the problem does not carry over to this case. Moreover we are interested in an approximate solution of this problem. It turns out that the standard stochastic Galerkin approach, which is widely used in practice nowadays, does not work in general. So we introduce an alternative stochastic Galerkin approach yielding a sequence of approximate solutions converging to the exact solution in the natural topology. Furthermore we present an example where the solutions of the standard stochastic Galerkin approach fails to converge to the exact solution in the natural topology.

A derivative-free approximation scheme for SPDEs with commutative noise

C. Leonhard and A. Rößler

Universität zu Lübeck, Germany

An infinite dimensional version of a derivative-free approximation scheme for finite dimensional stochastic (ordinary) differential equations is introduced. The proposed scheme can be applied to a certain class of semilinear stochastic partial differential equations (SPDEs) in the case of multiplicative commutative noise. Especially, the order of convergence and the efficiency of the new scheme will be discussed. This is joint work with Claudine Leonhard.

Analysis of the Ensemble Kalman Filter for Inverse Problems

C. Schillings and A. Stuart

University of Warwick, United Kingdom

The ideas from the Ensemble Kalman Filter introduced by Evensen in 1994 can be adapted to inverse problems by introducing artificial dynamics. In this talk, we will discuss an analysis of the EnKF based on the continuous time scaling limits, which allows to derive estimates on the long-time behavior of the EnKF and, hence, provides insights into the convergence properties of the algorithm. In particular, we are interested in the properties of the EnKF for a fixed ensemble size, in order to better understand current practice, and to suggest future directions for development of the algorithm. Results from various numerical experiments supporting the theoretical findings will be presented.

Full discretisation of semi-linear stochastic wave equations driven by multiplicative noise

R. Anton[a], D. Cohen[a], S. Larsson[b] and X. Wang[c]

[a] Umeå University, Sweden

[b] Chalmers University of Technology and University of Gothenburg, Sweden

[c] Central South University, China

A fully discrete approximation of the semi-linear stochastic wave equation driven by multiplicative noise is presented. A standard linear finite element approximation is used in space and a stochastic trigonometric method for the temporal approximation. This explicit time integrator allows for mean-square error bounds independent of the space discretisation and thus do not suffer from a step size restriction. Furthermore, it satisfies an almost trace formula (i. e., a linear drift of the expected value of the energy of the problem). Numerical experiments are presented and confirm the theoretical results.

How can SPDE simulations become more efficient?

A. Lang

Chalmers University of Technology, Sweden

Efficiency is an important aspect when simulating stochastic differential equations. The time to wait for a result on a regular desktop computer explodes quickly when more than simple examples are considered. In this talk we discuss how recent theoretical results help to decrease the necessary computational effort in terms of complexity and constants.

Deterministic approximations of PDEs via SDE approximations, the Feynman-Kac formula, and interpolation

K. Debrabant[a] *and E.R. Jakobsen*[b]

[a] University of Southern Denmark, Denmark

[b] Norwegian University of Science and Technology, Trondheim

In this talk, we show that numerical schemes for SDEs induce approximations of linear PDEs . We prove monotonicity of the PDE schemes and various L^p stability results, discuss consistency and the truncation error and provide convergence results and error estimates.

Quadratic invariant preserving methods for SDEs and redundant order conditions

S. Anmarkrud and A. Kværnø

Norwegian University of Science and Technology, Norway

In a recent paper Hong et.al. (APNUM, 2015) presented a set of conditions for stochastic Runge-Kutta (SRK) methods, as well as partitioned Runge-Kutta (SPRK) methods to preserve quadratic invariants. In this talk, we will derive a set of order conditions for SPRKs, based on rooted tree theory. It will then be shown that for both SRKs and SPRKs, by imposing the conditions for the preservation of quadratic invariants, most of the order conditions becomes redundant. Roughly speaking, there is only one condition for each unrooted tree. This is an extension of the results given for classical RK methods by Sanz-Serna and Abia (SINUM 1991).

MS20 – Stochastic partial differential equations: Analytical and numerical aspects

Organized by: Erika Hausenblas, Sylvie Roelly, Mechthild Thalhammer

Conservation laws with stochastic forcing

G. Vallet

University of Pau, France

The aim of this talk is to present a result of existence and uniqueness of the entropy solution to a class of stochastic nonlinear conservation laws.

What is the importance of strong vs. weak error analysis when computing stochastic partial differential equations?

A. Lang

Chalmers University of Technology, Sweden

The simulation of a stochastic partial differential equation relies heavily on the quantity of interest. Different methods lead to different "solutions" but also need different computational complexity. The goal of this talk is to show the importance of strong and weak error analysis for approximation schemes and why one should do better than bounding the weak error by the strong one.

The stochastic $p(\omega, t, x)$-Laplace equation with cylindrical Wiener process

A. Zimmermann

Universität Duisburg-Essen, Germany

We propose a nonlinear parabolic problem of $p(\omega, t, x)$-Laplace type in the framework of Orlicz Lebesgue and Sobolev spaces with variable random exponents with a stochastic forcing by a cylindrical Wiener process. We give a result of existence and uniqueness of the solution, for additive and multiplicative problems.

SPDE-based sampling methods for fractional processes

J. Voss

University of Leeds, United Kingdom

A series of recent papers (see [1], [2], and [3] for a selection) introducted SPDE-based sampling techniques, where SPDEs are used as the basis of MCMC methods on function space. These techniques allow to sample from a wide range of distributions on function spaces, including the solutions of SDEs, bridges of stochastic processes and the posterior distribution in filtering problems. This leads to algorithm for sampling bridges of SDEs and for solving non-linear filtering/smoothing problems. This talk explores how SPDE-based sampling techniques can be extended to sample from more general processes on path space, including fractional Brownian motion and derived processes.

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[2] M. Hairer, A.M. Stuart, and J. Voss: Analysis of SPDEs Arising in Path Sampling, Part II: The Nonlinear Case. Annals of Applied Probability, vol. 17, no. 5, pp. 1657-1706, 2007.
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The Forward-Backward Stochastic Heat Equation: Numerical Analysis and Simulation

T. Dunst

Universität Tübingen, Germany

I report on recent results to numerically approximate the forward-backward stochastic heat equation. For this purpose, I start with showing strong convergence with optimal rates for a spatial discretization of the backward stochastic heat equation, which is then extended to strong optimal rates for the forward-backward stochastic heat equation from optimal stochastic control. A full discretization based on the implicit Euler method for a temporal discretization, and a least squares Monte-Carlo method are then proposed and simulation results are reported. This is a joint work with Andreas Prohl (U Tuebingen).

Analytical and numerical solutions of SPDEs driven by fractional Brownian motion

E. Issoglio

University of Leeds, United Kingdom

In this talk we consider a stochastic transport-diffusion equation where the velocity field is the formal derivative of a fBm with Hurst index $H > 1/2$.
We study the equation analytically in a pathwise sense and we make use of fractional Sobolev spaces, properties of the heat semigroup and fixed point arguments to show existence, uniqueness and regularity of a mild solution.

The main difficulty lies in the term involving the noise because formally it is a product between a function and a distribution.
The numerical simulation is also implemented in a pathwise way, hence effectively reducing the SPDE to a PDE with distributional coefficients. The fBm is approximated using a wavelet series expansion which automatically leads to an approximation of the above-mentioned product.
Joint work with John Armstrong.

On a Milstein-Galerkin finite element method for semilinear SPDEs

R. Kruse

Technical University Berlin, Germany

In this talk we consider a numerical approximation of semilinear stochastic partial differential equations consisting of a Milstein scheme and a Galerkin finite element method. We present a strong convergence result under global Lipschitz conditions on the increment function of the numerical scheme. The main ingredient in our error analysis is a more abstract stability concept for numerical one step methods. If time permits we also indicate a further application of this concept to multilevel Monte Carlo methods.

MS21 – Data-driven methods for statistical predictability

Organized by: John Harlim

Data-driven stochastic subgrid-scale parameterisation for tropical convection

G. Gottwald[a] *and K. Peters*[b]

[a] University of Sydney, Australia

[b] Max Planck Institute for Meteorology, Hamburg, Germany

Observations of tropical convection from precipitation radar and the concurring large-scale atmospheric state at two locations (Darwin and Kwajalein) are used to establish an effective subgrid-scale parameterisation for tropical convection. Two approaches are presented which rely on the assumption that tropical convection induces a stationary equilibrium distribution. In the first approach we parameterise convection variables such as convective area fraction as an instantaneous random realisation conditioned on the large-scale vertical velocities according to a probability density function estimated from the observations. In the second approach convection variables are generated in a Markov process conditioned on the large-scale vertical velocity, allowing for non-trivial temporal correlations. Despite the different prevalent atmospheric and oceanic regimes at the two locations, with Kwajalein being exposed to a purely oceanic weather regime and Darwin exhibiting land-sea interaction, we establish that the empirical measure for the convective variables conditioned on large-scale mid-level vertical velocities for the two locations are close. This allows us to train the stochastic models at one location and then generate time series of convective activity at the other location. The proposed stochastic subgrid-scale parameterisations adequately reproduce the statistics of the observed convective variables and we discuss how they may be used in future scale-independent mass-flux convection parameterisations.

Data driven prediction of chaotic dynamical systems using diffusion maps and reduced-order Gaussian process regression

Z. Y. Wan

MIT, United States of America

We consider the problem of short term prediction of high-dimensional chaotic dynamical systems possessing lower-dimensional attractors. By utilizing time-series of the dynamical system we first compute a small number of diffusion coordinates that describe the system attractor. We then formulate a data-driven stochastic dynamical model that captures the evolution on these coordinates. The latter consists i) of a data-driven mean vector field, and ii) a zero-mean stochastic component that captures the uncertainty induced by the un-modeled coordinates. Both the mean vector field and the stochastic fluctuation are estimated using a spatial Gaussian process regression over the reduced-order phase space of diffusion coordinates. We apply our framework in the Lorenz-96 system

and we compare its performance with existing approaches over different dynamical regimes ranging from low-dimensional attractors to very high-dimensional turbulent regimes.

Diffusion Forecast: A nonparametric modeling

J. Harlim, T. Berry and D. Giannakis

The Pennsylvania State University, United States of America

I will discuss a nonparametric modeling approach for forecasting stochastic dynamical systems on low-dimensional manifolds. The key idea is to represent the discrete shift maps on a smooth basis which can be obtained by the diffusion maps algorithm. In the limit of large data, this approach converges to a Galerkin projection of the semigroup solution of the backward Kolmogorov equation of the underlying dynamics on a basis adapted to the invariant measure. This approach allows one to evolve the probability distribution (quantify uncertainties) of non-trivial dynamical systems with equation-free modeling.

Data-driven Methods for Nonparametric Forecasting of Dynamical Systems

D. Giannakis[a], *T. Berry*[b], *J. Harlim*[b] *and Z. Zhao*[a]

[a] New York University, United States of America

[b] The Pennsylvania State University, United States of America

We discuss two nonparametric techniques for predicting the future evolution of observables of dynamical systems from observations of the past. The first approach is a generalization of Lorenz's analog forecasting technique: Using local similarity kernels and Takens delay-coordinate maps, we select states (analogs) in the historical record of observations which closely resemble the current initial data, and make weighted ensemble forecasts following the evolution of those states. The second approach approximates the solution semigroup of dynamical systems on manifolds through a Galerkin projection of the shift map in an empirical basis constructed through the diffusion maps algorithm. We present applications in atmosphere ocean science, and discuss connections between the two techniques.

MS22 – Probabilistic numerical analysis of differential equations

Organized by: Ben Calderhead

Probabilistic Meshless Methods for Nonlinear PDEs

M. Girolami

University of Warwick, United Kingdom

Recent work by Conrad et al. [2015] establishes probabilistic foundations for models of the numerical error arising in the numerical solution by finite element approximation of ordinary and partial differential equations. This talk develops complementary probabilistic methodology for numerical solution by meshless methods. We derive optimality results for reconstruction rates and motivate active learning in order to minimise solution uncertainty.

Numerical Methods for Deterministic Differential Equations

K. Zygalakis

University of Southampton, United Kingdom

Numerical solutions of differential equations contain inherent uncertainties due to the finite dimensional approximation of a function. In modelling scenarios where the quantification of uncertainty is a key goal it is therefore important to study the uncertainty introduced by the numerical method, in order to determine its importance relative to other uncertainties, such as those caused by noisy data or by model error. This work is concerned with a probabilistic methodology for doing so. We demonstrate an approach which gives rise to root mean square convergence rates which are consistent with the underlying deterministic method. Furthermore, we employ the method of modified equations to demonstrate enhanced rates of convergence to stochastic or random perturbations of the original deterministic problem. Ordinary differential equations are used to illustrate the approach.
This is joint work with Patrick Conrad, Mark Girolami, (both Warwick, Statistics), Andrew Stuart(Warwick Mathematics) and Simo Sarkka (Aalto BECS)

Probabilistic ODE solvers in Statistics and Computing

P. Henning

Max Planck Institute for Intelligent Systems, Germany

Probabilistic numerical algorithms for the solution of ordinary differential equations offer new ways of modelling various sources of uncertainty, both within the computation of the solver itself and the ODE problem to be solved. Recent results have tightened the conceptional link between inference and computation in this area, identifying

classic solvers, e.g. subsets of the Runge-Kutta family, with certain classic statistical estimation methods. I will highlight some of these connections, then present a few applications for the measure of uncertainty implied by them, in medical imaging and computational statistics. The emerging picture is that, where probabilistic measures of uncertainty can be calibrated even just vaguely, but at low computational overhead, new application areas emerge.

Frank-Wolfe Bayesian Quadrature: Probabilistic Integration with Theoretical Guarantees

F. Briol

University of Warwick, United Kingdom

Probabilistic numerics aims to solve numerical problems from a statistical inference point of view. In the context of integration, methods such as Bayesian Quadrature demonstrate impressive empirical performance but lack theoretical analysis. This talk will present Frank-Wolfe Bayesian Quadrature (FWBQ), the first probabilistic integrator which admits theoretical convergence guarantees. Under FWBQ, convergence to the true value of the integral is shown to be exponential in the number of function evaluations and posterior contraction rates are proven to be super-exponential. In simulations, FWBQ is competitive with state-of-the-art methods and out-performs alternatives based on Frank-Wolfe optimisation.

MS23 – Recent advances in inverse problems

Organized by: Lidia Aceto, Christine Böckmann

The capability of variational source conditions in regularization

B. Hofman

TU Chemnitz, Germany

It is well-known for thirty years that specific conditions concerning the smoothness of solutions are required in order to obtain convergence rates in regularization of ill-posed problems formulated as linear or nonlinear operator equations in Hilbert spaces. Originally, rate results for such problems were based on source conditions of range-type, i.e. the solution has to belong to the range of some linear operator closely connected with the forward operator or its linearization. Since ten years range-type source conditions also play a prominent role for convergence rates in Banach space regularization. However, in the case of nonlinear ill-posed equations in Hilbert and Banach spaces additional conditions with respect to the structure of nonlinearity of the forward operator are necessary. It is a substantial advantage of variational source conditions, which have been developed since 2007, that they combine solution smoothness and nonlinearity conditions. Variational source conditions express the interplay of error terms in the pre-image space and changes of the forward operator in the image space in form of variational inequalities which have to be satisfied for all regularized solutions under consideration.
In this talk, based on variational source conditions, there are presented new results on Tikhonov-type ℓ^1-regularization for linear ill-posed problems with injective forward operators under the condition that the sparsity assumption slightly fails, but the solution is still in ℓ^1. Specifically, new ideas refer to the improvement of recently published convergence rates results and their extension to non-compact linear forward operators. One part of the talk is devoted to the relationships between Nashed's types of ill-posedness and mapping properties of the forward operator like compactness and strict singularity. The focus of another aspect of the talk is on the applicability of variational source conditions to Lavrentiev-type regularization in a Hilbert space setting when the forward operator is monotone. As in Tikhonov-type regularization also in Lavrentiev-type regularization appropriate variational source conditions have the potential to yield convergence rates.
This is joint work with Barbara Kaltenbacher, Elena Resmerita (Alpen Adria University Klagenfurt) and Jens Flemming, Ivan Veselić (TU Chemnitz). The research is partially supported by the Deutsche Forschungsgemeinschaft (DFG) under grant HO 1454/8-2.

A Singular Value Decomposition for Atmospheric Tomography

R. Ramlau

Johannes Kepler Universität Linz, Austria

The image quality of ground based astronomical telescopes suffers from turbulences in the atmosphere. Adaptive Optics (AO) systems use wavefront sensor measurements of incoming light from guide stars to determine an

optimal shape of deformable mirrors (DM) such that the image of the scientific object is corrected after reflection on the DM. An important step in the computation of the mirror shapes is Atmospheric Tomography, where the turbulence profile of the atmosphere is reconstructed from the incoming wavefronts. We present several reconstruction approaches and will in particular focus on reconstructions based on a singular value decomposition of the underlying operator.

Boundary Value Methods for inverse Sturm-Liouville problems

C. Magherini, L. Aceto and P. Ghelardoni

University of Pisa, Italy

An inverse Sturm-Liouville problem consists of recovering the potential function of the Sturm-Liouville differential operator starting from the knowledge of suitable spectral data. The existence and uniqueness of its solution has been proved for several formulations of the same.
Recently, numerical procedures for the solution of the symmetric, the two-spectra and the half inverse problems have been proposed in [3,4] which look for a continuous approximation of the unknown potential belonging to suitable function spaces of finite dimension. In order to effectively compute such approximation a sequence of direct problems has to be solved. This is done by applying one of the Boundary Value Methods introduced in [1,2] which generalize the classical Numerov scheme. The resulting procedures for the three inverse problems have provided competitive results with respect to other techniques available in the literature.
In this talk, the mentioned methods will be described and some numerical results, confirming their effectiveness, will be presented.
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Variable stepsize finite difference schemes for the approximation of whispering gallery modes in prolate and oblate spheroidal cavities

P. Amodio[a], G. Settanni[a], T. Levitina[b] and E.B. Weinmüller[c]

[a] Università degli Studi di Bari Aldo Moro, Italy

[b] TU Braunschweig, Germany

[c] Vienna University of Technology, Austria

The aim of this talk is to point out the obtained progress in the numerical simulation of the so-called Whispering Gallery Modes (WGMs) occurring inside prolate and oblate spheroidal cavities. The calculation of such modes

is difficult, since the model equation exhibits full variety of oscillations, while the WGMs are localized inside a very narrow strip in the near-equatorial domain of a cavity and show extremely large gradients inside this exited domain.
Following the idea inerithed from our previous research, we reformulate the problem in terms of separated equations: the two ODEs related to the angular and radial coordinates form a singular self–adjoint two parameter Sturm–Liouville problem which may be approximated by BVP methods.
We propose an efficient and reliable approach combining the Prüfer angle technique, applied to provide a starting good approximation for the parameters, and high order finite difference schemes with a variable stepsize based on the error equidistribution, to reach high accuracy in the computation of the fast oscillating components and to improve the evaluation of eigenvalues.
We illustrate the approach by numerical simulations concerning highly localized WGMs inside both prolate and oblate spheroidal cavities.
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MS24 – Enhanced Sampling Methods

Organized by: Elena Akhmatskaya, Chus Sanz-Serna, Tijana Radivojevic

Efficient updates for belief distributions

S. Reich

University of Potsdam, Germany

I will discuss the implementation of sequential Monte Carlo methods for updating belief distributions. Instead of using importance-resampling algorithms, I will focus on efficien implementations of the transform method [2] using copulas and regularised optimal transport problems [1].

Ref.

[1] M. Cuturi, Sinkhorn distances: Lightspeed computation of optimal transport. In advances in Neural Information Processing Systems 26, pages 2292-2300, 2013

[2] S. Reich, A non-parametric ensemble transform method for Bayesian inference, SIAM J Sci. Comput. 35, A 2013-2024, 2013.

Accelerating Simulations of Reaction-Diffusion Mechanochemistry in Acto-Myosin Networks

G. Papoian and J. Komianos

University of Maryland, United States of America

Acto-myosin networks are an integral part of the cytoskeleton of eukaryotic cells and play an essential role in determining cellular shape and movement. Acto-myosin network growth and remodeling in vivo is based on a large number of chemical and mechanical processes, which are mutually coupled and spatially and temporally resolved. To investigate the fundamental principles behind the self-organization of these networks, we have developed detailed physico-chemical, stochastic models of actin filament growth dynamics, where the mechanical rigidity of filaments and their corresponding deformations under internally and externally generated forces are taken into account. Our simulations reveal how different acto-myosin micro-architectures emerge in response to varying the network composition. Traditional simulation methods are not fast enough to reach timescales necessary for observing significant rearrangements of actomyosin micro-architectures, which require from hundreds to thousands of seconds. We developed a number of accelerated modeling approaches, in particular, based on leveraging the salient timescale separations in these systems, to enhance sampling and reach physically and biologically interesting timescales.

Adaptive multi-stage integrators with optimal energy conservation

M. Fernández-Pendás[a], *E. Akhmatskaya*[b] *and J.M. Sanz-Serna*[c]

[a] Basque Centre for Applied Mathematics - BCAM, Bilbao, Spain

[b] IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

[c] Departamento de Matemáticas, Universidad Carlos III, Madrid, Spain

We present a system specific numerical integrating scheme based on the optimal choice of a two-stage integrator from the family of the multi-stage symplectic integrators [1] for achieving an efficient sampling in molecular simulations of a given system with a chosen integration time-step.
The proposed adaptive scheme seeks for the integrator, which provides the best energy conservation and thus, potentially, the bigger acceptance rates in the Metropolis test of the hybrid Monte Carlo (HMC) methods [2, 3]. The search is done through the proper analysis of the integration time-step and the physical system for which the simulation is performed. As a result, the new scheme relies on a system specific parameter, which is calculated prior the simulation once a simulated system and a time-step are defined. In contrast, the scheme in [1] uses the fixed, system independent parameter.
In addition, the novel scheme identifies the range of the allowed time-steps for the simulated system and offers, if required, the appropriate integrator for any choice of a time-step within the range.
The scheme can be naturally extended to three- and four-stage numerical integrators.
The adaptive scheme is implemented in the modified GROMACS software package [4, 5, 6], which allows its application in molecular dynamics (MD), Hybrid Monte Carlo (HMC) and Generalized Hybrid Monte Carlo (GHMC) simulations. We have modified previously the GROMACS software for achieving better accuracy and sampling performance through the use of hybrid Monte Carlo methods and multi-stage numerical integrators.
We also analyse the accuracy and performance of this novel adaptive scheme in HMC and GHMC simulations for constrained and non-constrained dynamics. The performance and sampling of the scheme is compared with the "standard" velocity Verlet algorithm and the velocity two-stage integrator with the fixed parameter [1].
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Predicting RNA topologies by a Monte Carlo graph sampling approach

T. Schlick

New York University, United States of America

Recent research has revealed the surprising essential biological roles of RNA molecules as editors of the genetic message and regulators of transcription. To better understand RNA biological functions, knowledge of its three-dimensional structure is required. In this talk, recent work on applying graph theory representations of RNA secondary structures combined with Monte Carlo sampling of coarse-grained graphs based on knowledge-based potentials will be described. The combined hierarchical approach for predicting RNA junction topologies, sampling RNA graph space, and analyzing resulting energy landscapes leads to an efficient and effective method for predicting global arrangements of RNA three-dimensional structures.
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Optimal scaling of the transient phase of Metropolis Hastings algorithms

T. Lelièvre

École des Ponts ParisTech, France

Following the approach of Roberts et al., we study the Random Walk Metropolis algorithm with Gaussian proposals when the target probability measure is the n-fold product of a one-dimensional law. It is well known that in the large n limit, starting at equilibrium and using a diffusive rescaling in time, one ends up with a diffusion. By studying this limiting equation, an optimal acceptance probability rate can be deduced. We will show how to generalize these results when the assumption of stationarity is removed.
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A Markov Jump Process for More Efficient Hamiltonian Monte Carlo

A.B. Berger[a,c], *M. Mudigonda*[a,c], *M.R. Deweese*[a,c] *and J. Sohl-Dickstein*[b]

[a] Redwood Institute for Theoretical Neuroscience

[b] Stanford University

[c] University of California at Berkeley

Monte Carlo with discrete time sampling steps is limited by the fact that its transition rates must be less than or equal to 1. By deriving an HMC algorithm that is a continuous time Markov jump process, we are able to

escape this constraint. This allows us to propose new transition rates that lead to improved mixing, as measured both by the spectral gap and autocorrelation on several ex-ample problems. We release the algorithm as an open source python package.

Employing modified Hamiltonians for sampling enhancement in statistical simulation

T. Radivojevic[a] *and E. Akhmatskaya*[a,b]

[a] BCAM - Basque Center for Applied Mathematics, Bilbao, Spain

[b] IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Sampling with modified (shadow) Hamiltonians in hybrid Monte Carlo methods can dramatically improve efficiency of molecular simulation at different scales compared with conventional molecular dynamics and hybrid / Monte Carlo simulations [1-5]. We introduce modified Hamiltonians in Hamiltonian Monte Carlo [6] for enhancing sampling in statistical simulation, and demonstrate advantages of the proposed method in different statistical models through a comparison with well established Hamiltonian Monte Carlo based methods.

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Emulation of Higher-Order Tensors in Manifold Monte Carlo Methods for Bayesian Inverse Problems

M. Girolami

University of Warwick, UK

The Bayesian approach to Inverse Problems relies predominantly on Markov Chain Monte Carlo methods for posterior inference. The typical nonlinear concentration of posterior measure observed in many such Inverse Problems presents severe challenges to existing simulation based inference methods. Motivated by these challenges the exploitation of local geometric information in the form of covariant gradients, metric tensors, Levi-Civita connections, and local geodesic flows, have been introduced to more effectively locally explore the configuration space of the posterior measure. However, obtaining such geometric quantities usually requires extensive computational effort and despite their effectiveness affect the applicability of these geometrically-based Monte Carlo methods. In this talk we explore one way to address this issue by the construction of an emulator of the model

from which all geometric objects can be obtained in a much more computationally feasible manner. The main concept is to approximate the geometric quantities using a Gaussian Process emulator which is conditioned on a carefully chosen design set of configuration points, which also determines the quality of the emulator. To this end we propose the use of statistical experiment design methods to refine a potentially arbitrarily initialized design online without destroying the convergence of the resulting Markov chain to the desired invariant measure. The practical examples considered in this paper provide a demonstration of the significant improvement possible in terms of computational loading suggesting this is a promising avenue of further development.

MS25 – Advanced multilevel Monte Carlo methods

Organized by: Håkon Hoel, Kody Law, Raul Tempone

MLMC for reflected diffusions

M. Giles[a], *E. Mueller*[b], *R. Scheichl*[b] *and T. Shardlow*[b]

[a] University of Oxford, United Kingdom

[b] University of Bath, United Kingdom

When simulating the motion of particles, with or without mass, subject to random forces, the Euler-Maruyama discretisation with a uniform timestep of h gives $O(h)$ strong convergence if the volatility is uniform, but this degrades to $O(h^{1/2})$ when there are reflecting boundary conditions. A consequence of this is that the variance for the corresponding estimator used in Multilevel Monte Carlo (MLMC) degrades from $O(h^2)$ to $O(h)$, significantly increasing the computational complexity to achieve a certain user-specified accuracy. In this work, we show that a slight modification to the estimator leads to a tighter coupling between the coarse and fine path simulations, and even though it does not improve the order of strong convergence it does improve the order of the MLMC estimator. The effectiveness of the new coupling will be illustrated by numerical experiments.

An Efficient Forward-Reverse Expectation-Maximization Algorithm for Statistical Inference in Stochastic Reaction Networks

A. Moraes[a], *R. Tempone*[a], *P. Vilanova*[a] *and C. Bayer*[b]

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

[b] Weierstrass Institute for Applied Analysis and Stochastics, Germany

In this work, we present an extension to the context of Stochastic Reaction Networks (SRNs) of the forward-reverse representation introduced in "Simulation of forward-reverse stochastic representations for conditional diffusions", a 2014 paper by Bayer and Schoenmakers.
We apply this stochastic representation in the computation of efficient approximations of expected values of functionals of SNR bridges, i.e., SRNs conditioned to its values in the extremes of given time-intervals.
We then employ this SNR bridge-generation technique to the statistical inference problem of approximating the reaction propensities based on discretely observed data. To this end, we introduce a two-phase iterative inference method in which, during phase I, we solve a set of deterministic optimization problems where the SRNs are replaced by their reaction-rate Ordinary Differential Equations (ODEs) approximation; then, during phase II, we apply the Monte Carlo version of the Expectation-Maximization (EM) algorithm starting from the phase I output.
By selecting a set of over dispersed seeds as initial points for phase I, the output of parallel runs from our two-phase method is a cluster of approximate maximum likelihood estimates.
Our results are illustrated by numerical examples.

A multilevel adaptive reaction-splitting simulation method for stochastic reaction networks

P.A. Vilanova, A. Moraes and R. Tempone

King Abdullah University of Science and Technology, Saudi Arabia

To produce efficient simulations, we automatically classify the reactions channels into the fast and slow classes. To this end, we first introduce the concept of the level of activity of a reaction channel, which depends on the current state of the system.

Then, we propose a low cost heuristic that allows us to adaptively split the set of reaction channels into two subsets characterized by either a high or low level of activity. Based on a time splitting technique, the increments associated with high activity channels are simulated using the tau-leap method while those associated with low activity channels are simulated using an exact method.

This path simulation technique, which we name mixed method, is amenable for coupled path generation and a corresponding multilevel Monte Carlo algorithm.

To estimate expected values of observables of the system at a prescribed final time, our method bounds the global computational error to be below a prescribed tolerance, TOL, within a given confidence level. This goal is achieved with a computational complexity of order $O(TOL^{-}2)$, the same as with a pathwise exact method, but with a smaller constant.

We also present a novel control variate technique based on the stochastic time change representation by Kurtz, which may dramatically reduce the variance of the coarsest level at a negligible computational cost.

Our numerical examples show substantial gains with respect to the standard Stochastic Simulation Algorithm (SSA).

The forward-reverse method for Markov bridges and applications to statistical inference

C. Bayer and J. Shoenmakers

WIAS, Germany

In this paper we derive stochastic representations for the finite dimensional distributions of a multidimensional diffusion or more general Markov process on a fixed time interval, conditioned on the terminal state. The conditioning can be with respect to a fixed point or more generally with respect to some subset. The representations rely on a reverse process connected with the given (forward) process as introduced by Milstein, Schoenmakers and Spokoiny in the context of density estimation. The corresponding Monte Carlo estimators have essentially root-N accuracy, and hence they do not suffer from the curse of dimensionality. We improve the performance of the algorithm using the multilevel Monte Carlo approach. We also present an application in statistical inference of Stochastic Reaction Networks, using the forward-reverse algorithm as part of the EM algorithm.

Monte Carlo Methods and Mean Field Approximation for Stochastic Particle Systems

A.L. Haji Ali and R. Tempone

King Abdullah University of Science and Technology, Saudi Arabia

I discuss using single level and multilevel Monte Carlo methods to compute quantities of interests of a stochastic particle system in the mean-field. In this context, the stochastic particles follow a coupled system of Ito stochastic differential equations (SDEs). Moreover, this stochastic particle system converges to a stochastic mean-field limit as the number of particles tends to infinity. In this talk, I start by recalling the results that first appeared in (Haji-Ali, 2012) where I developed different versions of Multilevel Monte Carlo (MLMC) for particle systems, both with respect to time steps and number of particles and proposed using particle antithetic estimators for MLMC. In that work, I showed moderate savings of MLMC compared to Monte Carlo. Next, I expand on these results by proposing the use of our recent Multi-index Monte Carlo method to obtain improved convergence rates.

Multi-Index Monte Carlo

R.F. Tempone[a], *A.L. Haji Ali*[a] *and F. Nobile*[b]

[a] CEMSE, KAUST, Thuwal, Saudi Arabia

[b] MATHICSE-CSQI, EPF de Lausanne, Lausanne, Switzerland

We propose and analyze a novel Multi-Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The MIMC method is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Inspired by Giles's seminal work, we use in MIMC high-order mixed differences instead of using first-order differences as in MLMC to reduce the variance of the hierarchical differences dramatically. This in turn yields new and improved complexity results, which are natural generalizations of Giles's MLMC analysis and which increase the domain of the problem parameters for which we achieve the optimal convergence, $O(TOL^{-2})$. Moreover, in MIMC, the rate of increase of required memory with respect to TOL is independent of the number of directions up to a logarithmic term which allows far more accurate solutions to be calculated for higher dimensions than what is possible when using MLMC. We motivate the setting of MIMC by first focusing on a simple full tensor index set. We then propose a systematic construction of optimal sets of indices for MIMC based on properly defined profits that in turn depend on the average cost per sample and the corresponding weak error and variance. Under standard assumptions on the convergence rates of the weak error, variance and work per sample, the optimal index set turns out to be the total degree (TD) type. In some cases, using optimal index sets, MIMC achieves a better rate for the computational complexity than the corresponding rate when using full tensor index sets. We also show the asymptotic normality of the statistical error in the resulting MIMC estimator and justify in this way our error estimate, which allows both the required accuracy and the confidence level in our computational results to be prescribed. Finally, we include numerical experiments involving a partial differential equation posed in three spatial dimensions and with random coefficients to substantiate the analysis and illustrate the corresponding computational savings of MIMC.

Multilevel ensemble Kalman filtering

H. Hoel[a], *K.J.H. Law*[b] *and R. Tempone*[b]

[a] Department of Mathematics, University of Oslo, Norway

[b] Applied Mathematics and Computational Sciences, KAUST, Saudi Arabia

The ensemble Kalman filter (EnKF) is a sequential filtering method that uses an ensemble of particle paths to estimate the means and covariances of the Kalman filter by the use of sample moments, i.e., the Monte Carlo method. EnKF is often both robust and efficient, but its performance may suffer in settings where the computational cost of accurate simulations of particles is high. The multilevel Monte Carlo method (MLMC) is an extension of classical Monte Carlo methods which by sampling stochastic realizations on a hierarchy of resolutions may reduce the computational cost of moment approximations by orders of magnitude. In this work we have combined the ideas of MLMC and EnKF to construct the multilevel ensemble Kalman filter (MLEnKF). The main ideas of this method is to compute particle paths on a hierarchy of resolutions and to apply multilevel estimators on the ensemble hierarchy of particles to compute Kalman filter means and covariances. Theoretical results and a numerical study of the performance gains of MLEnKF over EnKF will be presented.

Multilevel Sequential Monte Carlo Samplers

A. Beskos[a], *A. Jasra*[b], *K. Law*[c], *R. Tempone*[c] *and Y. Zhou*[b]

[a] University College London, United Kingdom

[b] National University of Singapore

[c] King Abdullah University of Science and Technology

Multilevel Monte-Carlo methods provide a powerful computational technique for reducing the computational cost of estimating expectations for a given computational effort. They are particularly relevant for computational problems when approximate distributions are determined via a resolution parameter h, with h=0 giving the theoretical exact distribution (e.g. SDEs or inverse problems with PDEs). The method provides a benefit by coupling samples from successive resolutions, and estimating differences of successive expectations. We develop a methodology that brings Sequential Monte-Carlo (SMC) algorithms within the framework of the Multilevel idea, as SMC provides a natural set-up for coupling samples over different resolutions. We prove that the new algorithm indeed preserves the benefits of the multilevel principle, even if samples at all resolutions are now correlated.

MS26 – Computational and stochastic methods in inverse problems

Organized by: Jana de Wiljes, Sebastian Reich

Inference of Functional Circadian Networks

L. Petzold

University of California Santa Barbara, United States of America

In mammals, the Suprachiasmatic Nucleus (SCN), a brain region of about 20,000 neurons, serves as the master circadian clock, coordinating timing throughout the body and entraining the body to daily light cycles. The extent to which cells in the SCN can synchronize and entrain depends on the communication network between individual cell oscillators. Characterization of that network is challenging, due to the dynamics of the circadian oscillators and the stochastic noise inherent in discrete molecular chemical reactions. Statistical models based on information theoretic measures are well-suited for the analysis of stochastic information flow across networks. We have developed a methodology that uses information-theoretic measures on time course data to infer network structure, and tested its performance on data from computational models of networks of stochastic circadian oscillators with known connectivity. We then applied the method to experimental data, to infer the functional network for synchronization in mouse SCN slices. We will discuss the properties of the inferred networks.

Big Data and Big Models: on inverse problems that are too large to be solved

E. Haber

University of British Columbia, Canada

In recent years large data sets have been collected and analyzed, typically, by using some machine learning algorithms. However, many types of data demand a much more in-depth analysis that requires simulation, that is, solving partial differential equations, and optimization to estimate parameters.

In this talk we discuss examples for such data sets in earth science. We describe the setting in which vast amounts of geophysical data is collected from the air. We present the large scale modeling that is required to simulate such a data set and the inverse problems that arise from these types of problems. We show that by using traditional techniques these problems cannot be solved in reasonable time on reasonable hardware. We then discuss a new set of algorithms that enable us to solve such problems. These algorithms are based on a concept we call domain of interest computation for the forward coupled with stochastic programming for the inverse. We show that by using this combination we are able to solve very large scale inverse problems, using a rather modest hardware in reasonable time

Nonhomogeneous and nonstationary Markov regression

J. de Wiljes[a], *Lars Putzig and I. Horenko*[b]

[a] University of Potsdam, Germany

[b] Università della Svizzera Italiana, Switzerland

Dynamical systems with different characteristic behavior at multiple scales can be modeled with hybrid methods combining a discrete model (e.g., corresponding to the microscale) triggered by a continuous mechanism and vice versa.
A data-driven black-box-type framework is proposed, where the discrete model is parametrized with adaptive regression techniques and the output of the continuous counterpart (e.g., output of partial differential equations) is coupled to the discrete system of interest in the form of a fixed exogenous time series of external factors.
Data availability represents a significant issue for this type of coupled discrete continuous model, and it is shown that missing information/observations can be incorporated in the model via a nonstationary and nonhomogeneous formulation. This talk is based on work done in collaboration with Illia Horenko and Lars Putzig.

Data-Based Analysis of Extreme Events

O. Kaiser and I. Horenko

Università della Svizzera italiana, Switzerland

The concept of extreme events describes the above average behavior of a process, for instance, heat waves in climate or weather research, earthquakes in geology and financial crashes in economics. It is significant to study the behavior of extremes, in order to reduce their negative impacts. Key objectives include the identification of the appropriate mathematical/statistical model, description of the underlying dependence structure in the multivariate or the spatial case, and the investigation of the most relevant external factors.
This work presents a data-driven framework for spatio-temporal regression analysis of threshold excesses in a presence of unresolved covariates. Based on Extreme Value Theory and a nonparametric time-series analysis methodology, we design a semiparametric, nonstationary, and non-homogenous computational framework for regression analysis of spatio-temporal extreme events. The framework addresses the issue of unresolved covariates from the statistical point of view and goes beyond strong a priori assumptions like stationarity, locality or Markovian behavior. Further, the framework provides a pragmatic nonparametric and nonstationary description of the underlying spatial dependence structure. The performance of the method is demonstrated on real historical meteorological data.

A probabilistic stopping rule for randomized algorithms for inverse problems

U. Ascher and F. Roosta-Khorasani

University of BC, Canada

Iterative numerical algorithms are typically equipped with a stopping criterion, where the iteration process is terminated when some error or misfit measure is deemed to be below a given tolerance. This is a useful setting for comparing algorithm performance, among other purposes. However, in practical applications a precise value for such a tolerance is rarely known; rather, only some possibly vague idea of the desired quality of the numerical approximation is at hand. This leads us to think of approaches to relax the notion of exactly satisfying a tolerance value.

We concentrate on a probabilistic relaxation of the given tolerance. This allows derivation of proven bounds on the sample size of certain Monte Carlo methods. We describe an algorithm that becomes more efficient in a controlled way as the uncertainty in the tolerance increases, and demonstrate this in the context of some particular applications of inverse problems with sparse but many data sets.

Reduced Dimension and Sampling Approaches to Variational Inference

A. Sandu

Virginia Tech, United States of America

Four dimensional variational (4D-Var) approach formulates data assimilation as an optimization problem and computes a maximum aposteriori estimate of the initial condition and parameters of the dynamical system under consideration. The solution of large 4D-Var problems poses considerable challenges: the construction and validation of an adjoint model is an extremely labor-intensive process; strong-constraint 4D-Var is computationally expensive; and 4D-Var does not include posterior uncertainty estimates. In this talk we present several new ideas to tackle these challenges: solving the optimization problem using reduced order model surrogates, exploiting time parallelism, and constructing smoothers that sample directly from the posterior distribution using a Hamiltonian Monte Carlo technique.

A multi-grid approach to localization in ensemble Kalman filters

Y. Cheng, J. de Wiljes and S. Reich

University of Potsdam, Germany

One major issue data assimilation methods have to deal with, especially in practice, is the performance in high dimensional systems using a small number of ensembles/particles. The concept of localization has proven to be one way to go and has been implemented successfully for ensemble Kalman filters. However, one radius has to be chosen for all length scales. We propose an EnKF-based multi-grid approach that uses radial basis functions in order to extract information contained at different length scales of the signal.

Non-Gaussian data assimilation via a localized hybrid particle-ensemble Kalman filter

W. Acevedo[a], *N. Chutsagulprom*[b] *and S. Reich*[b]

[a] Freie Universität Berlin, Germany

[b] Universität Potsdam

Sequential importance re-sampling methods, typically referred to as particle filters, constitute a skillful approach to the assimilation of observations under strongly non-Gaussian conditions. However, particle filters are known to be liable to the 'curse of dimensionality', exhibiting a strong tendency to collapse for high-dimensional applications. In order to alleviate this undesired feature, we propose a hybrid methodology where the Ensemble Transform Kalman Filter (ETKF) and the Ensemble Transform Particle Filter (ETPF) are used sequentially. Furthermore, localization techniques are consistently applied to both filters, in order to minimize the impact of spurious correlations. The operation of the LETKF-LETPF scheme for a set of test models is discussed.

MS27 – Advances in Bayesian computation for large-scale differential equation models

Organized by: Youssef Marzouk

Statistical Approaches to finding Unbiased Solutions to Partial Differential Equations

M. Girolami

University of Warwick, United Kingdom

Partial Differential Equations (PDEs) are used to model many physical and natural systems, and so we may intrinsically be interested in the parameters driving our chosen PDE and so understand the underlying system. The resulting model observations are specified by the parameter values, the so called forward model, which in turn may be embedded within some statistical framework (Bayesian or frequentist) to conduct parameter estimation, the inverse problem. To find typical observations from a PDE with specified parameters we need to explicitly solve the PDE, this is typically achieved using finite element numerical methods.

An alternative approach to solving PDEs is to exploit their Feynman-Kac representation: Local solutions to certain classes of PDEs are equivalent to finding expectations with respect to the law of a complementary diffusion with some boundary conditions. Consequently, unbiased Monte Carlo estimates of solutions to PDEs can be obtained via repeated simulation from the complementary (killed) diffusion. Until recently, numerical approximations would have been required, biasing the result owing to discretisation error. However, recent advances in exact simulation and debiasing schemes mean that it is now possible to obtain unbiased local solutions to many PDEs. In this talk we detail how we have exploited this recent methodology to find unbiased solutions of a class of PDEs by exploiting the Feynman-Kac representation, along with some interesting non-trivial examples.

Joint work with Jake Carson (Warwick), Murray Pollock (Warwick)

Estimating large-scale chaotic dynamics

H. Haario

Lappeenranta University of Technology, South Karelia, Finland

Obvious likelihood approaches are not available for chaotic systems, due to the sensitivity of the trajectories to any perturbations in the calculations. For large systems, such as used for weather predictions, Ensemble Prediction Systems (EPS) are used to quantify the uncertainty. Here we extend EPS, with essentially no additional CPU costs, to online estimation by perturbing the model parameters as well. The estimation can be performed both by a covariance update process using importance weights, or by employing evolutionary (DE) optimisation. Here we emphasize the use of DE for multiple cost function situations.

Multilevel Sequential Monte Carlo Samplers

K. Law[a], *A. Beskos*[b], *A. Jasra*[c], *R. Tempone*[d] *and Y. Zhou*[c]

[a] ORNL, United States of America

[b] UCL, UK

[c] NUS, Singapore

[d] KAUST, Saudi Arabia

Consider the approximation of expectations w.r.t. probability distributions associated to the solution of partial differential equations (PDEs); this scenario appears routinely in Bayesian inverse problems. In practice, one often has to solve the associated PDE numerically, using, for instance finite element methods and leading to a discretization bias. In addition, the expectation cannot be computed analytically and one often resorts to Monte Carlo methods. In the context of this problem, it is known that a multilevel Monte Carlo (MLMC) approach can reduce the amount of computational effort to estimate expectations, for a given level of error. This is achieved via a telescopic sum of Monte Carlo approximations of coupled increments of expectations with respect to the probability distributions associated to progressively finer discretizations. In many practical problems of interest, one cannot achieve an i.i.d. sampling of the associated sequence of probability distributions. A sequential Monte Carlo (SMC) version of the MLMC method is introduced to deal with this problem. It is shown that under appropriate assumptions, the attractive property of a reduction of the amount of computational effort to estimate expectations, for a given level of error, can be maintained within the SMC context. The approach is numerically illustrated on the inversion of permeability given pressure measurements in a Darcy model.

High Order Quasi Monte-Carlo Integration for Bayesian Inverse Problems

C. Schwab

ETH, Switzerland

We present sparsity theory for elliptic and parabolic PDEs with uncertain input parameters, related to recently developed, deterministic, high-order Quasi-Monte Carlo quadratures known as digital nets. Admissible problems include (linear or semilinear) elliptic or parabolic partial differential equations with uncertain parameters, shape uncertainty and the corresponding Bayesian inverse problems as formulated in ???. A parametrization of the distributed uncertainty reduces the computational problem to an ntegration problem over infinite-dimensional parameter spaces. Based on a holomorphy condition on the parameteric dependence as in ???, we present regularity estimates for the parametric integrand functions and for uniform prior measure on the parameter uncertainty in classes of weighted reproducing kernel Hilbert spaces. Related recent results (joint with J. Dick, F. Kuo, T. LeGhia and D. Nuyens) on dimension independent convergence rates of the deterministic, higher order QMC quadrature for integrand functions in weighted function spaces will be presented. The density of the posterior measure in Bayesian inverse problems for PDEs with uncertain coefficients or uncertain domains is shown to belong to the class of admissible integrand functions with a hybrid of product and sPOD weights, making these problems now accessible to high order convergent methods.
This research has been supported in part by the Swiss National Science Foundation and by the European Research Council (ERC) under ERC AdG 247277.

Transport maps for Bayesian inference in high dimensions

A. Spantini and Y. Marzouk

Massachusetts Institute of Technology, United States of America

Characterizing the high dimensional posterior distributions that arise when inferring parameters or initial conditions of ODEs and PDEs in the Bayesian framework is a challenging task. One approach to this problem seeks to construct a deterministic transport map from a reference distribution to the posterior. Posterior samples can then easily be obtained by pushing forward reference samples through the map. In this talk, we discuss methods for identifying and exploiting low-dimensional structure in the computation of transport maps.
Formally, the transport map can be obtained as the solution of an optimization problem over a function space. We show that the first variation of this optimization objective can be analyzed and evaluated in closed form, and that it reveals low-dimensional structure that may be present in the inference problem. We then propose an algorithm that composes a sequence of transport maps, interleaved with rotations, that act on progressively fewer dimensions and that adapt to the structure of the target/posterior distribution. We demonstrate the algorithm on high-dimensional inference problems arising in ODEs and PDEs.

Gaussian Process Emulators in Bayesian Inverse Problems

A. Teckentrup and A. Stuart

University of Warwick, United Kingdom

A major challenge in the application of Markov chain Monte Carlo methods to large scale inverse problems, is the high computational cost associated with solving the governing equations for a given set of input parameters. To overcome this difficulty, we consider using a surrogate model that approximates the solution of the governing equations at a much lower computational cost. We focus in particular on Gaussian process emulators, and analyse the error in the posterior distribution resulting from this approximation.

Information Geometric Trust Region Kernels for MCMC

B. Calderhead

Imperial College London, United Kingdom

We introduce a new class of proposal kernels for use in Markov chain Monte Carlo for robustly sampling from strongly correlated and highly nonlinear probability distributions. We draw on ideas from information geometry and from the optimisation literature on trust region methods to suggest Monte Carlo kernels constructed using a regularised local Riemannian geometry. This methodology allows for efficient Bayesian inference in statistical models where the information content of the data is very low and the Fisher Information describing the local geometric curvature is numerically ill-conditioned. We demonstrate the approach using highly nonlinear ordinary differential equation models.

MS28 – Molecular dynamics

Organized by: Carsten Hartmann, Robert Skeel

Stratification of Markov processes for rare event simulation

J. Weare

University of Chicago, United States of America

I will discuss an ensemble sampling scheme based on a decomposition of the target average of interest into subproblems that are each individually easier to solve and can be solved in parallel. The most basic version of the scheme computes averages with respect to a given density and is a generalization of the Umbrella Sampling method for the calculation of free energies. We have developed a careful understanding of the accuracy of the scheme that is sufficiently detailed to
explain the success of umbrella sampling in practice and to suggest improvements including adaptivity. For equilibrium versions of the scheme we have developed error bounds that reveal that the existing understanding of umbrella sampling is incomplete and leads to a number of erroneous conclusions about the scheme. Our bounds are motivated by new perturbation bounds for Markov Chains that we recently established and that are substantially more detailed than existing perturbation bounds for Markov chains. They demonstrate, for example, that equilibrium umbrella sampling is robust in the sense that in limits in which the straightforward approach to sampling from a density becomes exponetially expensive, the cost to achieve a fixed accuracy with umbrella sampling can increase only polynomially.
I will also discuss extensions of the stratification philosophy to the calculation of dynamic averages with respect a given Markov process. The scheme is capable of computing very general dynamic averages and offers a natural way to parallelize in both time and space.

Using Bayes formula to estimate rates of rare events in transition path sampling simulations

M. Athènes

CEA, France

Transition path sampling is a method for estimating the rates of rare events in molecular systems based on transforming an ensemble that contains a small fraction of reactive trajectories into a biased ensemble wherein these rare trajectories have become frequent. Unfortunately, the extent of the transformation is such that the bias can not be removed using the reweighting scheme associated with free energy perturbation. As a result, multistate reweighting schemes are traditionally implemented to postprocess data collected from staged simulations. Herein, we show how Bayes formula allows to construct a biased sample containing an enhanced fraction of reactive trajectories and to directly estimate the transition rate from this sample. We apply the approach to the migration of a vacancy in iron.

Efficient rare event simulation in molecular dynamics

C. Schütte

Zuse Institute Berlin (ZIB), Germany

We study rare events like conformation changes in molecular dynamics. The aim is to devise novel efficient importance sampling strategies that speed up the sampling of rare events and yield estimators for rare event statistics with small variance and good convergence properties. This aim is achieved by using techniques from stochastic optimal control. We will discuss the theoretical connection between importance sampling in path space and optimal control, and the algorithmic realization of the resulting rare event estimators. In very high dimensions, computation of the optimal controls is a significant challenge and thus model reduction techniques are required that help to reduce the problem to low dimensions, e.g., to some reaction coordinates. We will outline the algorithmic set-up for realizing model reduction for optimal control problems and discuss the resulting performance in application to some test systems.

Numerical Continuation Methods for Stochastic Systems

C. Kuehn

Vienna University of Technology, Austria

In this talk, I am going to explain a route to extend numerical continuation schemes to stochastic problems. The paradigm intertwines abstract analytic reduction with efficient practical numerical parameter studies of large classes of stochastic differential equation models. The method allows to investigate local fluctuations, scaling laws, switching times, and potentially many other phenomena. Examples will be given from SODEs arising in mathematical biology as well via a classical SPDE model.

Adaptive multilevel splitting techniques

T. Lelièvre

École des Ponts ParisTech, France

We will discuss algorithms to sample rare events and which are based on interacting replicas. More precisely, we will discuss the Adaptive Multilevel Splitting algorithm which has been proposed by F. Cérou and A. Guyader in 2007. We will discuss the efficiency of the algorithm and present some results concerning the unbiasedness of the estimator, whatever the choice of the importance function and the number of replicas. This has practical consequences on the use of this algorithm, which are illustrated through various numerical experiments.
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Numerical methods for sampling from the Quasistationary Distribution of a Diffusion

N. Bou-Rabee

Rutgers University, United States of America

In this talk, I will present joint work with Gideon Simpson (Drexel), on multi-dimensional diffusions which are absorbed (or killed) once they leave a specified domain. Associated with this process is a quasistationary distribution (QSD), which describes the long time (statistical) behavior of the diffusion, conditioned on non-absorption. Diffusions with absorption appear in a variety of applications, notably molecular dynamics, where they capture metastable regions of the underlying diffusion on the larger state space, without absorption. The talk presents a continuous-time, Fleming-Viot process for sampling the QSD that consists of N replicas of a Markov Chain Approximation (MCA) of the diffusion. The MCA represents the effect of the absorbing Dirichlet boundary condition in a natural and efficient way. This capability is in stark contrast to discrete-time approximations of the diffusions, such as the Euler-Maruyama scheme, which require small time steps and ad hoc corrections to accurately capture the boundary effects. This Fleming-Viot process is easy to implement, and entails running the N replicas of the MCA until one of them exits, at which point one of the non-absorbed particles splits into two particles. For large N, the replicas' empirical distribution converges at a first-order rate to the QSD of the MCA. Moreover, the QSD of the MCA is exact for arithmetic Brownian motion (Brownian motion with constant drift), and in general, second-order (spatially) accurate. Numerical tests verify these properties, and in addition, illustrate that the method applies to diffusions with multiplicative noise and whose domains are complex or unbounded with energetic and/or entropic characteristics. We also apply the method to QSDs arising in population and Brownian dynamics.

On the numerical treatment of dissipative particle dynamics and related systems

X. Shang and B. Leimkuhler

University of Edinburgh, United Kingdom

We review and compare numerical methods for particle-based modelling of complex fluids and polymers. The class of methods considered includes dissipative particle dynamics (DPD) as well as extended stochastic-dynamics models incorporating a generalized pairwise thermostat scheme, in particular, a stochastic pairwise Nose-Hoover-Langevin (PNHL) method. To this end, splitting methods are developed and studied in terms of their thermodynamic accuracy, two-point correlation functions, and convergence. In terms of computational efficiency as measured by the ratio of thermodynamic accuracy to CPU time, we report significant advantages in simulation for the PNHL method compared to popular alternative schemes (up to an 80% improvement), without degradation of convergence rate. The momentum-conserving thermostat technique described here provides a consistent hydrodynamic model in the low-friction regime, but it will also be of use in both equilibrium and nonequilibrium molecular simulation applications owing to its efficiency and simple numerical implementation.

Simulating Large-Scale Chromatin Fibers

T. Schlick

Courant Institute, United States of America

Understanding chromosome tertiary organization and its role in control of gene expression represents one of the most fundamental open biological challenges. Chromatin structure and gene expression are intimately related because the complex nature and dynamics of protein-bound DNA folding in the living cell regulates gene activity at a large range of spatial and temporal scales. Recent advances in experimental studies of chromatin using nucleosome structure determination, ultra-structural techniques, single-force extension studies, and analysis of chromosomal interactions have revealed important chromatin characteristics under various internal and external conditions. Modeling studies, anchored to high-resolution nucleosome models, have explored many related questions systematically. In this talk, I will describe recent findings regarding chromatin structure and function using a combination of coarse-grained modeling and large-scale all-atom molecular dynamics simulations of chromatin fibers. In particular, I will describe how such multiscale modeling can successfully address questions regarding the effects of epigenetic chemical modifications and the structure of condensed chromosomes in the metaphase cell cycle.

References:
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R. Collepardo-Guevara and T. Schlick, Proc. Natl. Acad. Sci. USA 111: 8061–8066 (2014).
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MS29 – Mathematical models and numerical methods for image processing

Organized by: Adérito Araújo, Sílvia Barbeiro, Eduardo Cuesta

Some degenerate equations inspired by image processing

P. Guidotti

University of California, Irvine, United States of America

The talk will focus on the analysis of a class of degenerate parabolic equations motivated by applications to image processing.

Image processing by means of complex diffusion and FV methods

E. Cuesta[a], *A. Durá*[a], *A. Araújo*[b] *and S. Barbeiro*[b]

[a] University of Valladolid, Spain

[b] University of Coimbra, Portugal

In this talk a finite volume method for a complex diffusion PDE based models is presented. In these models the solution $u : \Omega \times (0, T] \to C$, is complex?valued due to the fact that diffusion is here governed by a complex term $D(x, t, u)$. The complex diffusion model has been already proposed for image processing in the literature in the framework of PDEs. The main idea behind this model is based on considering the restored image as a complex function u evolving in time according to a multi?scale process, where the restoration is handled by means of the complex-valued diffusion term D from the noisy original image in a nonlinear way. The smoothing-enhancing process, typical of the nonlinear real models for denosing is here shared by the real and imaginary parts of the image u. The talk will be focused on the description of the finite volume method applied to discretize a complex IBVP, and its applications to image processing. Comparison with other numerical approaches, and with finite volume schemes for real models will be emphasized.

A Decomposition Framework for Image Denoising Algorithms

M. Bertalmío

Universitat Pompeu Fabra, Spain

In this talk we consider an image decomposition model that provides a novel framework for image denoising. The model computes the components of the image to be processed in a moving frame that encodes its local geometry

(directions of gradients and level-lines). Then, the strategy we develop is to denoise the components of the image in the moving frame in order to preserve its local geometry, which would have been more affected if processing the image directly. Experiments on a whole image database tested with several denoising methods show that this framework can provide better results than denoising the image directly, both in terms of PSNR and SSIM metrics.
Joint work with Gabriela Ghimpeteanu and Thomas Batard.

Computational methods for tracking cells in 4D images

K. Mikula

Slovak University of Technology Bratislava, Slovak Republic

In the talk we present new method for tracking cells in 4D biomedical images (3D+time image sequences). The method is based on extraction of the cell trajectories as smooth centered paths inside 4D spatio-temporal tree structures obtained by segmentation of 4D images. In the presented approach, the 4D segmentation is obtained by creating a spatio-temporal tubes around the cell identifiers given as a result of suitable image filtering followed by a cell detection algorithm. Then a computation of constrained distance functions inside 4D segmentation is performed by solving numerically a spatially 4D eikonal equation. Since this is a large-scale computational problem in case of real 4D image data, the parallel implementation is necessary and thus developed. By a proper combination of computed distance functions we build a potential field which is backtracked in steepest descent direction in order to get the cell trajectories. Consequently, the cell lineage tree can be constructed by detecting merging trajectories when going backward in time indicating mitosis and thus a branching node of the cell lineage tree. Our work is motivated by the recent research in biology and medicine where the reconstruction of cell population dynamics is crucial for obtaining the cell lineage trees and study of formation and evolution of morphogenetic structures. Such research is related to embryonic development of organisms as well as to anticancer drug design.
This is a common work with Robert Spir and Nadine Peyrieras.

MS30 – Surface matching for image processing tasks

Organized by: Thomas Batard, Marcelo Bertalmio

Harmonic Flow for Histogram Matching- Application to Color Transfer between two Images

T. Batard and M. Bertalmío

University Pompeu Fabra, Spain

We present a method to perform histogram matching between two color images based on the concept of harmonic mapping between Riemannian manifolds. The key idea is to associate the histogram of a color image to a Riemannian manifold. In this context, the energy of the matching between the two images is measured by the Dirichlet energy of the mapping between the Riemannian manifolds. Then, we assimilate optimal matchings to critical points of the Dirichlet energy. We use a gradient descent flow with boundary condition to reach those critical points, and we present an application to color transfer between two images.

Convolutional neural networks on non-Euclidean domains

D. Boscaini[a], J. Masci[a], S. Melzi[b], M. Bronstein[a], U. Castellani[b] and P. Vandergheynst[c]

[a] University of Lugano, Switzerland

[b] University of Verona, Italy

[c] EPFL, Switzerland

Convolutional neural networks (CNN) have been proposed over two decades ago, and have experienced a renaissance in the recent few years in the computer vision and machine learning communities due to their state-of-the-art performance on a variety of image analysis tasks. However, in the domain of 3D shape analysis, these methods are practically unknown and unused.

We propose ShapeNet, a generalization of the CNN paradigm to non-Euclidean manifolds. Our construction is based on a local intrinsic representation of manifold structures that are then passed through a cascade of filters and linear and non-linear operators. The coefficients of the filters and linear combination weights are optimization variables that are learned to minimize a task- specific cost function. We use ShapeNet to learn invariant shape feature descriptors that significantly outperform recent state-of-the-art methods, and show that previous approaches such as heat and wave kernel signatures, optimal spectral descriptors, and intrinsic shape contexts can be obtained as particular configurations of ShapeNet.

Currents and normal cycles models for curve or surface registration. Applications in computational anatomy

J.A. Glaunès

Université Paris Descartes, France

Computational Anatomy is the geometrical and statistical study of the shape variability of organs based on the analysis of medical images. Designing efficient mathematical frameworks and algorithms for estimating optimal deformations between images or geometrical elements extracted from the images is fundamental in such studies. Some years ago, diffeomorphic methods for matching curves and surfaces have been developed using the mathematical notion of currents. At a discrete level, curves and surfaces are approximated in this framework by sums of vector-valued Dirac functionals which encode both position and tangential information. The key point is the ability to define and compute reproducing kernels and their corresponding Hilbert norms, which are used as matching criterions for curves or surfaces. I will present this setting and applications of such registration algorithms for the analysis of brain imaging datasets, and for a study of the human ear morphometry for research in audio. I will also present a new framework based on second-order currents called normal cycles which encode also curvature information. This new model appears to give more accurate results as it enforces matching between corresponding points of high curvature in both shapes. Moreover, it does not require to specify an orientation on the sub-manifolds, as opposed to the currents model. This is a very useful property in practice, specifically for curves composed of several disconnected components and branches. This new model is also related to another model based on varifolds, recently introduced by Nicolas Charon.

Contour Manifolds and Optimal Transport in Variational Image Segmentation

B. Schmitzer[a] *and C. Schnörr*[b]

[a] Université Paris-Dauphine, France

[b] Universität Heidelberg, Germany

Parametrized contours and region indicator functions are popular representations for shape with complimentary strengths. While contours allow for sophisticated shape modelling on corresponding manifolds, directly employing them in image segmentation functionals usually yields highly non-convex problems. Indicator functions are naturally compatible with the framework of convex variational image segmentation, however their natural linear structure is not well-adapted to shape-modelling.
Using the Riemannian structure of the 2-Wasserstein space, one can link both representations and combine their advantages.
In this talk we will detail this relation and provide context from the viewpoint of image segmentation, as motivation. As a potential application we discuss the construction of isometry invariant shape priors for object segmentation, which can be optimized globally. Numerical results are discussed along with open questions concerning both theory and applications.

MS31 – New aspects and applications of structure preserving numerical methods

Organized by: Takaharu Yaguchi

Energy-preserving discrete gradient schemes for the Hamilton equation based on the variational principle

A. Ishikawa and T. Yaguchi

Kobe University, Japan

Physical conservation laws are from the variational principle.

The conventional discrete gradient method is the framework for deriving energy-preserving schemes, however, is not based on this principle.

In this talk, we propose a new framework which discretizes the Hamilton equations while preserving the energy by application of the variational principle and the discrete gradients.

Moreover, if the Hamiltonian is separable, this framework gives explicit energy-preserving schemes.

Parasitism control for symmetric multivalue methods: theory and practice

A.T. Hill and T. Norton

University of Bath, United Kingdom

Parasitism, or weak instability, is a theoretical disadvantage of structure–preserving linear multistep and general linear methods. In practice, however, variants of the theoretically parasitic Leapfrog method continue to be used, especially in Meteorology.

In this talk, we consider how to choose a starting method, finishing method and parasitic filter, in order to minimize parasitism and retain geometric properties. We also present

numerical results which demonstrate that, when suitable choices are made, the Leapfrog method and other explicit symmetric multivalue methods are capable of approximate long–time preservation of invariants for several challenging Hamiltonian problems.

Stiff Problems in High Fidelity Visual Computing

D.L. Michels

Stanford University, United States of America

To take into account a multitude of physical effects, high fidelity simulations are nowadays of growing interest for analyzing and synthesizing visual data. In contrast to most numerical simulations in engineering, local accuracy is secondary to the global visual plausibility. Global accuracy can be achieved by preserving the geometric nature and physical quantities of the simulated systems for which reason geometric integration algorithms like symplectic methods are often considered as a natural choice. Additionally, if the underlying phenomena behaves numerically stiff, a non-geometric nature comes into play requiring for strategies to capture different timescales accurately.
In this talk, the use of hybrid semi-analytical (exponential) integrators for modeling and design applications is presented. The advantageous behavior is demonstrated across a broad spectrum of complex models that include deformable solids, trusses, textiles, and molecular structures, including damping, collision responses, friction, and non-linear material behavior.

Infinite dimensional Lie groups in numerical analysis

G. Bogfjellmo

Norwegian University of Science and Technology, Norway

Many phenomena in numerical analysis can be studied by expanding a function in series over some index set. The combinatorial formulas arising from composing such series can in some cases be formulated via the co-product in a Hopf algebra, with the interesting series forming a character group.
The most prominent example of this construction arising in numerical analysis is the Butcher group.
We explore the topological aspects of these groups, specifically showing if the Hopf algebra is graded and connected, the group of characters becomes a locally convex Lie group modelled on an infinite dimensional case.
The talk is based on joint work with Rafael Dahmen, TU Darmstadt and Alexander Schmeding, NTNU Trondheim.

MS32 – Optimal transport in image and shape analysis

Organized by: Jan Lellmann, Carola Schönlieb

A generalized model for optimal transport of images including dissipation and density modulation

J. Maas[b], *M. Rumpf*[a], *C. Schönlieb*[c] *and S. Simon*[a]

[a] University of Bonn, Germany

[b] IST Austria

[c] University of Cambridge, United Kingdom

In this contribution a new model in which the optimal transport and the metamorphosis perspectives are combined is presented. For a pair of given input images geodesic paths in the space of images are defined as minimizers of a resulting path energy. To this end, the underlying Riemannian metric measures the rate of transport cost and the rate of viscous dissipation. Furthermore, the model is capable to deal with strongly varying image contrast and explicitly allows for sources and sinks in the transport equations which are incorporated in the metric related to the metamorphosis approach by Trouvé and Younes. In the non-viscous case with source term existence of geodesic paths is proven in the space of measures. The proposed model is explored on the range from merely optimal transport to strongly dissipative dynamics. For this model a robust and effective variational time discretization of geodesic paths is proposed. This requires to minimize a discrete path energy consisting of a sum of consecutive image matching functionals. These functionals are defined on corresponding pairs of intensity functions and on associated pairwise matching deformations. Existence of time discrete geodesics is demonstrated. Furthermore, a finite element implementation is proposed and applied to instructive test cases and to real images. In the non-viscous case this is compared to the algorithm proposed by Benamou and Brenier including a discretization of the source term. Finally, the model is generalized to define discrete weighted barycentres with applications to textures and objects.

A total-variation Wasserstein flow applied to image denoising problems

C. Schönlieb[a], *M. Benning*[b], *L. Calatroni*[a] *and B. Duering*[b]

[a] University of Cambridge, United Kingdom

[b] University of Sussex, United Kingdom

We consider a nonlinear fourth-order diffusion equation modelling the denoising task of image densities. Such equation can be formally interpreted as the gradient flow of the Total Variation regularisation functional with respect to the 2-Wasserstein metric in the space of probability densities. In order to solve the model numerically, we present an implicit time-stepping scheme based on a primal-dual method for computing the subgradient of the total variation semi-norm relaxing the constraint on the dual variable through a penalty term. The numerical

solutions of the scheme respect the positivity, mass preservation properties of the underlying PDE as well as the gradient flow structure.

Entropic Regularization of Wasserstein Gradient Flows

B. Schmitzer

Université Paris-Dauphine, France

Jordan, Kinderlehrer and Otto have shown how several well-known PDEs can be interpreted as gradient flows in Wasserstein space. Today this is a popular point of view in physical sciences and game theory: beyond merely providing some beautiful intuition it serves as a tool for analytical and numerical investigation of PDEs. However, the involved optimal transport problem can quickly become a computational bottleneck. As a remedy we propose entropic regularization of optimal transport in the gradient flow scheme to allow the application of computationally efficient matrix scaling algorithms. In this talk we will briefly review gradient flows in Wasserstein space. Then the regularized variant is introduced. We show convergence to the original scheme and discuss numerical efficiency of the scheme.

Structure-texture decomposition by transport norms

D. Lorenz

TU Braunschweig, Germany

We show that distances based on optimal transport can be used to separate certain noise and texture components in images. While noise and texture have several similar characteristics such as both high and low frequencies and local oscillations, it turns out that their behavior under transport is fairly different. This allows to set up variational models to separate noise, texture and cartoon parts with a single variational model. We describe this model, show connections to previous texture models and also describe a low-cost computational framework for the optimal transport norms.

MS33 – Mathematical modelling in pharmacology and drug development

Organized by: Wilhelm Huisinga

The role of mathematical modeling in drug discovery, development and therapy optimization

W. Huisinga

Universität Potsdam, Germany

Mathematical modeling plays a key role in model-informed drug discovery and development as well as the optimization of drug therapies. This talk gives an introduction into the topic and an overview of different mathematical approaches used in drug discovery and development and therapy optimization. It is followed by three talks giving insight into specific applications/problems.

Modeling and simulation of complex pharmacometric models with Monolix

M. Lavielle

Inria, France

Population models describe biological and physical phenomena observed in each of a set of individuals, and also the variability between individuals. This approach finds its place in domains like pharmacometrics when we need to quantitatively describe interactions between diseases, drugs and patients. This means developing models that take into account that different patients react differently to the same disease and the same drug. The population approach can be formulated in statistical terms using mixed effects models.
Such framework allows one to represent models for many different data types including continuous, categorical, count and time-to-event data. This opens the way for the use of quite generic methods for modeling these diverse data types. In particular, the SAEM (Stochastic Approximation of EM) algorithm implemented in the Monolix software is extremely efficient for maximum likelihood estimation of population parameters, and has been proven to converge in quite general settings.
Monolix is associated with Mlxtran, a declarative language designed for encoding hierarchical models, including complex mixed effects models. Mlxtran is also a particularly powerful solution for encoding dynamical systems represented by a system of ordinary differential equations. Mlxtran is also used by Simulx, a R and Matlab function for easily computing predictions and simulating data from complex mixed effects models (http://simulx.webpopix.org).

Model-based treatment planning in reproductive medicine

S. Röblitz[a], *S. Schäfer*[b], *T. Dierkes*[b] *and R. Ehrig*[b]

[a] Freie Universität Berlin, Germany

[b] Zuse Institute Berlin (ZIB), Germany

Successful pregnancy is based on physiological events like adequate follicle maturation, ovulation, ovum fertilization, corpus luteum formation and endometrial implantation. These processes are controlled by hormones whose secretion follows a strictly balanced chronological regime. Endocrine diseases like polycystic ovarian syndrome or endometriosis as well as certain environmental and lifestyle factors are known to have a negative impact on fertility. Modern techniques in reproductive medicine like in-vitro fertilization or intracytoplasmic sperm injection have increased the chances for successful reproduction. However, current success rates vary significantly among clinics, still reaching only about 35% even in well functioning centers. This is mainly due to the usage of different treatment protocols and limited knowledge about individual variability in the dynamics of reproductive processes. Hence, the aim of our research is to provide a model-based clinical decision support system for reproductive endocrinologists that enables the simulation and optimization of treatment strategies in-silico. The talk focuses on the development and validation of a mathematical model for the human menstrual cycle, its specification in terms of individual patients, and its coupling to a treatment protocol model which allows to evaluate the success rate of different treatment strategies. The results are joint work with the researchers involved in the EU project PAEON.

MS34 – Parametric Model Order Reduction: Challenges and Solutions

Organized by: Christian Himpe, Ulrike Baur

Parametric Model Order Reduction via Bilinearization

P. Benner

Max Planck Institute for Dynamics of Complex Technical Systems, Germany

Parametric model order reduction (PMOR) for linear parametric or parameter-varying systems is omnipresent in engineering design applications. There exist numerous families of projection-based PMOR methods, but they all lack optimality properties regarding minimization of an error norm. We will discuss an approach based on transforming (analytically) a linear parametric system to a bilinear system, for which model reduction methods based on error minimization exist. We will illustrate the effectiveness of this approach using classical benchmark examples as well as industrial applications.

Reduced basis method for parameter-dependent Lyapunov equations with application in parametric model reduction

N.T. Son[a] *and T. Stykel*[b]

[a] Thai Nguyen University of Sciences, Vietnam

[b] Universität Augsburg, Germany

In this talk, we consider model reduction of parametric control systems using balanced truncation. This model reduction approach requires the numerical solution of parameter-dependent Lyapunov equations. We present a reduced basis method for solving such equations. Assuming an affine parameter dependence in the matrix coefficients, this method allows the offline-online decomposition. In the offline stage, the Lyapunov equations are solved for suitably chosen parameters and their solutions are collected to form the low-dimensional projection subspace. In the online stage, one computes an approximate solution for any parameter value using the Galerkin projection. We derive a posteriori error estimates for reduced basis approximations and present some results of numerical experiments.

Reduced Basis Approximation of Large Scale Parametric Algebraic Riccati Equations

A. Schmidt

University of Stuttgart, Germany

We consider the application of the Reduced Basis (RB) methodology for parametrized continuous time Algebraic Riccati Equations (AREs). The ARE is a nonlinear matrix valued equation with numerous applications for instance in the field of optimal feedback control or optimal state estimation for linear systems. Large scale problems that typically arise from semidiscretized partial differential equations often result in infeasible computation times when considering multi-query scenarios for varying parameters or real-time applications. We hence show how the RB method can be used for obtaining approximate solutions rapidly
while being able to quantify and control the resulting error by means of rigorous error bounds between the reduced solution and the true solution. Under the usual assumption of parameter separability we show how the calculation can be performed rapidly online with a complexity only depending on the reduced dimension. This is possible due to a expensive offline phase where a problem adapted solution space is constructed through a procedure called Low Rank Factor Greedy. This algorithm exploits a low rank structure in the solution matrices of the ARE and subsequently adds compressed information from so called low rank factors to the basis. A Galerkin projection results in small AREs that can be solved rapidly. In the online phase, the error can be rigorously quantified by a residual based error bound. We furthermore provide error statements for the linear quadratic regulator problem for linear and time invariant systems, when the reduced solution of the ARE is used as a surrogate for the true (expensive) solution for the definition the feedback controller.

Productivity-quality-energy a conflict triangle requiring PMOR of Machine Tool Models

J. Saak

Max Planck Institute for Dynamics of Domplex Technical Systems, Germany

Modern machine tools are highly complex and optimized devices. They consist of many building blocks that have been modelled and understood very well separately over the years. coupling the single models to assembly groups or entire machines is making the models so large and introduces so many parameters that full order simulations and control are unreachable when considering the development time demands by the market.
The large models can however be interpreted as networks of parametrized nodal systems. In order to get a high performance reduced order model, network reductions need to be undertaken in two ways. First the networks node model require PMOR approximations in order to preserve the coupling parameters. Second the network needs to be investigated further to eliminate such nodes that do not, or do least influence the actual target: the deviation of the tool center point from its desired position driven by the heat induced by the machining process. We will report on the research undertaken in the DFG/CRC-96 treating these problems.

MS35 – Numerical multiscale methods for oscillatory problems

Organized by: Richard Tsai, Gil Ariel

Multiscale methods for wave propagation problems

O. Runborg

KTH, Sweden

Wave propagation problems with rapidly varying coefficients are computationally costly to solve by traditional techniques because the smallest scales must be represented over a domain determined by the largest scales of the problem. We consider numerical methods for such wave propagation in the framework of the heterogeneous multiscale method. These methods couple simulations on macro- and microscales for problems with rapidly oscillating coefficients. The complexity is significantly lower than that of traditional techniques with a computational cost that is essentially independent of the microscale. In this talk we show analysis of how the method works in the long time case, where the macroscale solution show dispersive behavior, and how the method, although designed for wave problems, can be beneficial for solving multiscale elliptic problems.

Numerical homogenization methods for quasilinear multiscale PDEs

A. Abdulle[a], *Y. Bai*[a], *M. Huber*[a] *and G. Vilmart*[b]

[a] EPF Lausanne, Switzerland

[b] University of Geneva, Switzerland

We study the finite element heterogeneous multiscale method (FE-HMM) for two different classes of nonlinear multiscale PDEs with highly oscillatory coefficients.

We first consider nonlinear elliptic problems of nonmonotone type where the micro cell problems arising from homogenization theory are linear. We prove optimal convergence rates of the FE-HMM and show how the coupling of the method with the reduced basis technique (RB-FE-HMM) considerably improves the efficiency by drastically reducing the number of degrees of freedom.

We then focus on a class of nonlinear parabolic problems of monotone type for which the micro cell problems are now nonlinear. We introduce a novel linearized scheme that is only based on linear micro problems, which permits an efficient implementation, and present recently obtained optimal a priori error estimates which are fully discrete in time and space.

Publications and preprints available at: http://www.unige.ch/ vilmart/publications.html

Variance-reduced simulation of the effective dynamics of slow-fast stochastic differential equations

G. Samaey

KU Leuven, Belgium

We consider slow-fast stochastic differential equations for which an effective dynamics exists in terms of a relatively low number of macroscopic state variables and for which a direct simulation at the macroscopic level involves the computation of averages over the invariant measure of the fast subsystem for fixed values of the macroscopic state variables. Because the fast subsystem is often high-dimensional, these averaged quantities are usually computed using a Monte Carlo method, which leads to statistical noise on the computed results. We discuss algorithms that reduce the variance of this noise by an appropriate coupling of stochastic processes in consecutive time steps. We provide theoretical results and illustrate the method on a series of model problems with increasing complexity.

Multiscale parareal methods for highly oscillatory dynamical systems

R. Tsai

KTH Royal Institute of Technology, Sweden

We introduce a new parallel in time (parareal) algorithm which couples multiscale integrators with fully resolved fine scale integration and computes highly oscillatory solutions for a class of ordinary differential equations in parallel. The algorithm computes a low-cost approximation of all slow variables in the system.
The fast phase-like variables are computed using the parareal iterative methodology and an alignment algorithm. The method may be used either to enhance the accuracy and range of applicability of the multiscale method in approximating only the slow variables, or to resolve all the state variables.

Contributed Talks

Session CS01 – Stiff ODEs

Performance Evaluation of Quadruple and Octuple Precision Implicit Runge-Kutta ODE solvers

T. Kouya

Shizuoka Institute of Science and Technology, Japan

We show implementation details and performance evaluation of our multiple precision ODE solvers (BIRK) based on explicit and implicit Runge-Kutta (IRK) methods with QD, GQD libraries and MPFR. Especially for fully IRK methods, mixed precision iterative refinement method can accelerate to solve linear equations in its inner iteration process. QD and GQD, which provide quadruple and octuple precision floating-point arithmetic on CPUs and GPUs, can also be effective in order to solve some chaotic problems. In our talk, we demonstrate that BIRK is useful to solve such problems.

$\mathbf{A-\overline{A}-V}$ SGLMs

A. Ezzeddine

Lebanese International University, Lebanon

This paper considers an special construction of second derivative general linear methods (SGLMs) for the numerical integration of stiff initial value problems in ordinary differential equations. The introduced technique decreases the complexity of finding coefficients matrices of the methods. The constructed SGLMs of orders 3 and 4 which posses Runge-Kutta stability property, are A- and L-stable. Efficiency of the constructed methods is confirmed by numerical experiments.

Practical experiments with second derivative methods for stiff ODEs

G. Hojjati and A. Abdi

University of Tabriz, Islamic Republic of Iran

In this paper, we construct the second derivative general linear methods in the Nordsieck form for the numerical solution of stiff systems of first order ordinary differential equations. The constructed methods are L–stable of order $p = s + 1$, where s is the number of internal stages, and stage order $q = p$. The implementation issues including the starting procedures, stage predictors, local error estimation and the changing stepsize are examined. Numerical experiments indicate reliability of the error estimates and efficiency of the methods in a variable stepsize environment.

Construction and implementation of two-stage second derivative methods for stiff ODEs

A. Abdi and G. Hojjati

University of Tabriz, Islamic Republic of Iran

We consider the class of second derivative general linear methods (SGLMs) for the numerical solution of first order ordinary differential equations. In this large family of the methods, we construct two–stage A– and L–stable methods of order up to 6 with low error constants. By equipping some of these methods to variable stepsize, we will present some numerical experiments for fixed and variable stepsize implementations of these methods to show efficiency of them.

Session CS02 – Splitting methods

Adaptive High-order Time-Splitting Methods for Systems of Evolution Equations. Part II: Applications in Quantum Dynamics and Pattern Formation

O. Koch[a], *W. Auzinger*[b], *H. Hofstätter*[b], *M. Quinn*[b] *and M. Thalhammer*[c]

[a] University of Vienna, Austria

[b] Vienna University of Technology, Austria

[c] University of Innsbruck, Austria

We present high-order splitting time integrators for nonlinear evolution equations. Methods for splitting into two or three operators are introduced together with a rigorous error analysis and asymptotically correct defect-based error estimators. Our error analysis applies to equations of Schrödinger type, but also extends to parabolic problems within the appropriate functional analytic framework for either periodic or Dirichlet boundary conditions. The proposed methods are furthermore demonstrated to be highly successful for adaptive time-integration also in a parallel environment, with good scaling in the number of processors, and to produce efficient and accurate simulations of intricate dynamics as in models from quantum dynamics or pattern generation. Highly relevant models in the scope of our methods are the Gross-Pitaevskii equation, the Gray-Scott system or the Gierer-Meinhart model, which are efficiently solved.

Splitting schemes, order conditions, and optimized pairs

W. Auzinger[a], *H. Hofstätter*[a], *D. Ketcheson*[b] *and O. Koch*[c]

[a] Vienna University of Technology, Austria

[b] KAUST, Saudi Arabia

[c] University of Vienna, Austria

We describe an algorithm for the automatic generation of systems of polynomial equations representing order conditions for higher-order splitting schemes for the integration of evolution equations. This algorithm is based on combinatorial properties of Lyndon-Shirshov bases in free Lie Algebras. Since the number of terms in the resulting equations rapidly increases with the desired order, a parallel realization of the algorithm has been implemented for the purpose of speed-up. Splitting into two or three operators is considered, and a number of schemes obtained is presented. Our main focus is on pairs of schemes, where one of them is the 'worker', and its partner provides a local error estimate. We explain how optimized versions of such pairs of schemes can be constructed, and we present a number of examples.

Convergence of adaptive splitting and finite element methods for the Schrödinger-Poisson equation

W. Auzinger[b], *T. Kassebacher*[a], *O. Koch*[c] *and M. Thalhammer*[a]

[a] University of Innsbruck, Austria

[b] Vienna University of Technology, Austria

[c] University of Vienna, Austria

Operator splitting methods combined with hp-finite element approximations are studied for the full discretization of the Schrödinger-Poisson equation. As in each splitting step the nonlinear interaction potential is conserved exactly, splitting methods promise significant computational advantages as compared to standard time integration methods. Equipped with asymptotically correct a posteriori local error estimators for automatic stepsize control, the approach leads to reliable and efficient approximations. The provided stability and error analysis extends the work of Lubich ('07) for the Strang splitting method, incorporating the additional influence of the finite element space discretization.
This is joint work with Winfried Auzinger (Vienna University of Technology), Othmar Koch (University of Vienna), and Mechthild Thalhammer (University of Innsbruck).

Overcoming order reduction in reaction-diffusion splitting

Alexander Ostermann and L. Einkemmer

University of Innsbruck, Austria

Splitting methods constitute an important class of time integration schemes for evolution equations: one decomposes the vector field into disjoint parts, integrates the resulting sub-problems separately (on an appropriate time interval), and finally combines the single flows in the right way to obtain the sought-after numerical approximation. A standard example is given by reaction-diffusion equations, where the diffusion is modeled by the Laplacian and the reaction by a (locally acting) non-linearity, respectively. Separating the diffusion from the reaction gives, on the one hand, a free heat equation that can often by solved efficiently by fast Fourier techniques and, on the other hand, a set of ordinary differential equations that describe the local reactions at each grid point.
However, the above approach requires some care if the problem is endowed with non-periodic boundary conditions. In this case, a straightforward application of splitting will often lead to a strong order reduction and consequently to computational inefficiency. In the talk, we will exemplify the problem of boundary conditions in splitting methods with the help of typical examples. Based on these observations and further theoretical investigations, we will present some remedies to greatly avoid such order reductions.
The talk is based on the paper L. Einkemmer and A. Ostermann, Overcoming order reduction in diffusion-reaction splitting. Part 1: Dirichlet boundary conditions. To appear in SIAM J. Sci. Comput., 2015.

Session CS03 – Time fractional differential equations

Finite element approximation for time fractional parabolic optimal control problems - a priori error estimates

M. Kandasamy

Periyar University, India

In this paper, a numerical theory based on finite element approximations for time fractional parabolic optimal control problems is presented and analyzed. The state and co-state variables are approximated by the piecewise linear functions and the control is approximated by piecewise constant functions. We derive, a priori error estimates for both the control variable and the state variables. We illustrate with a numerical example to confirm our theoretical results.

Numerical solution of time-fractional reaction-diffusion systems

K. Burrage[a], *A. Cardone*[b], *B. Paternoster*[b] *and R. D'Ambrosio*[b]

[a] University of Oxford, UK, and Queensland University of Technology, Australia

[b] University of Salerno, Italy

Fractional differential systems model many dynamical phenomena all associated with memory aspects. These include anomalous diffusion in transport dynamics, the response of viscoelastic materials under mechanical stress, some biological processes in rheology and the kinetics of complex systems in spatially crowded domains. In recent years, considerable attention has been paid to fractional reaction-diffusion systems, where the fractional derivative index alpha produces new effects with respect to the classical model. For example, in the nonlinear model [1], when 0<alpha<1, a relaxation process arises, and when 1<alpha<2 periodic solutions may occur. In this talk we analyse the numerical treatment of time-fractional reaction-diffusion systems. As the solution depends on all its past history, numerical step-by-step methods are computationally expensive. On the other hand spectral methods can avoid the discretization of the 'heavy tail' and are exponentially convergent [2]. We propose a numerical scheme consisting of a spectral method through time, on a basis of functions suitably chosen for the problem, and a finite-difference method through space, whose coefficients are adapted according to the qualitative behaviour of the solution. Finally we illustrate preliminary numerical results on some significant test equations.

[1] V. Gafiychuk, B. Datsko, and V. Meleshko. Mathematical modeling of time fractional reaction-diffusion systems. J. Comput. Appl. Math., 220(1-2):215-225, 2008.

[2] M. Zayernouri and G. Em Karniadakis. Fractional spectral collocation method. SIAM J. Sci. Comput., 36(1):A40-A62, 2014.

An efficient difference scheme for the fractional Ginzburg-Landau equation

P. Wang and C. Huang

School of Mathematics and Statistics, Huazhong University of Science and Tehnology, People's Republic of China

In this talk, we present an efficient difference scheme for the nonlinear complex Ginzburg-Landau equation involving the fractional Laplacian. The scheme is based on the implicit midpoint rule for the temporal discretization and a weighted and shifted Grunwald difference operator for the spatial fractional Laplacian. This scheme is second-order in both time and space. Our focus is on a rigorous theoretical analysis for the scheme. In order to overcome the difficulty caused by the nonlocal property of the fractional Laplacian, we make a detailed study of the fractional approximation operator. The discrete fractional Gagliardo-Nirenberg inequality and an equivalence relation between an energy norm and the fractional Sobolev semi-norm are established. Then the scheme is proved to be unconditionally convergent in the l^2 norm with optimal order, in the sense that no restriction on the temporal step size in terms of the spatial discretization parameter needs to be assumed. Finally, numerical examples are given to validate the theoretical results and the effectiveness of the scheme.

A class of piecewise interpolating polynomial approximations for time-fractional differential equations

H. Zhou

Utrecht University, The Netherlands

In this talk we consider systems of fractional order (in time) differential equations. The fractional derivative of order between 0 and 1 is defined in the sense of Caputo. For the numerical approximation of such derivatives a class of implicit methods is constructed based on piecewise interpolating polynomials. We analyze the consistency and stability properties for a test equation. Numerical experiments will illustrate the performance and confirm the order of accuracy of the proposed techniques.

Session CS04 – Model reduction

Interpolary Model Reduction for Stokes-type Quadratic-Bilinear Systems

P.K. Goyal, J. Heiland, M.I. Ahmad and P. Benner

Max Planck Institute for Dynamics of Complex Technical Systems, Germany

In this talk, we focus on interpolatory model reduction for Stokes-type quadratic-bilinear descriptor systems. In case of linear system, extending standard interpolatory model reduction methods to descriptor systems without special treatment of the polynomial part of the transfer function, leads to an unbounded error in the H2 norm. This was
fixed recently in [S. Wyatt et. al., SISC 35(5):B1010-B1033, 2013]. Here, we consider similar problem for quadratic-bilinear descriptor systems. The approach is to transform the quadratic-bilinear descriptor system into an equivalent quadratic-bilinear ODE system using spectral projectors. This allows us to employ the two-sided interpolatory projection method [P. Benner et. al., SJSC 37(2):B239-B260, 2015] for model reduction of quadratic-bilinear descriptor systems, while ensuring bounded error in the H2 norm. In view of implementation, we propose an efficient method to compute the projection matrices by avoiding the explicit computation of spectral projectors. Numerical results, obtained from simulation of semi-discretized (Navier-)Stokes equations, show the efficiency of the proposed approach and a comparison with the direct implementation (without transforming the system into an equivalent ODE system).

Fully adaptive higher-order stochastic Galerkin FEM in low-rank tensor representation

M. Eigel[a]*, M. Pfeffer*[b] *and R. Schneider*[b]

[a] Weierstrass Institute (WIAS), Germany

[b] TU Berlin, Germany

PDE with stochastic data usually lead to very high-dimensional algebraic problems which easily become infeasible for numerical computations because of the dense coupling structure of the discretised stochastic operator. Recently, an adaptive stochastic Galerkin FEM based on a residual a posteriori error estimator was presented and the convergence of the adaptive algorithm was shown in [1,2]. While this approach leads to a drastical reduction of the complexity of the problem due to the iterative discovery of the sparsity of the solution, the problem size and structure still is rather limited. To allow for larger and more general problems, we exploit the tensor structure of the parametric problem by representing operator and solution iterates in the tensor train (TT) format [3]. The (successive) compression carried out with these representations can be seen as a generalisation of some other model reduction techniques, e.g. the reduced basis method.

We show that this model reduction approach facilitates the efficient computation of different error indicators related to the computational mesh, the active polynomial chaos index set, and the TT rank. In particular, the curse of dimensionality is avoided. Numerical examples demonstrate the efficiency of the fully adaptive approach.
[1] M. Eigel, C. J. Gittelson, C. Schwab, and E. Zander, "Adaptive stochastic Galerkin FEM", Comput. Methods Appl. Mech. Engrg., 270 (2014), pp. 247–269.
[2] M. Eigel, C. J. Gittelson, C. Schwab, and E. Zander, "A convergent adaptive stochastic Galerkin finite element method with quasi-optimal spatial meshes", WIAS preprint 1911.
[3] S. Holtz, T. Rohwedder, R. Schneider, "The Alternating Linear Scheme for Tensor Optimization in the Tensor Train Format", SIAM J. Sci. Comput., 2012, 34(2), A683?A713

Asymptotical Characterisation of Stiffness of Ordinary Differential Equations

P. Marschalik[a] *and R. Klein*[b]

[a] Johannes Gutenberg University Mainz, Germany

[b] Freie Universität Berlin, Germany

Motivated by multiscale asymptotics a new view on the mathematical structure of stiff behaviour of solutions of ordinary differential equation problems is given that is independent of numerical schemes or discretisations. Stiffness is introduced as an asymptotic property of the problem family that is said to occur if certain components of the family of solutions decay exponentially in the limit. The manifolds onto which these solution components relax are described.

Coarse-graining the dynamics of bursting neurons using an equation-free approach

A. Ben-Tal[a] *and I.G. Kevrekidis*[b]

[a] Massey University, New Zealand

[b] Princeton University, USA

A system of coupled bursting neurons often exhibits transitions from a quiescent state (no action potentials) to a bursting state (repeated train of action potentials followed by a period of no electrical activity) to a spiking state (continuous train of action potentials). However, in certain applications, the exact details of the complex dynamics that underlies these transitions may not be important and one would like to use a simplified model that captures the dynamics only roughly. We have developed a numerical method, based on an equation free approach that enables us to understand the type of bifurcations the simplified model should have. The method maps between the variables of a bursting neural network (for which the equations are known) and the variables of a simplified model (for which the equations are in principle unknown). By moving backward and forward between the variables of the detailed system and the variables of the simplified system using restriction and lifting operators, and simulating the detailed system for short periods of time, we can calculate the stationary solutions of the simplified model and their stabilities and create bifurcation diagrams for the simplified model. We illustrate our approach on a model of a single neuron that consists of 3 ordinary differential equations and show that the system could be simplified using 2 ordinary differential equations. We then show how our method can be applied to a network of several neurons. Our work is motivated by studies of the neural control of breathing.

Session CS05 – Delay differential equations

The IG-approach for nonlinear delay models: back to ODEs

R. Vermiglio[a], *O. Diekmann*[b], *D. Breda*[a] *and F. Scarabel*[c]

[a] Udine, Italy

[b] Utrecht, The Netherlands

[c] Helsinki, Finland

Nowadays delay models are proposed to describe a variety of problems in science and engineering. In fact, the introduction of the dependence on the past history allows a better description of the real-life phenomena and a more reliable prediction of their behavior. Delay models present a more complex dynamics since, opposite to ordinary differential equations (ODEs), they are infinite dimensional dynamical systems. Therefore their study needs to be complemented with efficient numerical methods. From a dynamical system point of view, a first relevant task concerns the stability of equilibria. Recently a numerical approach has been developed to this aim, which is based on the discretization of the infinitesimal generator (IG) associated to the linearized system. In this talk we present the extension of the so called lG-approach to nonlinear Delay Differential Equations (DDEs), Delay Equations (DEs), and coupled systems DDEs/DEs to reduce the original system to a nonlinear system of ODEs. This allows the use of proven and efficient tools for the analysis of bifurcation of ODEs, without resorting to the development of ad-hoc techniques for the original model. Some test examples are given.

The effect of impulsive birth and harvest pulses on a population dynamics model with feedback loops

A.-S. Frank[a,b] *and S. Subbey*[a,c]

[a] Institute of Marine Research (IMR), Norway

[b] Technical University Munich (TUM), Germany

[c] The Hjort Centre for Marine Ecosystem Dynamics, Bergen, Norway

This paper presents numerical analysis of a single-species and stage-structured Delay Differential Equation (DDE) model. The focus is on understanding (i) the effect of single or several harvest and birth pulses, and (ii) the role of delays, in regulating the dynamics of the perturbed system. We present numerical results, which sketch theoretically possible instances of the model behavior. On the basis of these results, we discuss the possible effects of impulsive perturbations on the dynamics of fish populations.

Analysis and Numerical Solutions of Linear Delay Differential-Algebraic Equations

P. Ha[a] *and V. Mehrmann*[b]

[a] Humboldt University of Berlin, Germany

[b] Technische Universität Berlin

The analysis and numerical solution of initial value problems for linear delay differential-algebraic equations (DDAEs) is discussed. Characteristic properties of DDAEs are analyzed and the differences between causal and noncausal DDAEs are studied. The method of steps is analyzed and it is shown that it has to be modified for general DDAEs. The classification of ordinary delay differential equations (DDEs) is generalized to DDAEs, and a numerical solution procedure for general retarded and neutral DDAEs is constructed. The properties of the algorithm are studied and the theoretical results are illustrated with a numerical example.

Application of two controls optimally in the treatment of HIV

H. Kheiri

University of Tabriz, Islamic Republic of Iran

In this paper, we apply optimal control theory to a system of ordinary differential equations describing the interaction of immune system with the human immunodeciency virus (HIV). Seeking to reduce the latent and infectious classes, we explore controls representing drug treatment strategies of this model. Using an objective function based on a combination of minimizing both latent and infectious T cell counts and associated costs, we solve for the optimal control in the optimality system. We apply a forward and backward numerical method for solving obtained system. At the end of the paper, the impact of combination of the strategies in the control of HIV are compared by numerical simulation.

Session CS06 – DAEs

Cosimulation Convergence Criteria for Hessenberg DAEs of Index 2

J. Pade and C. Tischendorf

Humboldt University of Berlin, Germany

The network approach to the modelling of complex technical systems results frequently in a set of coupled differential-algebraic equations (DAEs). Dynamic iteration methods, also referred to as cosimulation or waveform relaxation methods, are well-established since they allow for dedicated solvers and discretisation grids for the involved subsystems. Coupled DAE-systems may suffer from instability during a dynamic iteration. We present a convergence criterion for systems involving Hessenberg-DAEs of index 2.

A new projector-based decoupling for (linear) higher-index DAEs using automatic differentiation

D. Estévez Schwarz[a] *and R. Lamour*[b]

[a] Beuth Hochschule für Technik Berlin, Germany

[b] Humboldt Universität zu Berlin, Germany

For linear DAEs, automatic differentiation (AD) provides very accurate approximations for all relevant derivatives required for the analysis and solution of initial value problems. By the presented projector-based analysis of the original equations and their derivatives it becomes possible to describe the different types of components involved in the DAE. With this decoupling, index determination, consistent initialization, the diagnosis of singular points and the numerical solution using the Taylor series method become possible for higher-index linear DAEs. For nonlinear DAEs, the consideration of linearized systems yields, in principle, analogous results that allow a better understanding of unstructured DAEs. However, in practice we have to deal with all difficulties related to highly nonlinear equations. We will present our algorithms implemented in Python using the AD-software Algopy. The obtained results and open questions will be discussed and illustrated with several examples.

On Linear Operator-differential-algebraic Equations with Delay

C. Zimmer

TU Berlin, Germany

Constrained linear partial differential equations (lin. PDAEs) have an important role in modeling practical systems such as the incompressible linearized Navier-Stokes equation. On the other hand, time-delays occur

naturally in closed-loop controlled dynamical systems, since measurements, signal transmissions, and calculations of the control require a certain time.
The combination of lin. PDAEs and time-delays leads to a new mathematical object, which in includes a various number of challenges. In this talk, we investigate this kind of object in the abstract setting of linear operator-differential-algebraic equations with delay. In particular we consider semi-explicit systems and show existence as well as regularity results.

Session CS07 – SDEs

Numerical integration of coupled stochastic oscillators driven by random forces

H.A. de la Cruz Cansino[a], *J.C. Jimenez*[b] *and J. Zubelli*[c]

[a] FGV-Fundação Getulio Vargas, Brazil

[b] ICIMAF

[c] IMPA

In this work we consider a class of stable integrators for the effective numerical discretization of coupled stochastic oscillators driven by external random forces. We study the performance of the proposed methods, including the reproduction of some dynamical properties of stochastic harmonic oscillators and paths of nonlinear oscillators in general. Computer experiments illustrate the theoretical findings and the advantages of the proposed integrators in comparison with other conventional ones

Mean-square stiffness analysis of stochastic differential equations

A. Thalhammer and E. Buckwar

Johannes Kepler University Linz, Austria

Whereas the concept of stiffness of deterministic problems is well-examined, the notion of stiffness for stochastic differential equations (SDEs) has not been treated in detail yet. A reliable characterisation of stiffness in the stochastic setting is of great importance in practice, particularly if we are dealing with problems where a necessary reduction of time step sizes for explicit methods leads to significantly higher computational cost.

In this talk, we provide an overview of existing approaches to characterise stiffness for deterministic and stochastic problems. Furthermore, we extend a recently developed concept of stiffness for deterministic differential equations to the stochastic setting and link the proposed notion of stiffness in the mean-square sense with results from the stability theory of linear stochastic differential equations. Using these results, we conclude the talk by presenting numerical experiments with linear systems of SDEs coming from spatial discretisation schemes for stochastic partial differential equations.

Finite Element Method for Semi-linear Elliptic Stochastic Partial Differential Equation Driven by Additive Colored Noise

Y. Cao[a], *J. Hong*[b] *and Z. Liu*[b]

[a] Auburn University, America

[b] Chinese Academy of Science, People's Republic of China

We study finite element method for a boundary value problem of elliptic semi-linear SPDE driven by an additive colored noise, including the white noise as a special case. We analyze the regularity of the truncated solution (obtained by truncating the noise), and then give the error estimate between the exact solution and the truncated solution. Approximating the truncated equation by finite element method, we derive the error estimate between the truncated solution and the numerical solution. The effect of the noise on the accuracy of the approximation is illustrated. Results of the numerical experiments are provided to examine our theoretical results.

Ergodicity for a full-discrete scheme of the damped stochastic nonlinear Schrodinger equation

C. Chen, J. Hong and X. Wang

Chinese Academy of Science, People's Republic of China

We propose a full-discrete scheme of an ergodic stochastic Schrodinger equation, and the ergodicity of this scheme is studied. Utilizing spectral method in spatial direction, we obtain a finite-dimensional SDE. We show that this spatial semi- discrete scheme possesses a unique invariant measure (spatial invariant measure) which is a proper approximation of the original invariant measure to a small error. Furthermore, applying backward Euler scheme in temporal direction, the full-discrete scheme is obtained. We show also the numerical ergodicity of this scheme and the error between this invariant measure and the spatial one is of order 1/2.

Session CS08 – Structure preserving methods I

Nonholonomic mechanics for perfect fluids

A. Natale and C.J. Cotter

Imperial College London, United Kingdom

Perfect fluid models, such as the incompressible Euler equations, possess a remarkable geometric structure which can be described using the classical Lagrangian and Hamiltonian formalism. This structure is responsible for the numerous properties of the solutions, including conservation of energy and circulation, which directly descend from the symmetries of the system. Although powerful numerical techniques have been derived to tackle this class of problems, two main difficulties arise when dealing with fluids. Firstly, the infinite-dimensional nature of the problem requires a truncation that would preserve its variational nature. Secondly, numerical integrators should be designed in the Eulerian setting in order to avoid complications related to moving or deforming meshes. Pavlov et al. addressed both issues by approximating the Lie algebra of divergence-free vector fields by its action on piecewise constant functions defined on a triangulation of the computational domain and imposing a nonoholonomic constraint to obtain a sparse matrix algorithm. In this talk, we build on their results to develop a high order finite element geometric formulation of perfect incompressible fluids. The main idea of the method is to reinterpret the spatial discretization of the velocity fields as a nonholonomic constraint, and to define an isomorphism with a suitable Lie algebra. We present some preliminary results obtained with this formulation and we set the scene for further developments of the algorithm.

Pavlov, D. and Mullen, P. and Tong, Y. and Kanso, E. and Marsden, J. E. and Desbrun, M. (2011) Structure-preserving discretization of incompressible fluids. Physica D, 240 (6). pp. 443-458. ISSN 0167-2789.

Variational Integrators for Nonvariational PDEs

M. Kraus and o. Maj

Max-Planck-Institut für Plasmaphysik, Germany

Variational integrators provide a systematic way to derive geometric numerical methods for Lagrangian dynamical systems, which preserve a discrete multisymplectic form as well as momenta associated to symmetries of the Lagrangian via Noether's theorem.

An inevitable prerequisite for the derivation of variational integrators is the existence of a variational formulation for the considered dynamical system. Even though this is the case for a large class of systems, there are many interesting examples which do not belong to this class, e.g., equations of advection-diffusion type like they are often found in fluid dynamics or plasma physics.

We propose the application of the variational integrator method to so called adjoint Lagrangians, which formally allow us to embed any dynamical system into a Lagrangian system by doubling the number of variables. Thereby we are able to derive variational integrators for arbitrary systems, extending the applicability of the method significantly. A discrete version of the Noether theorem for adjoint Lagrangians yields the discrete momenta preserved by the resulting numerical schemes.

The theory is applied to dynamical systems from fluid dynamics and plasma physics like the advection equation, the Vlasov-Poisson system and magnetohydrodynamics, including numerical examples.

Preservation of Physical Properties of Stochastic Maxwell Equations with Additive Noise via Stochastic Multi-symplectic Methods

C. Chen, J. Hong and L. Zhang

Chinese Academy of Science, People's Republic of China

Stochastic Maxwell equations with additive noise are a system of stochastic Hamiltonian partial differential equations intrinsically, possessing the stochastic multi-symplectic conservation law. It is shown that the averaged energy increases linearly with respect to the evolution of time and the flow of stochastic Maxwell equations with additive noise preserves the divergence in the sense of expectation. Moreover, we propose three novel stochastic multi-symplectic methods to discretize stochastic Maxwell equations in order to investigate the preservation of these properties numerically. We made theoretical discussions and comparisons on all of the three methods to observe that all of them preserve the corresponding discrete version of the averaged divergence. Meanwhile, we obtain the corresponding dissipative property of the discrete averaged energy satisfied by each method. Especially, the evolution rates of the averaged energies for all of the three methods are derived which are in accordance with the continuous case. Numerical experiments are performed to verify our theoretical results.

Fast and structure-preserving numerical methods for partial differential equations

D. Furihata

Osaka University, Japan

We have developed some predictor-corrector numerical schemes based on the discrete variational derivative method for partial differential equations, like the linear multistep methods.
Those predictors and correctors are structure-preserving, and we can expect that their combinations are faster in computations than the normal structure-preserving nonlinear schemes in general.
We can also use some simpler predictors that are not structure-preserving in this context; however, we should investigate their properties carefully from the point of view of the structure inheritance.
In this talk, we introduce the predictor-corrector structure-preserving methods in detail and show some properties of them with some numerical computation results.

Session CS09 – Structure preserving methods II

Geometric integration on Lie groups using the Cayley transformation

M. Wandelt and M. Günther

University of Wuppertal, Germany

In this talk, we focus on geometric numerical integration on a Lie group using the Cayley transformation. We investigate a coupled system of differential equations that occurs in Lattice Quantum Chromodynamics. In this subject, one aims at computing expectation values of some operators to simulate elementary particles. In doing so, the Hybrid Monte Carlo Method is used. Here, Hamiltonian equations of motion have to be solved using integration on Lie groups and its corresponding Lie algebras. Usually, this is done via the Leapfrog method based on the exponential function. We examine the feasibility of the Cayley transformation instead and show its advantages compared to the exponential map, both theoretically and numerically.

Locally exact modifications of numerical schemes

J.L. Cieśliński

University of Bialystok, Faculty of Physics, Poland

It is well known that linear ODEs with constant coefficients, including the classical harmonic oscillator, admit explicit exact discretizations. In some cases one may use this fact directly, constructing structure preserving numerical schemes. As an example we present two different discretizations of the Kepler problem preserving all trajectories and constants of motion. Another idea, much more general, concerns nonlinear systems of ODEs. We consider a family of numerical schemes (a modification of an existing numerical scheme) and demand that its linearization exactly discretizes the linearized nonlinear system. As a result we get new numerical scheme, known as a locally exact modification of the initial scheme, which is surprisingly accurate for oscillations in the neighbourhood (not so small in fact) of stable equilibria. We present applications of our approach to discrete gradient methods and, in particular, locally exact modifications of the Average Vector Field method.

1. J.L.Cieśliński: On the exact discretization of the classical harmonic oscillator equation, J. Differ. Equ. Appl. 17 (2011) 1673.

2. J.L.Cieśliński: Locally exact modifications of numerical schemes, Comput. Math. Appl. 65 (2013) 1920.

3. J.L.Cieśliński: improving the accuracy of the AVF method, J. Comput. Appl. Math. 259 (2014) 233.

Discontinuous Galerkin methods for Hamiltonian ODEs and PDEs

Y. Sun

LSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, People's Republic of China

In this talk, we present the discontinuous Galerkin methods for solving Hamiltonian ODEs and PDEs. The geometric structure of the resulting numerical discretizations has been investigated. By choosing the suitable numerical fluxes the symplectic and multi-symplectic methods can be constructed based on the Galerkin variational discretizations. We apply the derived numerical methods to the nonlinear Schrodinger equation. The numerical experiments show that the numerical results can verify the corresponding theoretical analysis.

Session CS10 – Structure preserving methods III

A Numerical Method for a Dispersion Managed NLS

M. Mikl and T. Jahnke

Karlsruhe Institute of Technology, Germany

Modelling a dispersion managed optical fiber cable leads to a nonlinear Schrödinger equation (NLS) where the linear part is multiplied by a rapidly changing piecewise constant coefficient function. The occurring rapid oscillations in the solution implicate a severe step-size restriction for traditional time-integrators. In this talk, we present and analyze a novel first order time-integrator which does not suffer from this restriction. For the construction of this method we introduce an adiabatic transformation of the highly oscillating problem. We show that the transformed problem possesses a non-oscillating limit system and hence is in this spirit numerically more accessible. Finally, we motivate some ideas for the construction of higher order time-integrators.

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

P. Krämer and K. Schratz

Karlsruhe Institute of Technology, Germany

Solving the Maxwell-Klein-Gordon (MKG) equation in the non-relativistic limit regime is numerically very delicate as the solution becomes highly oscillatory in time. In order to resolve the oscillations, standard integration schemes require severe time step restrictions.

The idea to overcome this numerical challenge lies in the asymptotic expansion of the solutions, which allows us to filter out the high frequencies explicitly (see [Faou&Schratz,2014] for the case of the Klein-Gordon equation).

More precisely, this ansatz allows us to break down the numerical task to solving a non-oscillatory Schrödinger-Poisson system (SP), which can be carried out very efficiently without any additional time step restriction for example by applying splitting methods (cf. [Lubich,2008]). This formally derived non-relativistic limit of the MKG equation has already been studied from an analytical point of view in [Masmoudi&Nakanishi,2003].

In my talk I want to present the ideas of the convergence proof for the MKG equation to the SP system and give some numerical results.

Efficient methods for explicit time-dependence in semi-classical Schrödinger equations

P. Bader[a], *A. Iserles*[b], *P. Singh*[b] *and K. Kropielnicka*[c]

[a] La Trobe University, Australia

[b] University of Cambridge, UK

[c] University of Gdansk, Poland

We introduce a Zassenhaus decomposition technique that is used to boost high precision splitting methods to higher order thereby generating a hybrid algorithm. Identifying the correct algebra leads to significant improvements over our previous work (Bader et al. FoCM 14, 689 (2014)) and we show how to generalize the method for explicitly time-dependent potentials. In the case of oscillatory potentials, Magnus methods are expected to be superior and we demonstrate that the Zassenhaus split is versatile enough to be applied in this setting.

Session CS11 – Structure preserving methods IV

An Analysis on Asymptotic Behavior of Dissipative Numerical Integrators with Adaptive Time-stepping

S. Sato[a], *T. Matsuo*[a], *H. Suzuki*[a] *and D. Furihata*[b]

[a] The University of Tokyo, Japan

[b] Osaka University, Japan

The asymptotic behavior of continuous dissipative systems and dissipative numerical integrators with fixed time-stepping can be fully investigated by Lyapunov-type theorem on continuous and discrete dynamical systems, respectively. However, once adaptive time-stepping is involved, such theories cease to work, and usually the dynamics should be investigated in a backward way, such as in terms of pullback attractors. In this paper, we present a different approach?we stick to a forward definition of limit sets, and show that still we can establish a Lyapunov-type theorem, which reveals the precise asymptotic behavior of adaptive time-stepping integrators in the presence of a discrete Lyapunov functional.

Structure-preserving method for a certain class of dissipative differential equations

T. Yaguchi

Kobe University, Japan

It is known that certain autonomous dissipative differential equations can be derived as the Euler-Lagrange equation of the weighted variational principle.

In this contribution, we show that an energy-dissipative scheme is obtained by applying the technique to derive energy-preserving schemes to this variational structure. Application to the damped oscillator system is shown as an example.

The energy behaviour is also investigated theoretically and numerically.

A case study of the use of discrete gradient methods in image processing

V. Grimm[a], *R. McLachlan*[b], *D. McLachlan*[c], *R. Quispel*[c] *and C. Schönlieb*[d]

[a] Karlsruhe Intitute of Technology (KIT), Germany

[b] Massey University, New Zealand

[c] La Trobe University, Australia

[d] University of Cambridge, United Kingdom

Gradient flows appear all over image processing. Often, they represent gradient descent equations for the minimization of an energy functional as, for example, the Perona-Malik energy functional or the energy functionals for total variation (TV) denoising and deblurring. The emphasis is on minimization, and therefore the dissipation of energy, along the solution of the gradient descent equation.
It is of utter importance that the numerical method applied to the gradient flow preserves the dissipation of the discretized energy. The often used explicit Euler method suffers a severe step-size restriction under this requirement. As an alternative, we will discuss discrete gradient methods that are well-known methods of Geometric Numerical Integration, which preserve the dissipation of gradient systems. Under mild restrictions on the step-size, we will show that any discrete gradient method converges to a minimizer (or a set of minimizers) for convex functionals.
We will further promote the use of discrete gradient methods in image processing by several numerical experiments with nonlinear total variation (TV) deblurring and denoising experiments.

Second Order Conformal Symplectic Integrators for Damped Hamiltonian Systems

A. Bhatt, D. Floyd and B.E. Moore

University of Central Florida, United States of America

We introduce conformal symplectic integrators based on the classical Störmer-Verlet and implicit midpoint methods for linearly damped Hamiltonian systems. We discuss necessary and sufficient conditions for second order accuracy. These methods satisfy conformal symplecticity and conformal angular momentum for N-body system with distance dependent pairwise potential. Analysis for linear equations gives explicit relationships between the damping parameter and the time step size to reveal when the methods are most advantageous; essentially, the damping rate of the numerical solution is exactly preserved under these conditions. We apply these methods to a number of ODEs and PDEs. Additional structure preservation properties of these methods are revealed for PDEs, conformal total linear momentum in one case and a conformal Casimir in another case. Comparison of these methods with RK method and non-standard finite difference method demonstrates the usefulness and strengths of the methods.

Session CS12 – Structure preserving methods V

The cohesiveness of G-symplectic methods

J. Butcher

University of Auckland, New Zealand

G-symplectic methods are multistage multivalue methods which satisfy a condition similar to that of symplectic Runge–Kutta methods. In spite of their multivalue nature, experimental evidence shows that they approximately conserve symplectic behaviour and the invariance of quadratic invariants. Using the concept of cohesiveness, an attempt will be made to explain why this excellent behaviour persists for millions of time steps. It is shown that the deviation from perfect cohesiveness grows slowly as steps of the method are carried out.

Volume Preservation by Runge-Kutta Methods

P. Bader[b], *D. McLaren*[b], *GRW Quispel*[b] *and M. Webb*[a]

[a] Cambridge, United Kingdom

[b] La Trobe University, Melbourne, Australia

It is a classical theorem of Liouville that Hamiltonian systems preserve volume in phase space. Any symplectic Runge-Kutta method will respect this property for such systems, but Iserles, Quispel and Tse showed that no B-Series method can be volume preserving for all volume preserving vector fields (BIT 47 (2007)351-378). In this talk we show that despite this result, symplectic Runge-Kutta methods can be volume preserving for a much larger class of vector fields than Hamiltonian systems, and time permitting, discuss how some Runge-Kutta methods can preserve a modified measure exactly.

Session CS13 – Software and Implementation

A parallel version of MATSLISE, a Matlab package for solving Sturm-Liouville and Schrodinger equations

M. Van Daele and B. Devooght

Ghent University, Belgium

Matslise (Ledoux & Van Daele, 2005) is a graphical Matlab software package for the interactive numerical study of Sturm-Liouville problems (SLPs), which can generally be written as

$$(p(x)\,y')' + q(x)\,y = E\,w(x)\,y\,, \tag{1}$$

with appropriate boundary conditions. The package allows the fast and accurate computation of the eigenvalues E and the visualization of the corresponding eigenfunctions y. It is built upon high-order piecewise constant perturbation methods, also called the CP methods. In 2014, a successor code Matslise 2.0 was released. This new version is developed to work for a broad class of singular problems. This is realized by including the recent extension (Ledoux & Van Daele, 2010) of the CP algorithm from problems in Liouville normal form to the general Sturm-Liouville form and by using specially adapted algorithms in a narrow interval around the singularity.
An important property of the CP-methods for regular problems is that, before the actual computation of the eigenvalues and corresponding eigenfunctions, a mesh can be constructed such that the requested eigenvalues E_k with $\leq k_{\min} \leq k \leq k_{\max}$ can be computed within a given tolerance.
Then starting with the computation of $E_{k_{\min}}$, the eigenvalues are computed sequentially using E_k as initial guess in the Newton-iteration for approximating E_{k+1}.
In this talk, we discuss an adaptation of the CP-algorithm such that the computation of the eigenvalues and eigenvectors can be done in parallel. Experiments were carried out on a HPC infrastructure and on multi-core processors.

[1] V. Ledoux and M. Van Daele. Matslise: a Matlab package for the numerical solution of Sturm-Liouville and Schrdinger equations. ACM. T. Math. Software 31, 612-619, 2005.

[2] V. Ledoux and M. Van Daele. Solving Sturm-Liouville problems by piecewise perturbation methods, revisited. Comp. Phys. Commun. 181, 1335-1345, 2010.

A computational B-series toolkit for the analysis of Runge–Kutta Methods

T.J.T. Norton

University of Bath, United Kingdom

Any study of a Runge–Kutta method usually involves working with B-series. Such a study might require the evaluation of many B-series compositions, inversions, and other algebraic operations, which, if performed by

hand, can be quite cumbersome. However, by considering an object–oriented representation for B-series, many of these operations can be automated and performed rapidly and reliably.
In this talk, we discuss the development of a MATLAB toolkit for assisting B-series analysis. In particular, we will look at an object representation for rooted trees and B-series, and the common operations that are performed on these objects. Applications to general linear methods will also be considered.

OVDBDF - A Software Package for the Numerical Integration of differential algebraic equations

D. Bankmann and A. Steinbrecher

TU Berlin, Germany

Differential algebraic equations (DAEs) arise in many applications as multi-body systems or networks (e.g. electrical circuits) when modeling their dynamical behavior and can be obtained in particular via automatic modeling.
We consider DAEs in the most general form

$$(1) F(t, x, x') = 0,$$

where t is the independent variable, x the state vector and x' its derivative and the partial derivative of F with respect to x' is possibly singular.
In this context the so-called hidden constraints of the system play an important role in terms of numerical robustness. These are constraints that are not explicitly given in the equations (1). Failing to provide these constraints explicitly might lead to numerical drifts. There exist various (numerical) techniques to determine these constraints, e.g. the procedure mentioned in [1] for quasi-linear DAEs.
Thus, we can additionally impose

$$(2) G(t, x) = 0,$$

where G contains all the explicit and hidden constraints of the original system F, without changing the solution set.
In this talk we will present the solver OVDBDF for the numerical integration of such an overdetermined system fulfilling (1) and (2) that is based on the DASSL code for square nonlinear DAEs using backward difference formulas (BDF). A similar approach has been taken by QUALIDAES for quasi-linear DAEs using Radau IIA methods.
Besides a sophisticated stepsize and order control a key point for the robust and efficient numerical integration in OVDBDF is the precise consideration of the hidden constraints (2).
[1] Steinbrecher,A. Analysis of Quasi-Linear Differential-Algebraic Equations. Institut für Mathematik, Technische Universität Berlin, Berlin, Germany, number 11-2006. 2006.

Aspects of high performance computing using modern C++

L. Einkemmer

University of Innsbruck, Austria

Interpreted programming languages, such as Python and Matlab, are convenient in the development stage of numerical software. However, their performance is often hard to predict and for most applications it is at least

an order of magnitude worse compared to compiled languages such as Fortran or C. Due to this fact almost all high performance codes are written in either Fortran or C/C++.
In this talk we will consider implementations based on modern C++ that using the Boost library and template techniques succeed in providing a convenient high-level approach to code development, while still maintaining excellent performance characteristics. We will illustrate this approach on two scientific codes.
First, a resistive magnetohydrodynamics solver is considered. In this case the focus is on abstracting the implementation of the specific numerical scheme as well as the equations of motion from the remainder of the implementation (which is, for example, responsible for the MPI communication and the handling of the boundary conditions).
As a second example, we consider a Vlasov solver using the recently introduced semi-Lagrangian discontinuous Galerkin method. In this case the focus is on developing a dimension independent code that scales well on distributed memory systems (scaling results for the VSC-2 will be presented).
For both examples we will discuss performance and parallelization (using MPI) in some detail.

Session CS14 – Numerical methods for PDEs I

Gluing of Numerical Continuation and a Multiple Solution Method

C. Kuehn

Vienna University of Technology, Austria

In this talk, I shall outline a study of several elliptic PDEs (Lane-Emden-Fowler, Lane-Emden-Fowler with microscopic force, Caginalp) via the numerical continuation software pde2path. The main idea is to employ a gluing approach to determine a set of starting solutions for the continuation by exploiting the variational structures of the PDEs. In particular, the initialization problem of numerical continuation for PDEs is solved via a minimax algorithm to find multiple unstable solutions. Furthermore, for the Caginalp system, we illustrate the efficient gluing link of pde2path to the underlying mesh generation and the FEM MatLab pdetoolbox. Several interesting bifurcation diagrams and directly applicable conclusions about the three elliptic PDEs are obtained, in particular with respect to symmetry-breaking. The work is based upon the paper: "Efficient Gluing of Numerical Continuation and a Multiple Solution Method for Elliptic PDEs", C. Kuehn, arXiv:1406.6900

The effect of a sparse grad-div stabilization on control of stationary Navier-Stokes equations

A. Çibik

Gazi University, Turkey

This study presents a new divergence penalization stabilization for the optimal control of steady-state Navier Stokes equations. The effect of proposed stabilization is analyzed in terms of stability and velocity a priori error. The main difference of this method and usual grad-div stabilization arise in numerical computations. Since the proposed method produces block upper triangular matrices, it has an advantage in terms of implementation over usual grad-div stabilization, which produces fully coupled block matrices. The stability and convergence results are given for both state and adjoint state variables after stating the optimality conditions by using Lagrange approach. Numerical experiment, exposes the effectiveness of the method.

Session CS15 – Numerical methods for PDEs II

A multi-time-step coupling method for parabolic problems

M. Benes

Czech Technical University in Prague, Czech Republic

Evolution of time dependent physical quantities such as current, heat etc., in composite materials are modelled by initial boundary value problems for parabolic PDEs. These physical quantities follow different evolution patterns in different parts of the computational domain depending on the material properties, size of constituent material subdomains, coupling scheme, etc. Therefore, the stability and accuracy requirements of a numerical integration scheme may necessitate domain dependent time discretization. Parabolic problems are usually solved by discretizing spatially using finite elements and then integrating over time using discrete solvers. We propose an asynchronous multi-domain time integration scheme for parabolic problems. For efficient parallel computing of large problems, we present the dual decomposition method with local Lagrange multipliers to ensure the continuity of the primary unknowns at the interface between subdomains. The proposed method enables us to use domain dependent Rothe method on different parts of a computational domain and thus provide an efficient and robust approach to solving large scale problems.

A family of three-stage third order AMF-W-methods for the time integration of advection diffusion reaction PDEs

S. Gonzalez-Pinto[a], *D. Hernandez-Abreu*[a], *S. Perez-Rodriguez*[a] *and R. Weiner*[b]

[a] University of La Laguna, Spain

[b] Martin-Luther University, Halle-Wittenberg, Germany

A few three-stage W-methods for the time integration of semi-discretized advection diffusion reaction Partial Differential Equations (PDEs) are provided. In particular, two three-parametric families of W-methods of order three are obtained under a realistic assumption regarding the commutator of the exact Jacobian and the approximation of the Jacobian which defines the corresponding W-method. Specific methods are selected by minimizing error coefficients, enlarging stability regions or increasing monotonicity factors, and embedded methods of order two for an adaptive time integration are derived by further assuming first order approximations to the Jacobian. The relevance of the newly proposed methods in connection with the Approximate Matrix Factorization technique is discussed and numerical illustration on practical PDE problems revealing that the new methods are good competitors over existing integrators in the literature is provided.

A-Stable Higher Order Numerical Methods to Solve Partial Differrential Equations by Taylor Series

H. Hirayama

Kanagawa Institute of Technology, Japan

The arithmetic operations and functions of Taylor series can be defined by C++ language and Fortran. Using this, the solution of an ordinary differential equation can be expanded in Taylor series. The solution can be expanded up to arbitrary order,so the calculation formula of arbitrary order can be used instead of Runge-Kutta formula.Taylor series can be used for the evaluations of the errors and the optimal step size within given error allowance easily. In addition, we can transform Taylor series into Pade series, which give arbitrary order, high precision and A-stable formula for solving ordinary differential equation numerically.
The partial differential equations can be converted into the simultaneous ordinary differential equations by differentiating spatially. This ordinary differential equation can be easily solved by the Taylor series methods. The high precision and stable calculation can be done when we use this methods.

Padé Time Stepping Method of Rational Form for Solving PDEs

S. Algarni

King Fahd University of Petroleum & Minerals, Saudi Arabia

The purpose of this study is to investigate selected numerical methods that demonstrate good performance in solving PDEs. We adapt alternative method that involve rational polynomials. Padé time stepping (PTS) method, which is highly stable for the purposes of the present application and is associated with lower computational costs, is applied. Furthermore, PTS is modified for our study which focused on diffusion equations. Due to the rationality form of PTS, some numerical error occurs and then some a kind of control is imposed. Finally, numerical runs are conducted to obtain the optimal local error control threshold.

Session CS16 – Numerical methods for PDEs III

Discontinuous finite volume element discretization for coupled flow-transport problems arising in models of sedimentation

R. Bürger[a], *S. Kumar*[b] *and R. Ruiz-Baier*[c]

[a] Universidad de Concepción, Chile

[b] Indian Institute of Space Science and Technology, Thiruvananthapuram, India

[c] Université de Lausanne, Switzerland

The purpose of this study is to investigate selected numerical methods that demonstrate good performance in solving PDEs. We adapt alternative method that involve rational polynomials. Padé time stepping (PTS) method, which is highly stable for the purposes of the present application and is associated with lower computational costs, is applied. Furthermore, PTS is modified for our study which focused on diffusion equations. Due to the rationality form of PTS, some numerical error occurs and then some a kind of control is imposed. Finally, numerical runs are conducted to obtain the optimal local error control threshold.

On error estimates for some numerical methods with discrete TBC for the time-dependent Schrödinger equation

A. Zlotnik

Higher School of Economics, Russian Federation

We first deal with an initial-boundary value problem for the generalized time-dependent Schrödinger equation with variable coefficients in an unbounded multi-dimensional parallelepiped. To solve it, the Crank-Nicolson in time and the polylinear finite element in space method with the discrete transparent boundary conditions (TBC) is considered. We present its stability properties and derive error estimates $O(\tau^2 + h^2)$ uniform in time and in L^2 norm and mesh H^1 norm in space (a superconvergence result) under the Sobolev-type assumptions on the initial function.
We also derive error estimates for: (1) the Crank-Nicolson-any order FEM and the Numerov-Crank-Nicolson method for the 1D Cauchy problem on the whole axis; (2) the Numerov-Crank-Nicolson-Strang higher order splitting scheme for the problem in an unbounded strip.
The error estimates contain no the mesh steps in negative powers like for all other approximate TBCs.
The theoretical results are accompanied by computational ones on solving some 1D and 2D quantum mechanics problems.
1. A. Zlotnik. Error estimates of the Crank-Nicolson-polylinear FEM with the discrete TBC for the generalized Schrödinger equation in an unbounded parallelepiped, Finite Difference Methods: Theory and Appl. Proceedings of FDM-6. I. Dimov, I. Farago and L. Vulkov, eds. Lect. Notes Comput. Sci. Berlin, Springer, 2015, accepted.
2. A. Zlotnik, The Numerov-Crank-Nicolson scheme on a non-uniform mesh for the time-dependent Schrödinger equation on the half-axis, Kinetic and Related Models, 2015, accepted.

3. A. Zlotnik, A. Romanova. On a Numerov-Crank-Nicolson-Strang scheme with discrete transparent boundary conditions for the Schrödinger equation on a semi-infinite strip// Appl.Numer. Math. 2015. Vol. 93. P. 279-294.

Numerical solution of time-dependent Maxwell's equations for modeling light scattering in human eye's structures

A. Araújo, S. Barbeiro and M. Khaksar

CMUC, Department of Mathematics, University of Coimbra, Portugal

In this work we discuss the numerical discretization of the time-dependent Maxwell?s equations using a leap-frog type discontinuous Galerkin method. We focus on deriving stability and convergent estimates of fully discrete schemes. We consider anisotropic permittivity tensors, which arise naturally in our application of interest. An important aspect in computational electromagnetic problems is the implementation of the boundary conditions. We present some numerical examples to illustrate the theoretical results and also in the context of modeling scattered electromagnetic wave?s propagation through human eye?s structures. Finally, we also briefly discuss the multi-scale nature of the problem. In a small scale, we use Maxwell?s equations to compute parameters that could be used as inputs to larger scale simulations namely using Monte Carlo methods.

Session CS17 – Krylov subspace methods and exponential integrators

A convergence analysis for the shift-and-invert Krylov subspace method

T. Göckler and V. Grimm

Karlsruhe Institute of Technology (KIT), Germany

Time integration methods for stiff systems of ordinary differential equations often involve the action of a matrix function on a vector. The occuring matrices typically arise from a spatial discretization of a partial differential equation and have a huge field-of-values lying somewhere in the left complex half-plane. Refining the discretization, the norm of the matrix becomes very large. Therefore, the efficient and reliable approximation of a matrix function times a vector with a convergence rate independent of the norm of the matrix is a current topic of interest and research.
Recent advances have shown that rational Krylov subspace methods have a great advantage over standard Krylov subspace methods in this case. We therefore approximate the product of a matrix function and a vector in the shift-and-invert Krylov subspace which is spanned by the vector and the inverse of the matrix shifted by some value greater than zero.
By transforming the left complex half-plane to the unit disk, we obtain convergence results that depend on the smoothness of a transformed function on the boundary of this disk. In particular, we establish sublinear error bounds for the matrix phi-functions being of central importance in exponential integrators. A remarkable aspect of our analysis is the independence of the error from the norm of the considered discretization matrix.
Moreover, we discuss suitable choices for the shift in the rational Krylov subspace and illustrate our results by several numerical experiments.

Computing the action of the matrix exponential

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

[a] University of Innsbruck, Austria

[b] University of Verona, Italy

The Leja method is a well established scheme for computing the action of the matrix exponential. Due to a new backward error analysis the implementation of the method is further developed allowing for a more efficient method. From a scalar computation in high precision we predict the necessary number of scaling steps based only on a rough estimate of the field of values or norm of the matrix and the desired backward error.
We illustrate the developments in the implementation motivated by numerical experiments, where we give a special focus to the necessary matrix-vector products needed for the computation of the matrix exponential, for various classes of matrices. We can show that for a wide class of matrices the Leja method saves matrix-vector products in comparison to methods known from the literature. The numerical experiments include spatial discretization of time dependent partial differential equations and various prototypical test cases.

Exponential integrators for solving parabolic PDEs using Krylov subspaces

A. Schädle and G. Jansing

Heinrich-Heine-Universität, Germany

When discretizing parabolic boundary value problems using finite elements in space one obtains a system of the form $M\dot{u} = Au + g$, with a mass matrix M, a stiffness-matrix A, and an inhomogeneity g. Using exponential integrators to solve these systems numerically, we may use Krylov subspaces for computing the action of the matrix exponential or ϕ functions. There one typically has to solve m linear systems with M when building the M orthogonal m dimensional Krylov space $\mathcal{K}_m(M^{-1}A, b)$. Combining numerical inverse Laplace transform based on quadrature along a hyperbola in the complex plane with Krylov subspaces we are able to avoid the m linear system solves with the matrix M at the cost of forming a few, say L, Krylov subspaces $\mathcal{K}_m(\lambda M - A, b)$ with a complex parameter λ in the resolvent set of the stencil (M, A). It is known that the error arising from the numerical inverse Laplace transform decays exponentially in L. The solution of linear systems with M on the other hand can become expensive on unstructured, anisotropic grids and for finite elements using high degree polynomial basis functions. In this case the new method could be advantageous, as illustrated in the numerical experiments.

Numerical solution of the wave equation with acoustic boundary conditions

D. Hipp and M. Hochbruck

KIT - Karlsruhe Institute of Technology, Germany

In this talk we consider the wave equation with dynamic boundary conditions. In contrast to standard boundary conditions of Dirichlet, Neumann or Robin type, dynamic boundary conditions do not neglect the momentum on the boundary. A typical example are acoustic boundary conditions. Although the problem is well understood analytically, to the best of our knowledge, its numerical solution has not been studied so far.
First we illustrate the wave propagation for different dynamic and standard boundary conditions and review some known well-posedness results.
In the second part we derive, analyze and discuss a full discretization of the wave equation with acoustic boundary conditions on a two-dimensional domain. We use linear finite elements on the bulk of the domain and on its surface, respectively, for the spatial discretization. In order to prove its stability and convergence it is essential to study the energy exchange between the bulk and the boundary in detail.
The space discretization leads to a linear homogeneous system of ordinary differential equations whose solution is given by the matrix exponential operator. We discuss different options for the approximation of this exponential operator, namely Krylov subspace methods and rational approximations.
Finally, we illustrate our theoretical results by numerical examples.

Session CS18 – Uncertainty quantification and inverse problems

Efficient and structure-preserving numerical scheme applied to a continuous-time particle filter for a stochastic neural mass model

H. Hinterleitner, M. Ableidinger and E. Buckwar

Johannes Kepler University Linz, Austria

Neural mass models provide a useful framework for modelling mesoscopic neural dynamics and in this talk we consider the Jansen and Rit Neural Mass Model (JR-NMM). This system of ODEs has been introduced as a model in the context of electroencephalography (EEG) rhythms and evoked potentials and has been used for several applications, e.g. for detecting epileptic diseases. We propose a stochastic version of the JR-NMM which arises by incorporating random input and has the structure of a nonlinear stochastic oscillator. We simulate the stochastic JR-NMM by an efficient numerical scheme based on a splitting approach which preserves the qualitative behaviour of the solution. The final goal is to use the stochastic JR-NMM as the underlying model in a nonlinear filtering framework. We take advantage of our efficient numerical method in order to solve the inverse problem by a continuous-time particle filter.

Two-dimensional spheroid-particle model for the retrieval of the microphysical aerosol parameters via regularized inversion of lidar data

S. Samaras

University of Potsdam, Germany

A deeper understanding of the climate processes requires the investigation of the spatial and temporal variability of the microphysical properties of aerosol particles. Commonly used parameters such as the aerosol size distribution, the surface-area/volume concentration, the complex refractive index, and the single scattering albedo provide multilateral knowledge on aerosol type, growth, and shape, and Earth s radiation balance. Raman-elastic multi-wavelength lidar data have been widely used to measure the aerosol optical properties and to retrieve the size distribution through the inversion of the Mie forward model. While this model offers a reasonable treatment for spherically approximated particles, e.g. biomass burning aerosols, it no longer provides a viable description for the non-spherical case, since particle shape is known to have substantial effects for the scattering in side- and backward direction. In this work, we consider a spheroid-particle description generalizing to a two-dimensional size distribution which depends additionally on particle aspect ratio. T-matrix method is a technique for calculating the scattering and extinction cross sections for arbitrarily shaped particles, introduces a much higher level of computational complexity, which in turn makes real-time retrievals unviable. We circumvent this defect using precalculated look-up tables and a newly-developed alpha version of a retrieval software. We show that a retrieval with synthetic data is possible using the improved model along with regularization to account for the inherent instability of the inversion procedure. The general trend of the initial size distributions is captured in

our numerical experiments and the reconstruction quality depends on the data error level. Finally, our approach is applied to a real-life measurement case giving further insight for future improvements.

Regularizing a Volterra Integral Equation of the First Kind

S. Subbey

Institute of Marine Research, Norway

We consider the inverse problem of solving for the function u, when

$$\int_0^x K(x,t)u(t)\,dt = g(x),\ 0 \le x \le T. \tag{2}$$

Here, the kernel K and the function u are assumed to be exact, but the right hand side g represents observations and T is a fixed number. Equation (2) is a Volterra integral equation of the first kind. We deal with the particular case where g represents a sparse set of measurements at the points $\{x_1, \ldots, x_N\}$ of a fixed grid. The grid-points $x_1 < \ldots < x_N$ are assumed to be known exactly and the measured values g_i are approximations of the functional values $g(x_i)$. Then Eq. (2) may be replaced by

$$\int_0^{x_i} K(x_i,t)u(t)\,dt = g_i,\ i = 1, \ldots, N. \tag{3}$$

This problem occurs in porous media physics, and deriving u involves the unstable process of inverting a linear smoothing operator. The operator for this particular problem has no bounded inverse.
We show that a regularized solution of the inverse problem is obtained by constraining the solution space to monotone and convex functions. These constraints, which satisfy certain physical constraints, may be expressed in the form of linear inequalities. We then arrive at a solution which approximates the measured values as closely as possible, where the deviation is defined by a suitable norm. We present numerical experiments which compare different discretization schemes, and results for real experimental data.
Sam Subbey[1,2] and Sven-Åke Gustafson[3]
1. Inst. of Mar. Res., PB-1870, N-5817 Bergen, Norway
2. Institute of Informatics, University of Bergen, Postboks 7800, N-5020, Norway
3. Stavanger University, Dept. of Math. and Nat. Sciences, N-4036 Stavanger, Norway

Parametric uncertainty and global sensitivity analysis in a model of the carotid bifurcation: Identification and ranking of most sensitive model parameters

R. Gul and S. Bernhard

Freie Universität Berlin, Germany

In computational cardiovascular models, parameters are one of major source of uncertainty, which make the models unreliable and less predictive. In order to achieve predictive models that allow the investigation of the cardiovascular diseases, sensitivity analysis (SA) can be used to quantify and reduce the uncertainty in outputs

(pressure and flow) caused by input (electrical and structural) model parameters. In the current study, three variance based global sensitivity analysis (GSA) methods; Sobol, FAST and a sparse grid stochastic collocation technique based on the Smolyak algorithm, were applied on a lumped parameter model of carotid bifurcation. Sensitivity analysis was carried out to identify and rank most sensitive parameters as well as to fix less sensitive parameters at their nominal values (factor fixing). In this context, network location and temporal dependent sensitivities were also discussed to identify optimal measurement locations in carotid bifurcation and optimal temporal regions for each parameter in the pressure and flow waves respectively. Results show that, for both pressure and flow, flow resistance (R), diameter (d) and length of the vessel (l) are sensitive within right common carotid (RCC), right internal carotid (RIC) and right external carotid (REC) arteries, while compliance of the vessels (C) and blood inertia (L) are sensitive only at RCC. Moreover, Young?s modulus (E) and wall thickness (h) exhibit less sensitivities on pressure and flow at all locations of carotid bifurcation. Results of network location and temporal variabilities revealed, that most of sensitivity was found in common time regions i.e. early systole, peak systole and end systole.

Session CS19 – Monte Carlo methods

Martingale-based variance reduction in estimates of rare event statistics

H.C. Lie

Freie Universität Berlin, Germany

Rare events play an important role in the stochastic multiscale models of complex systems such as molecules. This has motivated the development of Monte Carlo algorithms for efficiently simulating rare events, and estimating rare event statistics. A natural requirement of such algorithms is that they feature variance reduction, in order to produce reliable estimates. We consider an algorithm, proposed by Hartmann and Schuette [J. Stat. Mech. Theor. Exp. pp. P11004 (2012)] that computes rare event statistics by solving a stochastic optimal control problem. Our aim is to show, using stochastic analysis and a simple example, how one may achieve both variance reduction in the Monte Carlo estimates and stability of the algorithm, by using a martingale-based control variate that derives from Girsanov's theorem.

Adaptivity and Guaranteed Error Control for Multi-Level Monte Carlo Methods

J. Neumann

Weierstrass Institute for Applied Analysis and Stochastics, Germany

Multi-level Monte Carlo methods have recently proven to help reduce the high computational cost of sampling based methods. So far, mainly uniform mesh sequences have been considered. This talk aims to provide insights in the combination of these techniques with adaptive finite element methods to perform adaptive mesh refinement of the mesh hierarchy used in the multi-level Monte Carlo simulation. Furthermore, error bounds for quantities of interest are derived for the stochastic setting where the stochastic error is controlled such that the determined bounds are guaranteed in probability. Numerical experiments examine the performance of the adaptive method for a posteriori error control and mesh refinement in Monte Carlo and multi-level Monte Carlo methods with respect to localised goals and reduction of the computational costs.

Adaptive importance sampling via minimization of estimators of cross-entropy, mean square, and inefficiency constant

T. Badowski

Free University of Berlin, Germany

Inefficiency constant, equal to product of variance of an estimator and its mean computation cost, can be used for quantifying the inefficiency of using unbiased estimators in Monte Carlo (MC) procedures. In case when mean computation cost is the same for different estimators, comparing their inefficiency constants reduces to comparing their variances or equivalently mean squares. We investigate adaptive methods for obtaining parameters of importance sampling (IS) distributions via minimization of well-known estimators of cross-entropy and mean square (of the IS estimator), as well as of new estimators of mean square and inefficiency constant. The received IS parameters can be used in separate IS MC procedures to estimate the quantity of interest. We develop single- and multi-stage minimization methods of such estimators for the families of IS distributions received from exponential change of measure and discrete Girsanov transformation up to a stopping time. We prove convergence and asymptotic properties of minimization results in our methods, in the proofs for the multi-stage methods utilising a novel uniform strong law of large numbers. We show that if the zero-variance IS parameter exists, then, under appropriate assumptions, minimization results of the new estimators converge to such parameter at a faster rate than such results of the well-known estimators, and a positive definite asymptotic covariance matrix of minimization results of the cross-entropy estimator is four times such matrix for the well-known mean square estimator. We introduce criteria for comparing asymptotic efficiency of stochastic optimization methods, applicable to methods minimizing estimators of functions considered in this work. In our numerical experiments for computing expectations of functionals of Euler scheme, minimization of the new estimators led to the lowest inefficiency constants and variances, followed by the well-known mean square estimator, and the cross-entropy one.

Global sensitivity analysis for random linear dynamical systems

Q. Liu and R. Pulch

University of Greifswald, Germany

We consider linear dynamical systems consisting of ordinary differential equations or differential algebraic equations. The input-output behaviour is specified by a transfer function in the frequency domain. In many applications the dynamical systems include a large number of physical parameters, which may exhibit uncertainties. For an uncertainty quantification, the parameters are replaced by random variables. Our aim is to quantify the sensitivity of the output with respect to a high-dimensional set of random parameters. Thus we examine the random-dependent transfer function. In particular, Sobol's total sensitivity coefficients are considered. We compare different numerical methods for this sensitivity analysis. On the one hand, quasi Monte-Carlo methods yield approximations of the sensitivity coefficients directly. On the other hand, Stroud cubature formulas can be applied in the computation of the expansions of the polynomial chaos, which allow for obtaining the sensitivities afterwards. We present numerical simulations of linear dynamical systems and compare the efficiency of different methods.

Session CS20 – Applications I

Direct simulation of interaction of water droplets and ice particles

M. Baumgartner and P. Spichtinger

Institute of Atmospheric Physics, Johannes Gutenberg University Mainz, Germany

We consider the growth or evaporation of cloud particles due to the diffusion of water vapor in a mixed-phase cloud, i.e. a cloud containing liquid water droplets and ice particles. This combination of cloud particles is of interest because it occurs frequently in the atmosphere. Since the water droplets and the ice particles have different saturation vapor pressures there are situations where the ice particles can grow while the droplets evaporate. The last process is called "Wegener-Bergeron-Findeisen process" and is important in the formation of precipitation. We solve the governing diffusion equation on a domain containing some cloud particles by a finite element method. Since the particles are small, we encounter a multiscale problem via the geometry of the domain. To avoid an expensive adaptation of the mesh to the small particles, we employ the extended finite element method and enrich the finite element ansatz-space. With a penalty method, we enforce the correct values of the solution at the cloud particles.

Non Fickian diffusion in porous media: second order approximations for the velocity and concentration

S. Barbeiro, S. Bardeji and J.A. Ferreira

CMUC, University of Coimbra, Portugal

Diffusion processes in porous media have traditionally been described using the classical parabolic advection-diffusion equation. However in different scenarios, significant discrepancies between experimental results and numerical simulations have been reported in the literature. To avoid such limitation, integro-differential equations have been proposed to replace the diffusion equation.

In this work we consider a system of quasilinear equations: an elliptic equation for the pressure and an integro-differential equation for the concentration defined in a two-dimensional spatial domain. We propose a numerical method based on a piecewise linear finite element method with convenient quadrature rules. We prove that the numerical pressure and concentration are second order convergent with respect to the spatial discretization, in the discrete H^1 and L^2 norms. For the time integration we use a first order implicit-explicit method.

Delay Differential Equations in Biosciences: Parameter estimation, sensitivity analysis and optimal control

F.A. Rihan

United Arab Emirates University, United Arab Emirates

In this contribution, we show the consistency of delay differential equations with biological systems with memory, in which we present a class of mathematical models with time-lags in immunology, physiology, epidemiology and cell growth. We also incorporate optimal control parameters into a delay model to describe the interactions of the tumour cells and immune response cells with external therapy. Sensitivity
analysis is an important tool for understanding a particular model, which is considered as an issue of stability with respect to structural perturbations in the model. We introduce a variational method to evaluate sensitivity of the state variables to small perturbations in the initial conditions and parameters appear in the model. The presented numerical simulations show the consistency of delay differential equations with biological systems with memory. The displayed results may bridge the gap between the mathematics research and its applications in biology and medicine.

A homotopy perturbation method for fractional-order convection-diffusion-reaction boundary-value problems

I. Ates

Utrecht University, The Netherlands

In this presentation, we describe the application of the homotopy perturbation method (HPM) to two-point boundary-value problems with fractional-order derivatives of Caputo-type. We illustrate the spectral convergence of HPM for convection-diffusion-reaction models and that it can be easily generated to different types of fractional differential equations. Numerical experiments are shown to demonstrate the effectiveness of HPM. The method is used to solve the linear and nonlinear fractional differential equations for which it is hard to find an analytical solution.

Session CS21 – Applications II

Nonlinear Modulation of Surface SH Waves in a Two Layered Hyperelastic Half Space

H.I. Var[a], E. Deliktas[b] and M. Teymur[b]

[a] Marmara University Turkey

[b] Istanbul Technical University Turkey

In this work the propagation of nonlinear surface shear horizontal (SH) waves in an hyperelastic half space coated with two different layers of uniform thickness is examined. The constituent materials are assumed to be homogeneous, isotropic, incompressible and having different mechanical properties. In the analysis it is assumed that between the linear shear velocities of the top layer, c_1, the bottom layer, c_2, and the half space, c_3, the inequality $c_1 < c_2 < c_3$ is valid. For the existence of SH waves, the phase velocity c of the wave must satisfy either the condition $c_1 < c_2 \leq c < c_3$ or the one $c_1 < c \leq c_2 < c_3$. In this study, the problem is examined under these two conditions. By employing the method of multiple scales, a nonlinear Schrödinger equation is derived for the nonlinear self modulation of the surface SH waves. It is observed that the existence of the envelope solitary waves depends on the nonlinear material parameters of the two layered half space as well as the thickness ratio of the layers. It is remarked that for short waves the nonlinear properties of the top layer dominates the modulation. On the other hand for long waves, nonlinear properties of the half space effects the nonlinear modulation most.

A numerical study of the small dispersion limit of the long wave-short wave interaction equations

E. Kesici, G. Topkarci and G. Muslu

Istanbul Technical University, Turkey

In this talk, we consider the long wave-short wave interaction equations with a small parameter ($0 < \epsilon << 1$)

$$
\begin{aligned}
i\epsilon\phi_t^\epsilon + \alpha\epsilon^2\phi_{xx}^\epsilon &= \beta u^\epsilon \phi^\epsilon \\
i\epsilon\psi_t^\epsilon + \alpha\epsilon^2\psi_{xx}^\epsilon &= \beta u^\epsilon \psi^\epsilon \\
u_t^\epsilon &= \mp\beta(|\phi^\epsilon|^2 + |\psi^\epsilon|^2)_x
\end{aligned}
$$

where the real-valued function $u^\epsilon(x,t)$ characterizes the long longitudinal wave and the complex-valued functions $\phi^\epsilon(x,t)$, $\psi^\epsilon(x,t)$ are the slowly varying envelopes of the short transverse waves [1].
The independent variables x and t denote spatial coordinate and time, respectively, and the parameters α and β are real constants. We study numerically the behavior of solutions to the long wave-short wave interaction equations in the limit $\epsilon \to 0^+$. For this aim, we present a finite difference method and Fourier spectral method. The conservation properties of numerical schemes are also discussed.
References

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A bilateral coupling approach to model the crosstalk phenomenon in electro-magnetic systems

H. Niroomand Rad and A. Steinbrecher

TU Berlin, Germany

Electro-magnetic systems consist of several electrical circuits, where each contained bunches of electrical elements such as capacitors, resistors and inductors. In such systems, the phenomenon of inducing electro-magnetic disturbances within electrical elements in addition to their influences in the entire electro-magnetic system is called crosstalk where it may cause the system to work improperly. Therefore, to avoid the system to malfunction, modeling, simulation and control of this phenomenon in the area of circuit simulation is of fundamental importance.
This talk is devoted only to modelling of the crosstalk phenomenon with respect to numerical issues. Our approach is focused on coupling of two equations, namely circuit equations and Maxwell equations, where to fully model the phenomenon, we propose bilateral coupling between them. That is, considering each set as an input-output system of equations, bilateral coupling allows the output of each system to be connected to the input of the other system. In this talk, we first present the set of Maxwell equations with suitable boundary conditions for every electrical element in which the disturbances are induced. Then, we introduce circuit equations considered for the electrical elements producing the electro-magnetic disturbances. In addition, we investigate the coupling and re-coupling relations in an operator based form and present them explicitly for the particular case of isotropic material.

Analytical solution of population balance equation involving aggregation and breakage in terms of modified approximation

Z. Pınar[a], *A. Dutta*[b] *and T. Özişç*[c]

[a] University of Namık Kemal, Turkey

[b] IKU Leuven, Belgium

[c] Ege University, Turkey

This study presents an effective analytical simulation to solve Population Balance Equation (PBE) involving particulate aggregation and breakage by making use of the appropriate solution(s) of associated complementary equation via Fibonacci&Lucas approximation (FLA). Travelling wave solutions of the complementary equation of a nonlinear PBE with appropriately chosen parameters is taken to be analogous to the description of the dynamic behavior of the particulate processes. For an initial proof-of-concept, a general case when the number of particles varies with respect to time is chosen. Three cases i.e. balanced aggregation and breakage and when either aggregation or breakage can dominate are selected and solved for their corresponding analytical solution. The results are then compared with the available analytical solution, based on Laplace transform obtained from standard literature and AEM which is proposed by Pinar et al. [20, 21, 27, 28]. In this study, it is shown that the solution approach proposed via Fibonacci&Lucas approximation is flexible and thereby more efficient than the analytical approach used in the literature.

Session CS22 – Applications III

A numerical approach to study the Kramers equation for finite geometries

A. Araújo[a], *A.K. Das*[b] *and E. Sousa*[a]

[a] CMUC, Department of Mathematics, University of Coimbra, Portugal

[b] Department of Physics, Dalhousie University, Halifax, Nova Scotia, Canada

The Kramers equation for the phase-space function, which models the dynamics of an underdamped Brownian particle, is the subject of our study. Numerical solutions of this equation for natural boundaries (unconfined geometries) have been well reported in the literature. But not much has been done on the Kramers equation for finite (confining) geometries which require a set of additional constraints imposed on the phase-space function at physical boundaries.

In this talk we present numerical solutions for the Kramers equation with a variety of potential fields – namely constant, linear, harmonic and periodic – in the presence of fully absorbing and fully reflecting boundary conditions. The choice of the numerical method and its implementation take into consideration the type of boundary conditions, in order to avoid the use of ghost points or artificial conditions. We study and assess the conditions under which the numerical method converges. Various aspects of the solutions for the phase-space function are presented and discussed in detail.

A boundary-value method for the space-fractional heat equation

P.A. Zegeling

Utrecht University, The Netherlands

Many different numerical approaches are available for approximating the space-fractional heat equation, usually yielding systems with (half-) full matrices. An alternative is to use a doubling-splitting approach to the operators, resulting in a banded-matrix structure. Analysis of the spectrum of the system reveals that a special treatment of the time-integration is needed to avoid numerical instabilities. Numerical experiments will illustrate the effectiveness of boundary-value methods, using the midpoint method extended with an implicit Euler final condition, to resolve this problem.

Theoretical results on the stability of the linear barycentric rational quadrature methods

S.A. Hosseini[a] *and A. Abdi*[b]

[a] Golestan University, Islamic Republic of Iran

[b] University of Tabriz, Islamic Republic of Iran

The stability analysis of the composite barycentric rational quadrature method (CBRQM) for the second kind Volterra integral equations introduced by Berrut et al., through application to the standard and the convolution test equations, will be surveyed. In each case, some theoretical results are achieved by providing corresponding recurrence relation and stability matrix.
Verification of these theoretical results is obtained by some numerical experiments. Numerical results confirm the analytic ones that the method is stable when the maximum value of absolute eigenvalues of the stability matrices is less than or equal to one.

Long-time behavior of Volterra integral equations on time scales and stability of numerical methods

E. Messina[a] *and A. Vecchio*[b]

[a] University of Napoli "Federico II", Italy

[b] C.N.R. National Research Council of Italy

Recently, there has been a growing interest in Volterra integral equations on time scales as they represent a powerful instrument for the mathematical representation of memory dependent phenomena in population dynamic, economy, etc. Here, we consider Volterra integral equations on time scales and present our study about the long-time behavior of their solutions. This study contains and extends some results of the classical stability theory for discrete and continuous Volterra equations and provides a potential tool for the stability analysis of numerical methods.

Session CS23 – Molecular dynamics and particle methods

A Fast Mollified Impulse Method for Flexible Water Simulations

L. Fath

Karlsruhe Institute of Technology, Germany

Atomistic simulations of ice friction with low shear speed require expensive computations. The highly oscillatory motion of bonds and angles in the water molecules restricts the (outer) step size of standard integrators to the femtosecond range. Unfortunately, physical processes such as friction, premelting and heat transport happen at a much slower scale in the nano- or microseconds or even slower.

Therefore we are interested in efficient multi-scale methods resolving the fastest (computationally cheap) dynamics but enabeling longer time steps on the expensive long-range forces.

The mollified impulse method avoids resonances in the integrator by filtering or mollifying only the slowest forces. Similar to the projected impulse method we developed a mollifier which resets the water molecules to their equilibrium positions. The new mollifier uses an idea based on corotation. It is cheap and very easy to implement in parallel but successfully avoids resonances at longer time steps. With this mollifier a step size at least twice as large compared to the standard impulse method can be used for ice friction simulations without sacrificing stability.

Canonical Symplectic Particle-in-Cell method for the Vlasov-Maxwell system

R. Zhang[a,c], *H. Qin*[a,b], *J. Liu*[a,c], *J. Xiao*[a,c], *Y. He* [a,c] *and Y. Wang*[a,c]

[a] University of Science and Technology of China, China

[b] Plasma Physics Laboratory, Princeton University, Princeton, USA

[c] Key Laboratory of Geospace Environment, CAS, China

Particle-in-Cell (PIC) simulation is the most important numerical tool in plasma physics and accelerator physics. However, its long term accuracy has not been established. To overcome this difficulty, we developed a canonical symplectic PIC method for the Vlasov-Maxwell system by discretizing the Marsden-Weinstein bracket. A fast local algorithm to solve the symplectic implicit time advance is discovered without root researching or global matrix inversion, enabling applications of the proposed method to plasma simulations with a large number, e.g., 109, of degrees of freedom.

Symmetric volume-preserving algorithms for charged particle dynamics

Y. He[a], *Y. Sun*[b], *J. Jiu*[a] *and H. Qin*[c]

[a] University of Science and Technology of China, People's Republic of China

[b] LSEC, Chinese Academy of Sciences, People's Republic of China

[c] Princeton University, Princeton,USA

The talk reports our recent development of the splitting technique for the charged particle motion under the Lorentz force. The source-free nature of the Lorentz vector field has been investigated. Based on the volume-preserving property of the dynamics, a class of numerical methods for advancing the charged particles in a general electromagnetic field has been constructed by splitting the classical evolution operator. This new class of numerical methods can conserve the reversibility of the system and the invariant volume form in phase space, and globally bound the numerical errors of energy, momentum, and some adiabatic invariants up to the order of the method over a very long simulation time. These derived numerical methods can be computed explicitly, and thus are effective for the long-term simulation of the multi-scale dynamics of plasmas.

Markov Chain Approximations of Controlled Diffusions

R. Banisch

Freie Universität Berlin, Germany

We study optimal control problems that arise if a particle performing overdamped Langevin Dynamics in an Energy landscape is subjected to an external force which can be adjusted by a controller. The task of the controller is to minimize a certain objective function. We focus on linear quadratic (LQ) control problems and show that they are dual to sampling problems which appear e.g. in Molecular Dynamics. A numerical method to approximately solve LQ control problems is derived. The method uses a logarithmic transformation together with a Galerkin projection onto a suitable space of basis functions. The result is a discretization of the entire control problem that replaces the continuous dynamics by a discrete Markov jump process, and preserves the most important structural properties. If the dynamics is metastable, then we propose to utilize the metastable structure by choosing a committor basis, guided by MSM theory. We derive error bounds for this choice which complement standard error bounds from the theory of finite elements. The method is flexible and can also incorporate other choices, e.g. piecewise polynomial or radial basis functions.

Session CS24 – Time-stepping methods

Functional Continuous Runge-Kutta Methods for Second Order Equations

A.S. Eremin

Saint-Petersburg State University, Russian Federation

This talk deals with numerical methods for retarded functional differential equations (RFDEs) of the second order in which the right-hand side is independent of the delayed function derivative.
Second order differential equations generally can be rewritten as a first order system and are solved with standard Runge-Kutta methods. However, in case of ordinary differential equations, if the right-hand side does not depend on the first derivative, much more efficient methods named after E. Nyström can be constructed.
Special explicit methods of Runge-Kutta type for solving RFDEs were first developed in the 1970's by Tavernini, who constructed several methods up to order four. But it is only in recent years that these methods have been expanded to a general class of methods called "Functional Continuous Runge-Kutta methods" for RFDEs. Functional Continuous Runge-Kutta methods (FCRKs) are reviewed in Acta Numerica 2009, where order conditions and examples of methods are presented.
The methods analogous to Runge-Kutta-Nyström methods can be developed for the RFDE problems with the right-hand side independent of the function derivative. They have the same order of convergence with less stages than the FCRKs for the corresponding first order equations, and are thus more efficient. However, the class of problems to which they are applicable is very limited.
Often second order RFDEs arise with a right-hand side which depends on the solution derivative at the current time, and on the solution but not its derivative at delayed times. Functional Continuous Runge-Kutta-Nyström methods are not applicable to such problems.
In the current work the construction of FCRKs for the second order equations without right-hand side dependency on the delayed solution derivative is discussed. It is shown that for the same convergence order (discrete and/or uniform) methods can be constructed with fewer stages than FCRKs for the corresponding first order equations. Order conditions and example methods are presented. Test problems are solved, demonstrating the declared convergence order of the new methods.

Effective order Runge-Kutta methods with free output

H. Podhaisky[a] *and J. Butcher*[b]

[a] Martin Luther University Halle-Wittenberg, Germany

[b] The University of Auckland, New Zealand

The concept of effective order was introduced in 1969. It makes it possible to reduce the number of order conditions for explicit Runge-Kutta methods considerably; for example, for $p = 5$, from 17 to 10. In particular, it is possible to construct methods of effective order five with only five stages. It might be asked why efficient

codes based on these methods are not available and widely used. One possible reason is that a finishing method, with additional cost, is needed whenever an output of the solution needs to be computed.
In this talk we will show that it is possible to construct methods for which essentially free output is available at the end of any step. This is achieved by re-using the stage values of the main method to provide an in-built finishing method. The main tool for this investigation is the composition of B-series.

Stability analysis of a type of explicit Runge-kutta methods for stochastic delay differential equations

T. Mitsui

Nagoya University, Japan

As relatively little is known about Runge-Kutta type method applied to stochastic delay differential system, we present an explicit Runge-Kutta Maruyama method for solving them. The mean-square stability properties of the numerical solutions generated by the Runge-Kutta method are investigated, and a sufficient condition for stability is obtained and applied to the stabilized explicit Runge-Kutta methods. Their stability is based on the boundedness of the shifted Chebyshev polynomials. Numerical experiments demonstrate effectiveness of the theoretical results.