SciCADE 2019

International Conference on Scientific Computation and Differential Equations

Innsbruck, July 22nd - 26th, 2019

Book of Abstracts

350
universität innsbruck
Wir bauen Brücken. Seit 1669

Monday

8:00am	**Registration** SoWi building							
8:45am	**Welcome Opening** Alexander Ostermann							
9:00am	**Plenary P1 - Hinke M. Osinga** The art of computing global manifolds							
10:00am	**Coffee Break**							
10:30am	**MS 07: Part 1** Geometry and structure preservation in numerical differential equations	**MS 03: Part 1** Asymptotic preserving schemes for kinetic problems	**MS 14: Part 1** Numerical methods for rare events and applications	**MS 22: Part 1** Optimal control problems with ODEs and DAEs	**MS 27: Part 1** Stability issues for stochastic, implicit-explicit, and parallel initial value problem solvers	**MS 28: Part 1** Selected topics in computation and dynamics: machine learning and multiscale methods	**CS 09** Schrödinger equations	**CS 10** Dynamical systems
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	SR 17
12:30pm	**Lunch**							
2:00pm	**MS 07: Part 2** Geometry and structure preservation in numerical differential equations	**MS 03: Part 2** Asymptotic preserving schemes for kinetic problems	**MS 14: Part 2** Numerical methods for rare events and applications	**MS 22: Part 2** Optimal control problems with ODEs and DAEs	**MS 27: Part 2** Stability issues for stochastic, implicit-explicit, and parallel initial value problem solvers	**MS 28: Part 2** Selected topics in computation and dynamics: machine learning and multiscale methods	**CS 02** Plasma physics	**CS 07** Time integration
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4:30pm	**Plenary P2** Germund Dahlquist Prize							
5:30pm	**Welcome Drink**							
6:00pm	**Guided Tour**							

Tuesday

9:00am	**Plenary P3 - Alison Marsden** Computational methods for blood flow simulation and personalized medicine in cardiovascular disease								
10:00am	**Coffee Break**								
10:30am	**MS 04: Part 1** Computational methods for quantum dynamic problems	**MS 06: Part 1** Wave problems	**MS 02: Part 1** Energy stable methods for gradient flows and applications	**MS 08: Part 1** Discrete integrable systems and numerical methods	**MS 12: Part 1** Numerical methods for plasma physics	**MS 39: Part 1** Recent developments in multirate and related numerical methods for multiscale problems	**MS 26: Part 1** Numerical approximation of stochastic systems	**CS 11** Boundaries and boundary layers	**CS 15** Partial differential equations
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 2	SR 3	SR 16	SR 17
12:30pm	**Lunch**								
2:00pm	**MS 04: Part 2** Computational methods for quantum dynamic problems	**MS 06: Part 2** Wave problems	**MS 02: Part 2** Energy stable methods for gradient flows and applications	**MS 08: Part 2** Discrete integrable systems and numerical methods	**MS 12: Part 2** Numerical methods for plasma physics	**MS 39: Part 2** Recent developments in multirate and related numerical methods for multiscale problems	**MS 26: Part 2** Numerical approximation of stochastic systems	**CS 08** Exponential integrators	**CS 13** Runge-Kutta methods
room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 2	SR 3	SR 16	SR 17
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4:30pm	**Plenary P4** New Talent Award								
5:45pm	**Special Session** **John C. Butcher** 45 years of B-series **Gerhard Wanner** How numerical analysis emerged in Innsbruck								
6:45pm	**Poster Session and Wine Reception**								

Wednesday

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room	HS 1	HS 2	HS 3	UR 1	UR 3		SR 16	SR 17
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4:30pm	**Plenary P7 - Katharina Schratz** Nonlinear Fourier integrators for dispersive equations							

Friday

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room	HS 1	HS 2	HS 3	UR 1	UR 3	SR 3	SR 16	SR 17
12:40pm	**Butcher Prize**							
12:45pm	**Plenary P9 - Jonathan Mattingly** Long time accuracy of some MCMC and Bayesian sampling schemes							
1:45pm	**Closing**							

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Discrete integrable systems and numerical methods

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Plenary Talks

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The art of computing global manifolds

Monday 04:30pm - 05:30pm
P2: Dahlquist Prize

Tuesday 09:00am - 10:00am
P3: Alison Marsden
Computational methods for blood flow simulation and personalized medicine in cardiovascular disease

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Wednesday 09:00am - 10:00am
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Thursday 09:00am - 10:00am
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Recent advance on numerical methods for oscillatory dispersive PDEs

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P8: Ernst Hairer
Numerics of charged particle dynamics in a magnetic field

Friday 12:45pm - 01:45pm
P9: Jonathan Mattingly
Long time accuracy of some MCMC and Bayesian sampling schemes

Room: Aula

Monday 09:00am - 10:00am

The art of computing global manifolds

Hinke M Osinga

University of Auckland, New Zealand

Global manifolds are the backbone of a dynamical system and key to the characterisation of its behaviour. They arise in the classical sense of invariant manifolds associated with saddle-type equilibria or periodic orbits and, more recently, in the form of finite-time invariant manifolds in system that evolve on multiple time scales. Dynamical systems theory relies heavily on the knowledge of such manifolds, because of the geometric insight that they can offer into how observed behaviour arises. In applications, global manifolds need to be computed and visualised so that quantitative information about the overall system dynamics can be obtained. This requires accurate numerical methods and a precise understanding of how the computations depend on various model parameters. The computation of global manifolds is a serious challenge, but an effort that pays off. This talk will focus on two case studies that represent the most recent developments in this area.

Room: Aula | Tuesday 09:00am - 10:00am

Computational methods for blood flow simulation and personalized medicine in cardiovascular disease

Alison Marsden

Stanford University, United States of America

Cardiovascular disease is the leading cause of death worldwide, with nearly 1 in 4 deaths caused by heart disease alone. In children, congenital heart disease affects 1 in 100 infants, and is the leading cause of infant mortality in the US. Patient-specific modeling based on medical image data increasingly enables personalized medicine and individualized treatment planning in cardiovascular disease patients, providing key links between the mechanical environment and subsequent disease progression. We will discuss recent methodological advances in cardiovascular simulations, including (1) optimization algorithms enabling customized treatments for individual patients, (2) uncertainty quantification tools to compute confidence in simulation predictions, and (3) novel methods for fluid structure interaction with incompressible tissues and wall mechanobiology. Clinical application of these methods will be demonstrated in two applications: 1) coronary bypass graft surgery and the biomechanics of vein graft failure, and 2) prediction of disease progression in pediatric patients with pulmonary hypertension. We will provide an overview of our open source SimVascular project, which makes our tools available to the scientific community (www.simvascular.org). Finally, we will provide an outlook on recent successes and challenges of translating modeling tools to the clinic.

Room: Aula

Wednesday 09:00am - 10:00am

Multiscale modelling of particles in membranes

Carsten Gräser

Freie Universität Berlin, Germany

Due to their rich structure the mathematical modelling of cell membranes is a challenging task. Even the restriction to very few aspects leads to coupled multiscale problems. We discuss the mathematical modelling of membranes with embedded membrane-shaping particles by hybrid approaches. The resulting models combine continuum membrane descriptions with discrete particle descriptions. While hybrid membrane-particle models are well-established in physics, the mathematical and numerical analysis of such models is still in its infancy. The talk will give an overview of recent results on modelling, analysis, and numerical treatment of coupled membrane-particle systems and on current work combining such models with concepts from statistical mechanics and molecular dynamics.

Room: Aula

Thursday 09:00am - 10:00am

Recent advance on numerical methods for oscillatory dispersive PDEs

Yongyong Cai

Beijing Computational Science Research Center, China, People's Republic of

Highly oscillatory dispersive PDEs, such as Klein-Gordon equation in the non-relativistic limit, Dirac equation in the non-relativistic limit, Schrodinger equation in the semi-classical limit, arise from many different areas, e.g. computational chemistry, plasma physics, quantum mechanics. These oscillatory PDEs usually exhibit solutions with high frequency waves in time and/or in space, and are generally computational expensive. In this talk, we report some recent advances on the numerical methods and analysis for some typical highly oscillatory dispersive PDEs.

Room: Aula | Thursday 04:30pm - 05:30pm

Nonlinear Fourier integrators for dispersive equations

Katharina Schratz

Karlsruhe, Germany

A large toolbox of numerical schemes for nonlinear dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever *non-smooth* phenomena enter the scene since the underlying PDEs have very complicated solutions exhibiting high oscillations and loss of regularity. This leads to huge errors, massive computational costs and ultimately provokes the failure of classical schemes. Nevertheless, *non-smooth phenomena* play a fundamental role in modern physical modeling (e.g., blow-up phenomena, turbulences, high frequencies, low dispersion limits, etc.) which makes it an essential task to develop suitable numerical schemes.
In this talk I present a new class of Fourier integrators for the nonlinear Schrödinger and Korteweg–de Vries equation at low-regularity. The key idea in the construction of the new schemes is to tackle and hardwire the underlying structure of resonances into the numerical discretization. This new approach offers strong geometric structure at low regularity and high oscillations – linking the finite dimensional discretization to powerful existence

Room: Aula

Friday 09:00am - 10:00am

Numerics of charged particle dynamics in a magnetic field

Ernst Hairer

Université de Genève, Switzerland

Combining the Lorentz force equations with Newton's law gives a second order differential equation in space for the motion of a charged particle in a magnetic field. The most natural and widely used numerical discretization is the Boris algorithm, which is explicit, symmetric, volumen-.preserving, and of order 2.
In a first part we discuss geometric properties (long-time behaviour, and in particular near energy conservation) of the Boris algorithm. This is achieved by applying standard backward error analysis. Near energy conservation can be obtained also in situations, where the method is not symplectic.
In a second part we consider the motion of a charged particle in a strong magnetic field. Backward error analysis can no longer be applied, and the accuracy (order 2) breaks down. To improve accuracy we modify the Boris algorithm in the spirit of exponential integrators. Special attention is paid to the approximation of the gyrocenter (guiding center). Theoretical estimates are obtained with the help of the modulated Fourier expansion of the exact and numerical solutions.
This talk is based on joint work with Christian Lubich.
Related publications (2017 - 2019) can be downloaded from http://www.unige.ch/ hairer/preprints.html

Room: Aula

Friday 12:45pm - 01:45pm

Long time accuracy of some MCMC and Bayesian sampling schemes

Jonathan Mattingly

Duke University, United States of America

I will give an overview of a number of methods used to control longtime averages in various computational algorithms. I will give a high level overview which tries to draw together some common themes as well as highlight the central difficulties. I will compliment this by some specific examples from Bayesian sampling where approximations are made to improve computational efficiencies and Markov Chain Monte Carlo where some standard mathematical assumptions are violated by systems of physical interest. If time permits, I will talk about some recent work around sampling in political applications.

Special Session

Room: Aula

Tuesday 05:45pm - 06:15pm
John Charles Butcher
45 years of B-series

Tuesday 06:15pm - 06:45pm
Gerhard Wanner
How numerical analysis emerged in Innsbruck

Room: Aula

Tuesday 05:45pm - 06:15pm

45 years of B-series

John Charles Butcher

University of Auckland, New Zealand

In the paper [Hairer, E. and Wanner, G. *Computing* **13** (1974), 1–15], the term “B-series" was introduced. Although the motivation was the analysis of numerical methods for differential equations, the Hopf algebra on which B-series are based, now has wide-ranging applications to various fields, including geometry, quantum field theory and stochastic processes.
In this 45 year anniversary, some of the combinatoric and algebraic structures, on which B-series are built, will be reviewed; together with an introduction to some of the applications to the analysis of numerical methods.

Room: Aula

Tuesday 06:15pm - 06:45pm

How numerical analysis emerged in Innsbruck

Gerhard Wanner

Geneva, Switzerland

Some twelve years ago, a professor of the University of Graz (the second largest university city in Austria after Vienna) asked me: "Mr. Wanner, you are from Innsbruck, right? How is it possible — Innsbruck is sooo small — how is it possible that such an important, widely visible, school of numerical analysis emerged there?" This talk tries to explain, how this was possible.

Invited Mini-Symposia

MS 01: Part 1
Multiscale methods and analysis for oscillatory PDEs

Room: HS 1

Thursday 10:30am - 11:00am
Philippe Chartier
Uniformly accurate methods for highly-oscillatory problems

Thursday 11:00am - 11:30am
Mohammed Lemou
Highly-oscillatory evolution equations with time-varying vanishing frequency: asymptotics and numerics.

Thursday 11:30am - 12:00pm
Christof Sparber
On the classical limit of a time-dependent self-consistent field system: Analysis and computation

Thursday 12:00pm - 12:30pm
Peter Alexander Markowich
Continuum Modeling of Transportation Networks with Differential Equations

Room: HS 1 | Thursday 10:30am - 11:00am

Uniformly accurate methods for highly-oscillatory problems

Philippe Chartier[1], **Mohammed Lemou**[1], **Florian Méhats**[1] **and Gilles Vilmart**[2]

[1] *Univ Rennes, INRIA-IRMAR, France*
[2] *University of Geneva, Switzerland*

We introduce a new methodology to design uniformly accurate methods for oscillatory evolution equations. The targeted models are envisaged in a wide spectrum of regimes, from non-stiff to highly-oscillatory. Thanks to an averaging transformation, the stiffness of the problem is softened, allowing for standard schemes to retain their usual orders of convergence. Overall, high-order numerical approximations are obtained with errors and at a cost independent of the regime.

Room: HS 1 Thursday 11:00am - 11:30am

Highly-oscillatory evolution equations with time-varying vanishing frequency: asymptotics and numerics.

Philippe Chartier[2,3], Mohammed Lemou[1,2,3], Florian Méhats[2,3] and Gilles Vilmart[4]

[1] *CNRS, France*
[2] *University of Rennes 1, France*
[3] *INRIA, France*
[4] *University of Geneva*

In asymptotic analysis and numerical approximation of highly-oscillatory evolution problems, it is commonly supposed that the oscillation frequency is either constant or, at least, bounded from below by a strictly positive constant uniformly in time. Allowing for the possibility that the frequency actually depends on time and vanishes at some instants introduces additional difficulties from both the asymptotic analysis and numerical simulation points of view. I will present a first step towards the resolution of these difficulties. In particular, we show that it is still possible in this situation to infer the asymptotic behavior of the solution at the price of more intricate computations and we derive a second order uniformly accurate numerical method.

Room: HS 1

Thursday 11:30am - 12:00pm

On the classical limit of a time-dependent self-consistent field system: Analysis and computation

Christof Sparber

University of Illinois at Chicago, United States of America

We consider a coupled system of Schrödinger equations, arising via the so-called time-dependent self-consistent field method. Using Wigner transformation techniques, we study the corresponding classical limit which results in a mixed quantum-classical model, closely connected to the well-known Ehrenfest system in molecular dynamics. In the second part of the talk, we present a time-splitting method for the coupled Schrödinger-Liouville system obtained above. We prove that our splitting scheme is stable, uniformly with respect to the semiclassical parameter, and, moreover, that it preserves a discrete semiclassical limit. Thus one can accurately compute physical observables using time-steps independent of the small semiclassical parameter.

Room: HS 1 | Thursday 12:00pm - 12:30pm

Continuum Modeling of Transportation Networks with Differential Equations

Peter Alexander Markowich

KAUST, Saudi Arabia

We present an ab-initio approach to the modeling of (biological) transportation networks, which leads to a highly complex nonlinear PDE system featuring (fractal-type) structures, locally large variations of solutions and moving ‚free boundaries‘ and thin transition layers. The system has applications in many different areas of biology (leaf venation, neural networks, blood flow. . . ..) and exploits the well known biological principle that transportation drives network growth.

MS 01: Part 2
Multiscale methods and analysis for oscillatory PDEs

Room: HS 1

Thursday 02:00pm - 02:30pm
Weizhu Bao
Multiscale methods and analysis for the Dirac equation in the nonrelativistic limit regime

Thursday 02:30pm - 03:00pm
Jia Yin
A fourth-order compact time-splitting Fourier pseudospectral method for the Dirac equation

Thursday 03:00pm - 03:30pm
Xiaofei Zhao
Uniformly accurate Particle-In-Cell methods for Vlasov equation with non-homogeneous strong magnetic field

Thursday 03:30pm - 04:00pm
Caroline Lasser
Non-adiabatic wave packet propagation with Gaussian beams

Room: HS 1 | Thursday 02:00pm - 02:30pm

Multiscale methods and analysis for the Dirac equation in the nonrelativistic limit regime

Weizhu Bao

National University of Singapore, Singapore

In this talk, I will review our recent works on numerical methods and analysis for solving the Dirac 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 and indefinite, 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 the time splitting Fourier pseudospectral (TSFP) method 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 Dirac equation. Rigorous error estimates show that the EWI spectral method has much better temporal resolution than the FDTD methods for the Dirac equation in the nonrelativistic limit regime. Based on a multiscale expansion of the solution, we present a multiscale time integrator Fourier pseudospectral (MTI-FP) method for the Dirac equation and establish its error bound which uniformly accurate in term of the small dimensionless parameter. Numerical results demonstrate that our error estimates are sharp and optimal. Finally, these methods and results are then extended to the nonlinear Dirac equation in the nonrelativistic limit regime.This is a joint work with Yongyong Cai, Xiaowei Jia, Qinglin Tang and Jia Yin.

Room: HS 1 | Thursday 02:30pm - 03:00pm

A fourth-order compact time-splitting Fourier pseudospectral method for the Dirac equation

Weizhu Bao and Jia Yin

National University of Singapore, Singapore

We propose a new fourth-order compact time-splitting (S_{4c}) Fourier pseudospectral method for the Dirac equation by splitting the Dirac equation into two parts together with using the double commutator between them to integrate the Dirac equation at each time interval. The method is explicit, fourth-order in time and spectral order in space. It is unconditional stable and conserves the total probability in the discretized level. It is called a compact time-splitting method since, at each time step, the number of sub-steps in S_{4c} is much less than those of the standard fourth-order splitting method and the fourth-order partitioned Runge-Kutta splitting method. Another advantage of S_{4c} is that it avoids to use negative time steps in integrating sub-problems at each time interval. Comparison between S_{4c} and many other existing time-splitting methods for the Dirac equation are carried out in terms of accuracy and efficiency as well as long time behavior. Numerical results demonstrate the advantage in terms of efficiency and accuracy of the proposed S_{4c}. Finally we report the spatial/temporal resolutions of S_{4c} for the Dirac equation in different parameter regimes including the nonrelativistic limit regime, the semiclassical limit regime, and the simultaneously nonrelativisic and massless limit regime.

Room: HS 1 | Thursday 03:00pm - 03:30pm

Uniformly accurate Particle-In-Cell methods for Vlasov equation with non-homogeneous strong magnetic field

Xiaofei Zhao

Wuhan University, China

I will present our recent work on 2D/3D Vlasov equation with non-homogeneous strong magnetic field. The problem has highly oscillatory characteristics with solution dependent frequency. In 2D case, benefited from a confinement property, we derived a suitable formulation of the characteristics and then proposed a two-scale integrator under the Particle-In-Cell discrestization. The proposed method has uniform accuracy in terms of the magnetic field and preserves the confinement in the discrete level. In 3D, we apply the Rodrigues' rotation formula. Uniformly accurate methods are obtained in either the linear case or the nonlinear case but with magnetic field of fixed intensity.

Room: HS 1 | Thursday 03:30pm - 04:00pm

Non-adiabatic wave packet propagation with Gaussian beams

Caroline Lasser

Technische Universität München, Germany

Highly oscillatory time-dependent Schrödinger-type equations appear prominently in solid-state physics and quantum molecular dynamics. Often their dynamics come by an additional scale due to non-adiabatic transitions. We present a new unified approach for constructing effective transition operators and analyse them in the framework of Gaussian beam propagation. Our results are joint work with Clotilde Fermanian-Kammerer and Didier Robert.

MS 02: Part 1
Energy stable methods for gradient flows and applications

Room: HS 3

Tuesday 10:30am - 11:00am
Zhen Zhang
A Multiple SAV approach to the energy stable scheme of the moving contact line problem

Tuesday 11:00am - 11:30am
Guanghui Hu
A structure preserving numerical scheme for time-dependent Kohn-Sham equation.

Tuesday 11:30am - 12:00pm
Haijun Yu
Efficient Energy Stable Schemes for Time-Fractional Phase-Field Systems

Tuesday 12:00pm - 12:30pm
Buyang Li
Energy-decaying extrapolated RK-SAV methods for the Allen-Cahn and Cahn-Hilliard equations

Room: HS 3

Tuesday 10:30am - 11:00am

A Multiple SAV approach to the energy stable scheme of the moving contact line problem

Zhen Zhang and Fengdai Kang

Southern University of Science and Technology, China, People's Republic of

We explore the numerical approximation for a phase-field model to the moving contact line (MCL) problem, governed by the Cahn-Hilliard equation with a dynamic moving contact line boundary condition. Based on the framework of the recently developed scalar Auxiliary Variable(SAV) approach, we introduce multiple scalar auxiliary variables (MSAVs) approach to deal with both the bulk and boundary energy. It enjoys the advantages of second order, unconditional energy stable numerical scheme, and only requires computing a linear, decoupled system with constant coefficients at each time step. Numerical experiments are presented to verrify the effectiveness and efficiency of the proposed schemes for mobility number in different scales.

Room: HS 3 | Tuesday 11:00am - 11:30am

A structure preserving numerical scheme for time-dependent Kohn-Sham equation.

Guanghui Hu

University of Macau, Macau S.A.R. (China)

In this talk, the background of time-dependent density functional theory is briefly reviewed first. Then several geometric structures preserved by the equation are introduced. It is important that these structures are preserved by the numerical schemes as well. Hence we introduce a fully discretised numerical scheme based on the implicit middle point rule as well as the h-adaptive finite element method. The scheme is shown to preserve the properties well, and we also develop an algebraic multigrid method to accelerate the simulations. Numerical experiments show the effectiveness of the proposed method.

Room: HS 3

Tuesday 11:30am - 12:00pm

Efficient Energy Stable Schemes for Time-Fractional Phase-Field Systems

Haijun Yu

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

For the time-fractional phase field models, the corresponding energy dissipation law has not been settled on both the continuous level and the discrete level. In this work, we shall address this open issue. More precisely, we prove that the time-fractional phase field models indeed admit an energy dissipation law of an integral type. In the discrete level, we propose a class of finite difference schemes that can inherit the theoretical energy stability. Our discussion covers the time-fractional gradient systems including the time-fractional Allen-Cahn equation, the time-fractional Cahn-Hilliard equation and the time-fractional molecular beam epitaxy models. Moreover, a numerical study of the coarsening rate of random initial states depending on the fractional parameter α reveals that there are several coarsening stages for both time-fractional Cahn-Hilliard equation and time- fractional molecular beam epitaxy model, while there exists a $-\alpha/3$ power law coarsening stage.
This talk is based on joint works with: Tao Tang (SUSTC) and Tao Zhou (AMSS).

Room: HS 3 | Tuesday 12:00pm - 12:30pm

Energy-decaying extrapolated RK-SAV methods for the Allen-Cahn and Cahn-Hilliard equations

Georgios Akrivis, Buyang Li and Dongfang Li

Hong Kong Polytechnic University, Hong Kong S.A.R. (China)

We construct and analyze a class of extrapolated and linearized Runge-Kutta (RK) methods, which can be of arbitrarily high order, for the time discretization of the Allen-Cahn and Cahn-Hilliard phase field equations, based on the scalar auxiliary variable (SAV) formulation. We prove that the proposed q-stage RK-SAV methods have qth-order convergence in time and satisfy a discrete version of the energy decay property. Numerical examples are provided to illustrate the discrete energy decay property and accuracy of the proposed methods.

MS 02: Part 2
Energy stable methods for gradient flows and applications

Room: HS 3

Tuesday 02:00pm - 02:30pm
Jiang Yang
Framework of monotone schemes for the Allen-Cahn equations preserving the maximum principle

Tuesday 02:30pm - 03:00pm
Hui Zhang
Linear, decoupled and unconditionally energy stable schemes for the binary fluid-surfactant model

Tuesday 03:00pm - 03:30pm
Jie Shen
Structure preserving schemes for complex nonlinear systems

Tuesday 03:30pm - 04:00pm
Zhi Zhou
Time-Fractional Allen-Cahn Equations: Analysis and Numerical Methods

Room: HS 3 | Tuesday 02:00pm - 02:30pm

Framework of monotone schemes for the Allen-Cahn equations preserving the maximum principle

Tao Tang and Jiang Yang

Southern University of Science and Technology, China, People's Republic of

It is well known that maximum principle is one intrinsic property of the Allen–Cahn equation. Various numerical schemes have been developed to preserve the maximum principle. The underlying challenges not only comes from the stiffness of Laplace operator but also comes from the strong nonlinear term. Hence, the construction of such numerical schemes and corresponding numerical analysis can be very tricky for some situations. In this work, we establish a framework of monotone schemes for the Allen-Cahn equations, in which only several concise and reasonable conditions are assumed. These conditions can guarantee both the unique solvability and the maximum principle. We apply this framework to well-studied numerical schemes in several literatures. It is found that the framework regain the exactly same results for the existing numerical schemes.

Room: HS 3 | Tuesday 02:30pm - 03:00pm

Linear, decoupled and unconditionally energy stable schemes for the binary fluid-surfactant model

Hui Zhang

Beijing Normal University, China, People's Republic of

Here, we develop a first and a second order time stepping schemes for a binary fluid-surfactant phase field model by using the scalar auxiliary variable approach. The free energy contains a double-well potential, a nonlinear coupling entropy and a Flory-Huggins potential. The resulting coupled system consists of a Cahn-Hilliard type equation and a Wasserstein type equation which leads to a degenerate problem. By introducing only one scalar auxiliary variable, the system is transformed into an equivalent form so that the nonlinear terms are treated semi-explicitly. Both the schemes are linear and decoupled, thus they can be solved efficiently. We further prove that these semidiscretized schemes in time are unconditionally energy stable. Some numerical experments are performed to validate the accuracy and energy stability of the proposed schemes.

Room: HS 3

Tuesday 03:00pm - 03:30pm

Structure preserving schemes for complex nonlinear systems

Jie Shen[1,2]

[1]*Purdue University, United States of America*
[2]*Xiamen University, China*

Many complex nonlinear systems have intrinsic structures such as energy dissipation or conservation, and/or positivity/maximum principle preserving. It is desirable, sometimes necessary, to preserve these structures in a numerical scheme.
I will first present a new approach to deal with nonlinear terms in a large class of gradient flows and Hamiltonian systems. The approach is not restricted to specific forms of the nonlinear part of the free energy or Hamiltonian. It leads to linear and unconditionally energy stable schemes which only require solving decoupled linear equations with constant coefficients. Hence, these schemes are extremely efficient and very accurate when combined with higher-order BDF schemes. However, this approach, in general, will not preserve positivity or maximum principle. I will then present a strategy to construct efficient energy stable and positivity preserving schemes for certain nonlinear evolution systems, such as the Poisson-Nernst-Planck (PNP) equation and Keller-Segel equation, whose solutions remain to be positive.

Room: HS 3

Tuesday 03:30pm - 04:00pm

Time-Fractional Allen-Cahn Equations: Analysis and Numerical Methods

Zhi Zhou

Hong Kong Polytechnic University, Hong Kong S.A.R. (China)

In this work, we consider a time-fractional Allen-Cahn equation, where the conventional first order time derivative is replaced by a Caputo fractional derivativewith order $\alpha \in (0,1)$. First, the well-posedness and (limited) smoothing property are systematically analyzed, by using the maximal L^p regularity of fractional evolution equations and the fractional Grönwall's inequality. We also show the maximum principle like their conventional local-in-time counterpart. Precisely, the time-fractional equation preserves the property that the solution only takes value between the wells of the double-well potential when the initial data does the same. Second, after discretizing the fractional derivative by backward Euler convolution quadrature, we develop several unconditionally solvable and stable time stepping schemes, i.e., convex splitting scheme, weighted convex splitting scheme and linear weighted stabilized scheme. Meanwhile, we study the discrete energy dissipation property (in a weighted average sense), which is important for gradient flow type models, for the two weighted schemes. Finally, by using a discrete version of fractional Grönwall's inequality and maximal ℓ^p regularity, we prove that the convergence rates of those time-stepping schemes are $O(\tau^\alpha)$ without any extra regularity assumption on the solution. We also present extensive numerical results to support our theoretical findings and to offer new insight on the time-fractional Allen-Cahn dynamics.

MS 03: Part 1
Asymptotic preserving schemes for kinetic problems

Room: HS 2

Monday 10:30am - 11:00am
Shi Jin
Random Batch Methods for Interacting Particle Systems

Monday 11:00am - 11:30am
Gabriella Puppo
Kinetic models of BGK type and their numerical integration

Monday 11:30am - 12:00pm
Giacomo; Pareschi Dimarco
Micro-macro generalized polynomial vhaos techniques for kinetic equations

Monday 12:00pm - 12:30pm
Liu Liu
A bi-fidelity method for the multiscale Boltzmann equation with random parameters

Room: HS 2 | Monday 10:30am - 11:00am

Random Batch Methods for Interacting Particle Systems

Shi Jin

Shanghai Jiao Tong University, China, People's Republic of

We develop random batch methods for interacting particle systems with large number of particles. These methods use small but random batches for particle interactions, thus the computational cost is reduced from $O(N^2)$ per time step to $O(N)$, for a system with N particles with binary interactions. On one hand, these methods are efficient Asymptotic-Preserving schemes for the underlying particle systems, allowing N-independent time steps and also capture, in the $N \to \infty$ limit, the solution of the mean field limit which are nonlinear Fokker-Planck equations; on the other hand, the stochastic processes generated by the algorithms can also be regarded as new models for the underlying problems. For one of the methods, we give a particle number independent error estimate under some special interactions. Then, we apply these methods to some representative problems in mathematics, physics, social and data sciences, including the Dyson Brownian motion from random matrix theory, Thomson's problem, distribution of wealth, opinion dynamics and clustering. Numerical results show that the methods can capture both the transient solutions and the global equilibrium in these problems.
This is a joint work with Lei Li (Shanghai Jiao Tong University) and Jian-Guo Liu (Duke University)

Room: HS 2 Monday 11:00am - 11:30am

Kinetic models of BGK type and their numerical integration

Gabriella Puppo

La Sapienza Università di Roma, Italy

Kinetic models of BGK type are simplified kinetic models that are suited to study weakly off equilibrium effects. In this contribution, I will discuss recent developments on this topic, considering more realistic effects than are usually included in standard BGK models. In particular, I will discuss mixtures of gases, and polyatomic effects.
All these models contain in explicit form the target equilibrium distribution. This allows to tailor numerical methods to the particular predicted relaxation, enforcing asymptotic preserving properties naturally within the time discretisation.

Room: HS 2

Monday 11:30am - 12:00pm

Micro-macro generalized polynomial vhaos techniques for kinetic equations

Giacomo Dimarco[1], Lorenzo Pareschi[1] and Mattia Zanella[2]

[1] *University of Ferrara, Italy*
[2] *Politecnico di Torino, Italy*

Kinetic equations play a major role in the modelling of large systems of interacting particles/agents with a proved effectiveness in describing real world phenomena ranging from plasma physics to biological dynamics. Their formulation has often to face with physical forces deduced through experimental data and of which we have at most statistical information. Hence, we consider the presence of random inputs in the form of uncertain parameters as a structural feature of the kinetic modelling. In this talk, we will consider uncertainty quantification for Vlasov-Fokker-Planck equations through a micro-macro numerical approach based on stochastic Galerkin methods which preserve the large time distribution of the system.

Room: HS 2 | Monday 12:00pm - 12:30pm

A bi-fidelity method for the multiscale Boltzmann equation with random parameters

Liu Liu

University of Texas at Austin, United States of America

In this talk, we study the multiscale Boltzmann equation with multi-dimensional random parameters by a bi-fidelity stochastic collocation (SC) method developed in [A. Narayan, C. Gittelson and D. Xiu, SIAM J. Sci. Comput., 36 (2014)]. By choosing the compressible Euler system as the low-fidelity model, we adapt the bi-fidelity SC method to combine computational efficiency of the low-fidelity model with high accuracy of the high-fidelity (Boltzmann) model. With a quite small number of high-fidelity asymptotic-preserving solver runs for the Boltzmann equation, the bi-fidelity approximation can capture well the macroscopic quantities of the solution to the Boltzmann equation in the random space. A priori estimate on the accuracy between the high- and bi-fidelity solutions in the case when the Knudsen number is small, together with a convergence analysis is established. Finally, we present extensive numerical experiments to verify the efficiency and accuracy of our proposed method. This is a joint work with Xueyu Zhu.

MS 03: Part 2
Asymptotic preserving schemes for kinetic problems

Room: HS 2

Monday 02:00pm - 02:30pm
Christian Klingenberg
A Class of Asymptotic and Stationary Preserving Schemes for Kinetic Models

Monday 02:30pm - 03:00pm
Jingwei Hu
A second-order asymptotic-preserving and positivity-preserving exponential Runge-Kutta method for a class of stiff kinetic equations

Monday 03:00pm - 03:30pm
Giacomo Albi
IMEX multistep method for hyperbolic systems with relaxation

Monday 03:30pm - 04:00pm
Ruiwen Shu
On the uniform accuracy of the implicit-explicit backward difference formulae (IMEX BDF) for stiff hyperbolic relaxation systems and kinetic equations

Room: HS 2 | Monday 02:00pm - 02:30pm

A Class of Asymptotic and Stationary Preserving Schemes for Kinetic Models

Christian Klingenberg

Universität Würzburg, Germany

We are interested in the stationary preserving (SP) property of AP schemes for kinetic models. The trick in proving the SP property is to show that the macroscopic quantities can be updated time-explicitly while the discretization of the scheme is an IMEX discretization. One can see that any AP scheme with the property of updating the macroscopic quantities explicitly satisfies the SP property. As an example, three different AP schemes considered and proved to satisfy the SP property. The first two schemes solve the chemotaxis kinetic model and the third solves the Boltzmann equation. Several numerical test cases are performed to validate the SP property of each AP scheme.
This is joint work with Farah Kanbar and Min Tang.

Room: HS 2 | Monday 02:30pm - 03:00pm

A second-order asymptotic-preserving and positivity-preserving exponential Runge-Kutta method for a class of stiff kinetic equations

Jingwei Hu[1] **and Ruiwen Shu**[2]

[1] *Purdue University, United States of America*
[2] *University of Maryland, United States of America*

We introduce a second-order time discretization method for stiff kinetic equations. The method is asymptotic-preserving (AP) – can capture the Euler limit without numerically resolving the small Knudsen number; and positivity-preserving – can preserve the non-negativity of the solution which is a probability density function for arbitrary Knudsen numbers. The method is based on a new formulation of the exponential Runge-Kutta method and can be applied to a large class of stiff kinetic equations including the BGK equation (relaxation type), the Fokker-Planck equation (diffusion type), and even the full Boltzmann equation (nonlinear integral type). Furthermore, we show that when coupled with suitable spatial discretizations the fully discrete scheme satisfies an entropy-decay property. Various numerical results are provided to demonstrate the theoretical properties of the method.

Room: HS 2

Monday 03:00pm - 03:30pm

IMEX multistep method for hyperbolic systems with relaxation

Giacomo Albi[1], **Giacomo Dimarco**[2] **and Lorenzo Pareschi**[2]

[1] *University of Verona, Italy*
[2] *University of Ferrara, Italy*

In this talk, we consider the development of Implicit-Explicit (IMEX) Multistep time integrators for hyperbolic systems with relaxation. More specifically, we consider the case in which the transport and the relaxation part of such systems have different time and space scales. The consequence is that the nature of the asymptotic limit can differ, passing from an hyperbolic to a parabolic character. From the computational point of view, this causes many drawbacks that standard time integrators, even implicit ones, are not able to handle: loss of efficiency and loss of capability in describing the limit regime. In this work, we construct highly stable numerical methods which describe all the different regimes with high accuracy in time and space that are able to capture the correct asymptotic limit. Several numerical examples confirm the consistency and linear stability analysis and show that the proposed methods outperform existing ones.

Room: HS 2

Monday 03:30pm - 04:00pm

On the uniform accuracy of the implicit-explicit backward difference formulae (IMEX BDF) for stiff hyperbolic relaxation systems and kinetic equations

Ruiwen Shu[1] **and Jingwei Hu**[2]

[1] *University of Maryland, College Park, United States of America*
[2] *Purdue University, United States of America*

Many hyperbolic and kinetic equations contain a non-stiff convection part and stiff relaxation or collision part (characterized by the stiffness parameter ε). For these type of problems, implicit-explicit (IMEX) Runge-Kutta or multi-step methods have been very popular and their performance is understood well in the non-stiff regime ($\varepsilon = O(1)$) and limiting regime ($\varepsilon \to 0$). However, in the mildly stiff regime (say, $\varepsilon = O(\Delta t)$), some uniform accuracy or order reduction phenomena have been reported numerically without much theoretical justification. In this work, we prove the uniform accuracy (an optimal priori error bound) of a class of IMEX multi-step methods — IMEX BDF for linear hyperbolic systems with stiff relaxation. The proof is based on the energy estimate with a new multiplier technique. For nonlinear hyperbolic and kinetic equations, we numerically verify the same property using a series of examples.

MS 04: Part 1
Computational methods for quantum dynamic problems

Room: HS 1

Tuesday 10:30am - 11:00am
Yan Wang
A low-regularity method for the nonlinear Dirac equation

Tuesday 11:00am - 11:30am
Jérémie Gaidamour
A parallel framework for the numerical simulation of Bose–Einstein condensates

Tuesday 11:30am - 12:00pm
Yue Feng
Long time error analysis of finite difference time domain methods for the nonlinear Klein-Gordon equation with weak nonlinearity

Tuesday 12:00pm - 12:30pm
Chunmei Su
Numerical methods and analysis for the logarithmic Schrodinger equation

Room: HS 1 | Tuesday 10:30am - 11:00am

A low-regularity method for the nonlinear Dirac equation

Yan Wang

Central China Normal University, China, People's Republic of

In this work, we consider the numerical integration of the nonlinear Dirac equation and the Dirac-Poisson system (NDEs) under rough initial data. We propose a ultra low-regularity integrator (ULI) for solving the NDEs which enables optimal first order convergence in H^r-norm for solution in H^r. In contrast to classical methods, ULI overcomes the numerical loss of derivatives and is therefore more efficient and accurate for approximating less regular solutions. Convergence theorems and the extension of ULI to second order are established. Numerical results are presented to confirm the theoretical results and for comparisons. This is a joint work with Katharina Schratz and Xiaofei Zhao.

Room: HS 1

Tuesday 11:00am - 11:30am

A parallel framework for the numerical simulation of Bose–Einstein condensates

Jérémie Gaidamour[1] **and Xavier Antoine**[2]

[1] *CNRS*
[2] *University of Lorraine, France*

We propose a parallel implementation of a spectral method for computing the ground states of rotating Bose–Einstein condensates (BEC) modeled by the Gross-Pitaevskii equation (GPE). Considering a standard pseudo-spectral discretization based on Fast Fourier Transforms (FFTs), the method consists in finding the numerical solution of a minimization problem with a preconditioned nonlinear conjugate gradient method. We present some scalability results for the 2D and 3D computation of the stationary states of BEC with fast rotation and large nonlinearities. The code takes advantage of existing HPC libraries and can itself be leveraged to implement other spectral methods or solve the dynamics of BEC problems.

Room: HS 1 | Tuesday 11:30am - 12:00pm

Long time error analysis of finite difference time domain methods for the nonlinear Klein-Gordon equation with weak nonlinearity

Weizhu Bao[1], **Yue Feng**[1] **and Wenfan Yi**[2]

[1]*National University of Singapore, Singapore*
[2]*Hunan University, P. R. China*

We establish error bounds of the finite difference time domain (FDTD) methods for the long time dynamics of the nonlinear Klein-Gordon equation (NKGE) with a cubic nonlinearity, while the nonlinearity strength is characterized by ε^2 with $0 < \varepsilon \leq 1$ a dimensionless parameter. When $0 < \varepsilon \ll 1$, it is in the weak nonlinearity regime and the problem is equivalent to the NKGE with small initial data, while the amplitude of the initial data (and the solution) is at $O(\varepsilon)$. Four different FDTD methods are adapted to discretize the problem and rigorous error bounds of the FDTD methods are established for the long time dynamics, i.e. error bounds are valid up to the time at $O(1/\varepsilon^\beta)$ with $0 \leq \beta \leq 2$, by using the energy method and the techniques of either the cut-off of the nonlinearity or the mathematical induction to bound the numerical approximate solutions. In the error bounds, we pay particular attention to how error bounds depend explicitly on the mesh size h and time step τ as well as the small parameter $\varepsilon \in (0, 1]$, especially in the weak nonlinearity regime when $0 < \varepsilon \ll 1$. Our error bounds indicate that, in order to get "correct" numerical solutions up to the time at $O(1/\varepsilon^\beta)$, the ε-scalability (or meshing strategy) of the FDTD methods should be taken as: $h = O(\varepsilon^{\beta/2})$ and $\tau = O(\varepsilon^{\beta/2})$. As a by-product, our results can indicate error bounds and ε-scalability of the FDTD methods for the discretization of an oscillatory NKGE which is obtained from the case of weak nonlinearity by a rescaling in time, while its solution propagates waves with wavelength at $O(1)$ in space and $O(\varepsilon^\beta)$ in time. Extensive numerical results are reported to confirm our error bounds and to demonstrate that they are sharp.

Room: HS 1 | Tuesday 12:00pm - 12:30pm

Numerical methods and analysis for the logarithmic Schrodinger equation

Weizhu Bao[1], **Carles Remi**[2], **Chunmei Su**[3] **and Qinglin Tang**[4]

[1] *National University of Singapore*
[2] *Université de Rennes 1*
[3] *Technical University of Munich*
[4] *Sichuan University*

We present a regularized Lie-Trotter splitting method for the logarithmic Schrödinger equation (LogSE) and establish its error bound. In order to suppress the round-off error and to avoid the blow-up of the logarithmic nonlinearity, a regularized logarithmic Schrödinger equation (RLogSE) is proposed with a small regularization parameter $0 < \varepsilon \ll 1$ and linear convergence is established between the solutions of RLogSE and LogSE in terms of ε. Then we use the Lie-Trotter splitting integrator to solve the RLogSE and establish its error bound $O(\tau^{1/2}\ln(\varepsilon^{-1}))$ with $\tau > 0$ the time step, which implies an error bound at $O(\varepsilon + \tau^{1/2}\ln(\varepsilon^{-1}))$ for the LogSE by the Lie-Trotter splitting method. Numerical results are reported to confirm the error bounds and to demonstrate rich and complicated dynamics of the LogSE.

MS 04: Part 2
Computational methods for quantum dynamic problems

Room: HS 1

Tuesday 02:00pm - 02:30pm
Xinran Ruan
Numerical methods for computing ground states of Bose-Einstein Condensates with higher order interaction

Tuesday 02:30pm - 03:00pm
Eric Polizzi
Scalable Algorithms for Real-Space and Real-Time First-Principle Calculations

Tuesday 03:00pm - 03:30pm
Karolina Kropielnicka
Symplectic integrator for the Klein-Gordon equation with space- and time- dependent mass under possible influence of laser impulses

Tuesday 03:30pm - 04:00pm
Emmanuel Lorin
Towards Perfectly Matched Layers for Fractional PDEs.

Room: HS 1 | Tuesday 02:00pm - 02:30pm

Numerical methods for computing ground states of Bose-Einstein Condensates with higher order interaction

Xinran Ruan[1] **and Weizhu Bao**[2]

[1]*Sorbonne Université, France*
[2]*National University of Singapore, Singapore*

The higher order interaction (HOI), which is crucial in the description of the Bose-Einstein condensate near Feshbach resonance, makes the computation of ground states more difficult due to the extra nonlinearity introduced. In this talk, I will show two numerical methods for the computation of the ground states, namely the normalized gradient flow method and the “rDF-APG" method. The two methods are specially designed to deal with the extra nonlinear term, i.e. the HOI term. Extensive numerical experiments indicate that both methods are stable and efficient.

Room: HS 1 | Tuesday 02:30pm - 03:00pm

Scalable Algorithms for Real-Space and Real-Time First-Principle Calculations

Eric Polizzi

University of Massachusetts, Amhers, United States of America

Realistic first-principle quantum simulations applied to large-scale atomistic systems pose unique challenges in the design of numerical algorithms that are both capable of processing a considerable amount of generated data, and achieving significant parallel scalability on modern high-end computing architectures. From atoms and molecules to nanostructures, we discuss how the FEAST eigensolver can considerably broaden the perspectives for enabling reliable and high-performance large-scale first-principle all-electrons DFT and real-time TDDFT calculations. We will present various simulation results with applications ranging from computational electronic spectroscopy of molecules, to plasmonic excitations in carbon-based nanostructures.

Room: HS 1 | Tuesday 03:00pm - 03:30pm

Symplectic integrator for the Klein-Gordon equation with space- and time- dependent mass under possible influence of laser impulses

Karolina Kropielnicka and **Karolina Lademann**

University of Gdańsk, Poland

We consider the numerical integration of the non-stationary Klein–Gordon equation with the position- and time-dependent mass, which may be under the influence of laser. The special structure of KG equation allows us to use commutators which can be computed easily. In the proposed method time-mesh is not influenced by highly oscillatory potential. Numerical examples and comparisons are demonstrated to illustrate effective results.

Room: HS 1 | Tuesday 03:30pm - 04:00pm

Towards Perfectly Matched Layers for Fractional PDEs.

Emmanuel Lorin

Carleton University, Canada

This talk is dedicated to the derivation of absorbing layers for space fractional evolution PDEs. Within this approach, widely used powerful FFT solvers can be adapted without much effort to compute Initial Boundary Value Problems (IBVP) for well-posed fractional equations with absorbing boundary layers. We analyze mathematically the method and propose some illustrating numerical experiments including fractional diffusion and Schroedinger equations.
This is a joint work with X. Antoine (IECL, Universite de Lorraine).

MS 06: Part 1
Wave problems

Room: HS 2

Tuesday 10:30am - 11:00am
Balázs Kovács
L^2 error estimates for wave equations with dynamic boundary conditions

Tuesday 11:00am - 11:30am
Daniel Appelo
WaveHoltz: iterative solution of the Helmholtz equation via the wave equation

Tuesday 11:30am - 12:00pm
Lise-Marie Imbert-Gerard
Generalized Plane Waves in two dimensions: beyond Helmholtz equation

Tuesday 12:00pm - 12:30pm
Maria Lopez Fernandez
Directional $\mathcal{H}^2$-Matrices for Helmholtz Problems with Complex Frequency

Room: HS 2 | Tuesday 10:30am - 11:00am

L^2 error estimates for wave equations with dynamic boundary conditions

David Hipp[1] **and Balázs Kovács**[2]

[1] *KIT, Germany*
[2] *University of Tübingen, Germany*

L^2 norm error estimates of semi- and full discretisations, using bulk–surface finite elements and Runge–Kutta methods, of wave equations with dynamic boundary conditions are studied. The analysis resides on an abstract formulation and error estimates, via energy techniques, within this abstract setting. Four prototypical linear wave equations with dynamic boundary conditions are analysed which fit into the abstract framework. For problems with velocity terms, or with acoustic boundary conditions we prove surprising results: for such problems the spatial convergence order is shown to be less than two. These can also be observed in the presented numerical experiments.

Room: HS 2 | Tuesday 11:00am - 11:30am

WaveHoltz: iterative solution of the Helmholtz equation via the wave equation

Daniel Appelo[1], **Fortino Garcia**[1] **and Olof Runborg**[2]

[1] *University of Colorado, Boulder, United States of America*
[2] *Royal Institute of Technology, Stockholm, Sweden*

Designing efficient iterative solvers for the Helmholtz equation is notoriously difficult and has been the subject of much research. The main two difficulties in solving the Helmholtz equation are the resolution requirements and the highly indefinite character of the discretized system of equations. Inspired by the work considered in the late 1990's by Bristeau, Glowinski, and Périaux (and recently revived by Grote et al.) on so called exact controllability methods, we introduce a novel idea that enables the use of time domain methods for wave equations to design frequency domain Helmholtz type solvers. Our approach yields an underlying linear operator corresponding to a symmetric positive definite matrix allowing us to both solve a nice coercive problem and accelerate convergence via Krylov methods such as conjugate gradient (CG). The resulting method is high order accurate and straightforward to parallelize.

Room: HS 2 | Tuesday 11:30am - 12:00pm

Generalized Plane Waves in two dimensions: beyond Helmholtz equation

Lise-Marie Imbert-Gerard[1] **and Guillaume Sylvand**[2]

[1] *University of Maryland, United States of America*
[2] *Airbus CRT / Inria*

We are interested in boundary value problems modeling wave propagation in frequency domain, in inhomogeneous and anisotropic media, and therefore in partial differential equations with variable coefficients. In particular we are interested in aero-acoustics where the inhomogeneous medium is represented by the variable density ρ, while the anisotropic flow is represented by the variable vector field $\mathbf{M}$.
Trefftz methods are commonly used for wave propagation problems in frequency domain, and rely on basis functions that solve exactly the driving equation, such as classical plane waves. In order to take advantage of Trefftz methods for problems with variable coefficients, in which case there is usually no known exact solution of the PDE to discretize the Trefftz formulation, Generalized Plane Waves (GPWs) have been developed as approximated solutions to the given PDE.
GPWs were initially introduced for the variable-coefficient Helmholtz equation in two dimensions. In this presentation we will extend the design and construction of GPWs beyond Helmholtz equation, and we will discuss their interpolation properties.

Room: HS 2 | Tuesday 12:00pm - 12:30pm

Directional $\mathcal{H}^2$-Matrices for Helmholtz Problems with Complex Frequency

Steffen Boerm[1], **Maria Lopez Fernandez**[2] **and Stefan A. Sauter**[3]

[1] *University of Kiel, Germany*
[2] *Sapienza University of Rome, Italy*
[3] *University of Zurich, Switzerland*

The sparse approximation of high-frequency Helmholtz-type integral operators has many important physical applications such as problems in wave propagation and wave scattering. The discrete system matrices are huge and densely populated and hence their sparse approximation is of outstanding importance. In our paper we will generalize the directional $\mathcal{H}^2$-matrix techniques from the "pure" Helmholtz operator $\mathcal{L}u = -\Delta u + \zeta^2 u$ with $\zeta = -\mathrm{i}\,k$, $k \in \mathbb{R}$, to general complex frequencies $\zeta \in \mathbb{C}$ with $\operatorname{Re}\zeta > 0$. In this case, the fundamental solution decreases exponentially for large arguments. We will develop a new admissible condition which contains $\operatorname{Re}\zeta$ in an explicit way and introduce the approximation of the integral kernel function on admissible blocks in terms of frequency-dependent directional expansion functions. We develop an error analysis which is explicit with respect to the expansion order and with respect to $\operatorname{Re}\zeta$ and $\operatorname{Im}\zeta$. This allows to choose the variable expansion order in a quasi-optimal way depending on $\operatorname{Re}\zeta$ but independent of, possibly large, $\operatorname{Im}\zeta$. The complexity analysis is explicit with respect to $\operatorname{Re}\zeta$ and $\operatorname{Im}\zeta$ and shows how higher values of $\operatorname{Re}\zeta$ reduce the complexity. In certain cases, it even turns out that the discrete matrix can be replaced by its nearfield part. Numerical experiments illustrate the sharpness of the derived estimates and the efficiency of our sparse approximation.

MS 06: Part 2
Wave problems

Room: HS 2

Tuesday 02:00pm - 02:30pm
Sébastien Imperiale
An efficient time discretisation of the incompressible elastodynamics equation in living tissues

Tuesday 02:30pm - 03:00pm
Daniel Ziegler
Parallel adaptive discontinuous Galerkin discretizations in space and time for visco-elastic and visco-acoustic waves.

Tuesday 03:00pm - 03:30pm
Marina Fischer
Wave Equation in a Periodic Waveguide with a Local Perturbation

Tuesday 03:30pm - 04:00pm
Maryna Kachanovska
Error analysis for local absorbing boundary conditions in fractal trees

Room: HS 2

Tuesday 02:00pm - 02:30pm

An efficient time discretisation of the incompressible elastodynamics equation in living tissues

Federica Caforio[1,2] **and** **Sébastien Imperiale**[2]

[1] *Computational Cardiology Laboratory, Institute of Biophysics, Medical University of Graz*
[2] *Inria & LMS, Ecole polytechnique, CNRS, Université Paris-Saclay*

The principal aim of this work is to provide an adapted numerical scheme for the approximation of elastic wave propagation in nearly-incompressible solids such as living tissue. The simulation in such media is computationally intensive due to the severe stability condition that is imposed on the time step of explicit methods. We construct an implicit/explicit, second-order time discretisation, that, by using penalisation techniques, provides an efficient way to deal with incompressibility: at the price of solving at each time step a scalar Poisson problem (that can be performed by various, efficient algorithms), the time step restriction is independent of the incompressibility parameters.

Room: HS 2 | Tuesday 02:30pm - 03:00pm

Parallel adaptive discontinuous Galerkin discretizations in space and time for visco-elastic and visco-acoustic waves.

Willy Dörfler, Christian Wieners and Daniel Ziegler

Karlsruher Institut für Technologie, Germany

We consider space-time Petrov-Galerkin methods for linear wave equations. Based on our results for Maxwell's equations and acoustic and elastic waves, our main focus lies now on the system for visco–elastic waves is heterogeneous media

$$\begin{aligned} \rho\,\partial_t \boldsymbol{v} &= \operatorname{div}\boldsymbol{\sigma} + \boldsymbol{f}\,, \\ \partial_t\boldsymbol{\sigma} &= 2\mu(1+L\tau_{\mathrm{S}})\operatorname{dev}\boldsymbol{\varepsilon}(\boldsymbol{v}) + \kappa(1+L\tau_{\mathrm{P}})\operatorname{div}\boldsymbol{v}\,\mathbf{I} + \sum_{l=1}^{L}\boldsymbol{\eta}_l\,, \\ \tau_{\sigma,l}\,\partial_t\boldsymbol{\eta}_l &= -2\mu\tau_{\mathrm{S}}\operatorname{dev}\boldsymbol{\varepsilon}(\boldsymbol{v}) - \kappa\tau_{\mathrm{P}}\operatorname{div}\boldsymbol{v}\,\mathbf{I} - \boldsymbol{\eta}_l\,, \qquad l = 1,\dots,L \end{aligned}$$

in $Q = (0,T)\times\Omega\subset\mathbb{R}^{1+d}$. Based on the framework of generalized standard materials this extends the system for velocity $\boldsymbol{v}$ and stress $\boldsymbol{\sigma}$ by memory tensors $\boldsymbol{\eta}_l$ describing the attenuation of elastic waves in geophysical applications. The visco–acoustic case corresponds to the case $\mu\to 0$ and $\boldsymbol{\sigma} = p\mathbf{I}$, where p is the the hydrostatic pressure.

We use a tensor product space-time mesh with a discontinuous Galerkin finite element method with full upwind flux for the spatial discretization and a Petrov–Galerkin discretization in time. For this setting we establish convergence by verifying discrete inf-sup stability with a constant independent of the polynomial degree of the finite element space. The full space-time linear system is solved by a parallel multilevel preconditioner.

The method is adaptive with variable polynomial degrees in the space-time cells with a refinement strategy based on a goal-oriented dual-weighted error estimator. This reduces the error with respect to a given goal functional within several adaptive iterations. In our numerical examples we choose a linear goal functional corresponding to a space-time region of interest and we show that the adaptive procedure clearly identifies the subset of the space-time cylinder which is required for the accurate evaluation of the goal functional.

Room: HS 2 | Tuesday 03:00pm - 03:30pm

Wave Equation in a Periodic Waveguide with a Local Perturbation

Marina Fischer

Heinrich-Heine-Universität, Düsseldorf, Germany

In this contribution we focus on the numerical computation of the wave equation in a periodic waveguide that is locally perturbed in a bounded domain. By using the Laplace transform in time we transfer our computations to the frequency domain and obtain a Helmholtz equation. Applying ideas by P. Joly and S. Fliss we derive transparent boundary conditions on the perturbed domain by solving local problems on one periodicity cell and extend the solution to the rest of the waveguide. With the inverse Laplace transform we then obtain transparent boundary conditions in the time domain which are now given as convolutions. On using convolution quadrature methods we are able to compute the solution of the wave equation in the perturbed domain. Besides, with the same technique the solution on the rest of the waveguide can be computed. In a numerical example we illustrate the performance of the proposed method.

Room: HS 2 | Tuesday 03:30pm - 04:00pm

Error analysis for local absorbing boundary conditions in fractal trees

Patrick Joly and **Maryna Kachanovska**

POEMS (UMR CNRS-ENSTA-INRIA), INRIA, France

We consider the problem of sound propagation in human lungs, modelled by a 1D weighted wave equation on a fractal tree. As the domain geometry is structurally infinite, to perform the numerical computations, it is necessary to be able to truncate it by imposing transparent boundary conditions. This is done by approximating the Dirichlet-to-Neumann operator. We prove that its symbol is a meromorphic function with real poles, which are the eigenvalues of the underlying weighted laplacian. Truncation of its symbol to a finite (N) number of terms results in a local in time approximation of the operator. The error induced by the truncation depends on the eigenvalues and conormal traces of the eigenfunctions. By deriving the asymptotics on eigenvalues of the weighted laplacian on the fractal tree, in the spirit of [Kigami, Lapidus 1993; Levitin, Vassiliev 1996] and extending bounds on eigenfunctions of [Barnett, Hassell 2011] we obtain an upper and lower bounds on the error as a function of N. The results are illustrated by numerical experiments.

MS 07: Part 1
Geometry and structure preservation in numerical differential equations

Room: HS 1

Monday 10:30am - 11:00am
Brynjulf Owren
An application of loopy trees to Kahan's method

Monday 11:00am - 11:30am
Milo Viviani
Lie–Poisson methods for isospectral flows and their application to long-time simulation of spherical ideal hydrodynamics

Monday 11:30am - 12:00pm
Antonella Zanna
On some symplectic P-stable additive Runge–Kutta Methods

Monday 12:00pm - 12:30pm
Molei Tao
Explicit high-order symplectic integration of nonseparable Hamiltonians

Room: HS 1

Monday 10:30am - 11:00am

An application of loopy trees to Kahan's method

Brynjulf Owren, Geir Bogfjellmo, Elena Celledoni, Robert Iain McLachlan and Reinout Quispel

NTNU, Norway

A popular research subject in recent years has been to identify first integrals and preserved measures in Kahan's method. Munthe-Kaas and Verdier have introduced a generalisation of Butcher series that they call aromatic series, indexed by loopy trees. We show how these trees can be used in the search for first integrals and preserved measures in the numerical integrator of Kahan. We also identify some necessary conditions for preserved measures of this form to exist.

Room: HS 1

Monday 11:00am - 11:30am

Lie–Poisson methods for isospectral flows and their application to long-time simulation of spherical ideal hydrodynamics

Klas Modin and Milo Viviani

Chalmers University of Technology, Sweden

The theory of isospectral flows comprises a large class of continuous dynamical systems, particularly integrable systems and Lie–Poisson systems. Their discretization is a classical problem in numerical analysis. Preserving the spectra in the discrete flow requires the conservation of high order polynomials, which is hard to come by. Existing methods achieving this are complicated and usually fail to preserve the underlying Lie–Poisson structure. Here we present a class of numerical methods of arbitrary order for Hamiltonian and non-Hamiltonian isospectral flows, which preserve both the spectra and the Lie–Poisson structure. The methods are surprisingly simple, and avoid the use of constraints or exponential maps. Furthermore, due to preservation of the Lie–Poisson structure, they exhibit near conservation of the Hamiltonian function. As an illustration, we apply the methods to long-time simulation of the Euler equations on a sphere. Our findings suggest that our structure-preserving algorithms, on the one hand, perform at least as well as other popular methods (i.e. CLAM) without adding spurious hyperviscosity terms, on the other hand, show that the conservation of the Casimir functions can be actually used to predict the final state of the fluid.

Room: HS 1 | Monday 11:30am - 12:00pm

On some symplectic P-stable additive Runge–Kutta Methods

Antonella Zanna

University of Bergen, Norway

Symplectic partitioned Runge–Kutta methods can be obtained from a variational formulation treating all the terms in the Lagrangian with the same quadrature formula. We construct a family of symplectic methods allowing the use of different quadrature formula for different parts of the Lagrangian. In particular, we study a family of methods using Lobatto quadrature (with corresponding Lobatto IIIA-IIIB symplectic method) and Gauss–Legendre quadrature combined in an appropriate way. The resulting methods are similar to additive Runge-Kutta methods. The IMEX method, using the Verlet and IMR combination is a particular case of this family.
The methods have the same favourable implicitness as the underlying Lobatto IIIA-IIIB pair. Differently from the Lobatto IIIA-IIIB, which are known not to be P-stable, we show that the new methods satisfy the requirements for P-stability.

Room: HS 1 | Monday 12:00pm - 12:30pm

Explicit high-order symplectic integration of nonseparable Hamiltonians

Molei Tao

Georgia Institute of Technology, United States of America

Symplectic integrators preserve the phase-space volume and have favorable performances in long time simulations. Methods for explicit symplectic integration have been extensively studied for separable Hamiltonians (i.e., H(q,p)=K(p)+V(q)), and they lead to both accuracy and efficiency. However, nonseparable Hamiltonians also model important problems. Unfortunately, implicit methods had been the only available symplectic approach with long-time accuracy for general nonseparable systems.
This talk will construct explicit symplectic integrators for nonseparable systems. These new integrators are based on a mechanical restraint that binds two copies of phase space together, and they can be made arbitrarily high-order. Using backward error analysis, KAM theory, and some additional multiscale analysis, a pleasant error bound is established for integrable systems. Numerical evidence of statistical accuracy for non-integrable systems (e.g., a finite-dimensional nonlinear Schrodinger equation) were also observed.

MS 07: Part 2
Geometry and structure preservation in numerical differential equations

Room: HS 1

Monday 02:00pm - 02:30pm
Tomasz Michal Tyranowski
Variational integrators for stochastic dissipative Hamiltonian systems

Monday 02:30pm - 03:00pm
François Gay-Balmaz
Variational discretization framework for geophysical fluid models

Monday 03:00pm - 03:30pm
Evan Gawlik
Structure-Preserving Finite Element Methods for Ricci Flow

Monday 03:30pm - 04:00pm
Ari Stern
Constraint-preserving hybrid finite element methods for Maxwell's equations

Room: HS 1

Monday 02:00pm - 02:30pm

Variational integrators for stochastic dissipative Hamiltonian systems

Michael Kraus[1,2] **and** **Tomasz Michal Tyranowski**[1]

[1] *Max Planck Institute for Plasma Physics, Germany*
[2] *Technische Universität München, Germany*

Variational integrators are derived for structure-preserving simulation of stochastic forced Hamiltonian systems. The derivation is based on a stochastic discrete Hamiltonian which approximates a type-II stochastic generating function for the stochastic flow of the Hamiltonian system. The generating function is obtained by introducing an appropriate stochastic action functional and considering a stochastic generalization of the deterministic Lagrange-d'Alembert principle. Our approach presents a general methodology to derive new structure-preserving numerical schemes. The resulting integrators satisfy a discrete version of the stochastic Lagrange-d'Alembert principle, and in the presence of symmetries, they also satisfy a discrete counterpart of Noether's theorem. Furthermore, mean-square and weak Lagrange-d'Alembert Runge-Kutta methods are proposed and tested numerically to demonstrate their superior long-time numerical stability and energy behavior compared to non-geometric methods. The Vlasov-Fokker-Planck equation is considered as one of the numerical test cases, and a new geometric approach to collisional kinetic plasmas is presented.

Room: HS 1 | Monday 02:30pm - 03:00pm

Variational discretization framework for geophysical fluid models

<u>François Gay-Balmaz</u>[1] **and Werner Bauer**[2]

[1] *CNRS Ecole Normale Superieure, France*
[2] *Inria Rennes*

We introduce a geometric variational discretization framework for geophysical ow models. The numerical scheme is obtained by discretizing, in a structure preserving way, the Lie group formulation of fluid dynamics on diffeomorphism groups and the associated variational principles. Being based on a discrete version of the Euler-Poincare variational method, this discretization approach is widely applicable. We present an overview of structure-preserving variational discretizations of various equations of geophysical fluid dynamics, such as the Boussinesq, anelastic, pseudo-incompressible, and rotating shallow-water equations. We verify the structure-preserving nature of the resulting variational integrators for test cases of geophysical relevance. Our framework applies to irregular mesh discretizations in 2D and 3D in planar and spherical geometry and produces schemes that preserve invariants of the equations such as mass and potential vorticity. Descending from variational principles, the discussed variational schemes exhibit a discrete version of Kelvin circulation theorem and show excellent long term energy behavior.

Room: HS 1

Monday 03:00pm - 03:30pm

Structure-Preserving Finite Element Methods for Ricci Flow

Evan Gawlik

University of Hawaii, United States of America

This talk will introduce a family of structure-preserving finite element methods for normalized Ricci flow in two dimensions. Our construction is based on two key ideas: computing scalar curvature by solving the differential equation that governs its temporal evolution, and approximating the metric tensor with Regge finite elements – piecewise polynomial (0,2)-tensor fields whose tangential-tangential components along edges are single-valued. The resulting methods preserve total area and obey a discrete analogue of the Gauss-Bonnet theorem. When piecewise constant Regge finite elements are used, the approximate curvature produced by the method coincides with the widely used angle defect from discrete differential geometry.

Room: HS 1 | Monday 03:30pm - 04:00pm

Constraint-preserving hybrid finite element methods for Maxwell's equations

Yakov Berchenko-Kogan and Ari Stern

Washington University in St. Louis, United States of America

Maxwell's equations describe the evolution of electromagnetic fields, together with constraints on the divergence of the magnetic and electric flux densities. These constraints correspond to fundamental physical laws: the nonexistence of magnetic monopoles and the conservation of charge, respectively. However, one or both of these constraints may be violated when one applies a finite element method to discretize in space. This is a well-known and longstanding problem in computational electromagnetics. We use domain decomposition to construct a family of primal hybrid finite element methods for Maxwell's equations, where the Lagrange multipliers are shown to correspond to a numerical trace of the magnetic field and a numerical flux of the electric flux density. Expressing the charge-conservation constraint in terms of this numerical flux, we show that both constraints are strongly preserved. As a special case, these methods include a hybridized version of Nédélec's method, implying that it preserves the constraints more strongly than previously recognized. These constraint-preserving properties are illustrated using numerical experiments in both the time domain and frequency domain. Additionally, we observe a superconvergence phenomenon, where hybrid post-processing yields an improved estimate of the magnetic field.

MS 08: Part 1
Discrete integrable systems and numerical methods

Room: UR 1

Tuesday 10:30am - 11:00am
Adrian Stefan Cirstea
Birational dynamics on non-relatively minimal elliptic surfaces for discrete Nahm-type equations.

Tuesday 11:00am - 11:30am
Mats Vermeeren
Continuum limits of integrable lattice equations

Tuesday 11:30am - 12:00pm
Charalambos Evripidou
Integrable reductions of the dressing chain

Tuesday 12:00pm - 12:30pm
Matteo Petrera
Kahan discretizations: old and new aspects

Room: UR 1 | Tuesday 10:30am - 11:00am

Birational dynamics on non-relatively minimal elliptic surfaces for discrete Nahm-type equations.

Adrian Stefan Cirstea

Horia Hulubei, National Institute of Physics and Nuclear Engineering, Romania

The desingularization of birational dynamical systems lift them to automorphisms of rational surfaces which, in many cases, are not relatively minimal. The Hirota-Kahan discretization of Nahm-type equations provides such cases and, using the blow-down structure, one can lift them to automorphisms of minimal elliptic surfaces. The linear action on the corresponding Picard lattice allows recovery of the higher order invariants found before by Petrera, Pfadler and Suris.

Room: UR 1 | Tuesday 11:00am - 11:30am

Continuum limits of integrable lattice equations

Mats Vermeeren

TU Berlin, Germany

Discretizing integrable differential equations in a way that preserves the integrability is a notoriously difficult problem. One explanation of this difficulty is that not just the given equation has to be discretized, but also all of its symmetries. This is particularly challenging in the case of integrable PDEs, which have an infinite hierarchy of symmetries. In this talk we discuss a slightly simpler way to connect discrete and continuous integrable systems, namely that of continuum limits. A well-chosen continuum limit procedure, which has its roots in the work of Tetsuji Miwa, can recover a full integrable hierarchy from a single lattice equation. We will discuss how integrability is carried over from the discrete equation to the continuous hierarchy, with particular focus on the variational structure of the equations. Hopefully, these insights can inspire new approaches to the problem of integrable discretization.

Room: UR 1 | Tuesday 11:30am - 12:00pm

Integrable reductions of the dressing chain

Charalambos Evripidou

University of Hradec Kralove, Czech Republic

In this talk I will show how we construct a family of integrable systems as reductions of the dressing chain, described in its Lotka-Volterra form. For any two non-negative integers k, n satisfying $n \geq 2k+1$ we obtain a Lotka-Volterra system which on the one hand is a reduction of the dressing chain of $2m+1$ variables and on the other hand is a deformation of an integrable reduction of the $2m+1$-dimensional Bogoyavlenskij-Itoh system, where $m = n-k-1$. The talk will be focused on the particular case $k = 0$ where we also constructed a family of discretizations of the obtained integrable systems, including their Kahan discretization. These discretizations are also Liouville and superintegrable.

Room: UR 1 | Tuesday 12:00pm - 12:30pm

Kahan discretizations: old and new aspects

Matteo Petrera

Technical University of Berlin, Germany

In this talk I will present the current state of research on the Kahan discretization of quadratic vector fields. In the last decade many efforts have been spent to understand why such a numerical integrator is as good as it is. Indeed, besides its algorithmic applicability, it preserves several geometric and dynamical properties of the the continuous system it discretizes. Among such properties, a prominent one is integrability, which is preserved in a remarkable number of cases. After presenting the main structural features of this discretization, I will provide some examples, thus focusing on some recent discoveries which highlight the rich geometry behind the obtained birational maps.

MS 08: Part 2
Discrete integrable systems and numerical methods

$\boxed{\textbf{Room:}\ \ \text{UR 1}}$

Tuesday 02:00pm - 02:30pm
Luis C. García-Naranjo
Structure preserving discretization of ϕ-simple nonholonomic systems

Tuesday 02:30pm - 03:00pm
Robert Iain McLachlan
The bicomplex of aromas: an extension of Butcher series

Tuesday 03:00pm - 03:30pm
Reinout Quispel
Using discrete Darboux polynomials to detect and determine preserved measures and integrals of rational maps. Part I

Tuesday 03:30pm - 04:00pm
Benjamin Kwanen Tapley
Using discrete Darboux polynomials to detect and determine preserved measures and integrals of rational maps. Part II

Room: UR 1 | Tuesday 02:00pm - 02:30pm

Structure preserving discretization of ϕ-simple nonholonomic systems

Luis C. García-Naranjo

UNAM, Mexico, TU Berlin, Germany.

Nonholonomic *phi*-simple systems form a remarkable class of nonholonomic mechanical problems with symmetry whose reduced equations of motion always possess an invariant measure and admit a formulation in conformally Hamiltonian form. We present a discretization of these systems, at fixed energy values, that preserves the geometric structure of the continuous problem and exhibits good energy behaviour.

Room: UR 1

Tuesday 02:30pm - 03:00pm

The bicomplex of aromas: an extension of Butcher series

Robert Iain McLachlan

Massey University, New Zealand

Butcher series involve elementary differentials, like $f'f$, which are invariant under affine maps. They occur both in numerical integration and in (some) integrable maps. However, they cannot be divergence-free, even if the vector field f is. Therefore we study series in all possible affine-invariant functions of f, which are called aromas. The simplest example is $f\nabla \cdot f$. Aromatic series arise in integrable maps, but, curiously, not yet directly in numerical integration. They form part of a larger object, the bicomplex of aromas, which allows us to construct and enumerate the divergence-free aromas.

Room: UR 1 | Tuesday 03:00pm - 03:30pm

Using discrete Darboux polynomials to detect and determine preserved measures and integrals of rational maps. Part I

Reinout Quispel

La Trobe University, Australia

Preservation of phase space volume (or more generally measure), first integrals (such as energy), and second integrals have been important topics in geometric numerical integration for more than a decade, and methods have been developed to preserve each of these properties separately [1]. Preserving two or more geometric properties simultaneously, however, has often been difficult, if not impossible. Then it was discovered that Kahan's 'unconventional' method seems to perform well in many cases [2,3,4]. Kahan himself, however, wrote: "I have used these unconventional methods for 24 years without quite understanding why they work so well as they do, when they work." The first approximation to such an understanding in computational terms was obtained in [4,5]: Kahan's method works so well because 1. It is very successful at preserving multiple quantities simultaneously,eg modified energy and modified measure. 2. It is linearly implicit 3. It is the restriction of a Runge-Kutta method However, point 1 above raises a further obvious question: Why does Kahan's method preserve both certain (modified) first integrals and certain (modified) measures? In this presentation we invoke Darboux polynomials to try and answer this question. The method of Darboux polynomials for ordinary differential equations was introduced by Darboux to detect rational integrals [6]. Very recently we have advocated the use of Darboux polynomials for discrete systems [7,8]. Darboux polynomials provide a unified theory for the preservation of polynomial measures and second integrals, as well as rational first integrals. In this new perspective the answer we propose to the above question is: Kahan's method works so well because it is good at preserving (modified) Darboux polynomials. If time permits we may discuss extensions to polarization methods [9]. This presentation will be spread over 2 talks. The first talk will be given by Reinout Quispel, and the second talk by Ben Tapley.

References:

[1] Hairer, Lubich & Wanner, Geometric Numerical Integration: Structure-preserving algorithms for ordinary differential equations, 2nd edition, Springer (2006).
[2] Kahan, Unconventional numerical methods for trajectory calculations, Unpublished lecture notes, 1993.
[3] Petrera, Pfadler & Suris, On integrability of Hirota-Kimura type discretizations, Regular and Chaotic Dynamics 16 (2011), 245–289.
[4] Celledoni, McLachlan, Owren & Quispel, Geometric properties of Kahan's method, J Phys. A 46 (2013), 025201.
[5] Celledoni, McLachlan, McLaren, Owren & Quispel, Integrability properties of Kahan's method, J. Phys. A 47 (2014), 365202.
[6] A nice introduction to Darboux polynomials, first integrals, second integrals of ODEs is given in: Goriely, Integrability and Nonintegrability of Dynamical Systems, World Scientific, Singapore, (2000) section 2.
[7] Celledoni, Evripidou, McLaren, Owren, Quispel & Tapley, Discrete Darboux polynomials and the search for preserved measures and integrals of rational maps, arxiv:1902.04685.
[8] Celledoni, Evripidou, McLaren, Owren, Quispel, Tapley & Van der Kamp, Using discrete Darboux polynomials to detect and determine preserved measures and integrals of rational maps, J Phys A 52 31LT01.
[9] Celledoni, McLachlan, McLaren, Owren & Quispel, Discretization of polynomial vector fields by polarization, Proc. R. Soc. A 471 (2015) 20150390, 10pp

Room: UR 1 | Tuesday 03:30pm - 04:00pm

Using discrete Darboux polynomials to detect and determine preserved measures and integrals of rational maps. Part II

Elena Celledoni[1], Charalampos Evripidou[2], David McLaren[2], Brynjulf Owren[1], Reinout Quispel[2], Benjamin Kwanen Tapley[1] and Peter van der Kamp[2]

[1]*Norwegian University of Science and Technology*
[2]*La Trobe University*

Preservation of phase space volume (or more generally measure), first integrals (such as energy), and second integrals have been important topics in geometric numerical integration for more than a decade, and methods have been developed to preserve each of these properties separately [1]. Preserving two or more geometric properties simultaneously, however, has often been difficult, if not impossible. Then it was discovered that Kahan's 'unconventional' method seems to perform well in many cases [2,3,4]. Kahan himself, however, wrote: "I have used these unconventional methods for 24 years without quite understanding why they work so well as they do, when they work." The first approximation to such an understanding in computational terms was obtained in [4,5]: Kahan's method works so well because 1. It is very successful at preserving multiple quantities simultaneously,eg modified energy and modified measure. 2. It is linearly implicit 3. It is the restriction of a Runge-Kutta method However, point 1 above raises a further obvious question: Why does Kahan's method preserve both certain (modified) first integrals and certain (modified) measures? In this presentation we invoke Darboux polynomials to try and answer this question. The method of Darboux polynomials for ordinary differential equations was introduced by Darboux to detect rational integrals [6]. Very recently we have advocated the use of Darboux polynomials for discrete systems [7,8]. Darboux polynomials provide a unified theory for the preservation of polynomial measures and second integrals, as well as rational first integrals. In this new perspective the answer we propose to the above question is: Kahan's method works so well because it is good at preserving (modified) Darboux polynomials. If time permits we may discuss extensions to polarization methods [9]. This presentation will be spread over 2 talks. The first part talk will be given by Reinout Quispel, and the second talk by Ben Tapley. References:
[1] Hairer, Lubich & Wanner, Geometric Numerical Integration: Structure-preserving algorithms for ordinary differential equations, 2nd edition, Springer (2006). [2] Kahan, Unconventional numerical methods for trajectory calculations, Unpublished lecture notes, 1993. [3] Petrera, Pfadler & Suris, On integrability of Hirota-Kimura type discretizations, Regular and Chaotic Dynamics 16 (2011), 245–289. [4] Celledoni, McLachlan, Owren & Quispel, Geometric properties of Kahan's method, J Phys. A 46 (2013), 025201. [5] Celledoni, McLachlan, McLaren, Owren & Quispel, Integrability properties of Kahan's method, J. Phys. A 47 (2014), 365202. [6] A nice introduction to Darboux polynomials, first integrals, second integrals of ODEs is given in: Goriely, Integrability and Nonintegrability of Dynamical Systems, World Scientific, Singapore, (2000) section 2. [7] Celledoni, Evripidou, McLaren, Owren, Quispel & Tapley, Discrete Darboux polynomials and the search for preserved measures and integrals of rational maps, arxiv:1902.04685. [8] Celledoni, Evripidou, McLaren, Owren, Quispel, Tapley & Van der Kamp, Using discrete Darboux polynomials to detect and determine preserved measures and integrals of rational maps, J Phys A 52 31LT01. [9] Celledoni, McLachlan, McLaren, Owren & Quispel, Discretization of polynomial vector fields by polarization, Proc. R. Soc. A 471 (2015) 20150390, 10pp

MS 09
Computational PDEs in cell biology

Room: HS 1

Friday 10:30am - 11:00am
Mariya Ptashnyk
Multiscale analysis and numerical simulations of signalling processes in biological tissues

Friday 11:00am - 11:30am
Christoph Haselwandter
The Mathematics of Mechanosensation

Friday 11:30am - 12:00pm
James Van Yperen
Numerical simulation of the Rice Blast fungus using curve shortening flow and reaction-diffusion on the curve

Room: HS 1 | Friday 10:30am - 11:00am

Multiscale analysis and numerical simulations of signalling processes in biological tissues

Mariya Ptashnyk[1] **and Chandrasekhar Venkataraman**[2]

[1] *Heriot-Watt University, United Kingdom*
[2] *University of Sussex, Brighton, United Kingdom*

In order to better understand development, growth and remodelling of biological tissues and organs a better understanding of interactions between cells in a tissue is required. Essential parts of communications between cells, as well as cell responses to external and internal stimuli, are governed by intercellular signalling processes. In this talk we consider derivation and analysis of mathematical models for cellular signalling processes on the level of a single cell. A coupled system of nonlinear bulk-surface partial differential equations is used to model the dynamics of signalling molecules in the inter- and intra-cellular spaces and of cell membrane receptors. Using multiscale analysis techniques we derive macroscopic two-scale model for signalling processes defined on the tissue level. Two-scale numerical method is developed and implemented for simulations of the macroscopic bulk-surface problem. The nonlinear coupling between microscopic and macroscopic scales induces formation of patterns in the dynamics of solutions of the macroscopic model for cellular signalling processes, which may correspond to heterogeneity in cellular response mechanisms.

Room: HS 1 | Friday 11:00am - 11:30am

The Mathematics of Mechanosensation

Christoph Haselwandter

University of Southern California, United States of America

The sense of touch is crucial for animal survival, and was already identified by Aristotle as one of the five fundamental senses. Yet, the molecular basis for mechanosensation in mammals is only beginning to be unraveled. Over the past few years it has been established that Piezo proteins underlie mechanosensation in a wide range of mammalian cells. Piezo is a membrane ion channel that gates open when mechanical force is applied to a cell membrane. How does Piezo transduce mechanical stimuli into electrical activity? Through membrane mechanical calculations, we show that the observed molecular structure of Piezo suggests a simple physical mechanism for how Piezo senses changes in cell membrane tension. We find that, in the absence of membrane tension, Piezo tends to locally curve the cell membrane into a minimal surface. The unique mathematical properties of this minimal surface amplify the sensitivity of Piezo to changes in membrane tension, rendering it exquisitely responsive. We assert that the shape of Piezo is an elegant example of molecular form evolved to optimize a specific function, in this case tension sensitivity.

Room: HS 1 | Friday 11:30am - 12:00pm

Numerical simulation of the Rice Blast fungus using curve shortening flow and reaction-diffusion on the curve

James Van Yperen and **Vanessa Styles**

Sussex, United Kingdom

The Rice Blast disease accounts for the annual losses of 11-18% of global rice yield. It is caused by the pathogen magnaporthe oryzae (Rice Blast fungus). Elements of its behaviour can be modelled using mean curvature flow coupled with a reaction-diffusion equation on the surface. We adapt a proposed 3D model to a 2D version in order to prove finite element error bounds for coupling of curve shortening flow with reaction-diffusion. We begin the talk with an introduction to the mechanics of the Rice Blast fungus we wish to model. We then review the mathematical machinery and literature used for the finite element method applied to curve shortening flow with prescribed normal contact to a fixed boundary. Finally we demonstrate our current model.

MS 10
Surface and geometric PDEs

Room: HS 1

Wednesday 10:30am - 11:00am
Christian Lubich
Convergence of an evolving finite element method for mean curvature flow

Wednesday 11:00am - 11:30am
Chandrasekhar Venkataraman
Lumped surface finite element methods for surface reaction diffusion systems

Wednesday 11:30am - 12:00pm
Ana Djurdjevac
PDEs on random hypersurafaces

Wednesday 12:00pm - 12:30pm
Hauke Sass
Space-Time Trace-FEM for Solving PDEs on Evolving Surfaces

Room: HS 1

Wednesday 10:30am - 11:00am

Convergence of an evolving finite element method for mean curvature flow

Balázs Kovács[1], **Christian Lubich**[1] **and Buyang Li**[2]

[1] *Univ. Tuebingen, Germany*
[2] *Hong Kong Polytechnic University*

Approximating the mean curvature flow by numerical methods was first addressed by Dziuk in 1990. He proposed a finite element method based on a weak formulation of the mean curvature flow as a (formally) heat-like partial differential equation, in which the moving nodes of the finite element mesh determine the approximate evolving surface. However, proving convergence of Dziuk's method or related evolving finite element methods for closed two-dimensional surfaces (or higher-dimensional hypersurfaces) has remained an open problem.
We here consider a different evolving finite element method for mean curvature flow of closed two-dimensional surfaces and prove optimal-order convergence over time intervals on which the evolving surface remains sufficiently regular. We study stability and convergence for both the finite element semi-discretization and the full discretization obtained with a linearly implicit backward difference time discretization. Our approach shares with Dziuk's method the property that the moving nodes of a finite element mesh determine the approximate evolving surface. However, the method presented here discretizes equations that are different from the equation discretized by Dziuk. In his approach, a weak formulation of the quasi-heat equation describing mean curvature flow is discretized, whereas in the present work evolution equations for the normal vector and the mean curvature are discretized, which then yield the velocity of the surface evolving under mean curvature flow. Evolution equations for geometric quantities on a surface evolving under mean curvature flow have been an important tool in the analysis of mean curvature flow ever since Huisken's 1984 paper , but apparently they have so far not been used in the numerical approximation of mean curvature flow.

Room: HS 1 | Wednesday 11:00am - 11:30am

Lumped surface finite element methods for surface reaction diffusion systems

Chandrasekhar Venkataraman

University of Sussex, United Kingdom

We consider the use of mass lumping in the surface finite element method for the approximation of semilinear systems of parabolic equations on surfaces. The approach allows us to prove discrete maximum principle type results for the discretised systems which in turn allows us to prove the existence of invariant regions for the discrete solutions through mimicking the analysis of the continuous systems. Throughout the talk, the analytical results presented will be supported by simulation results.

Room: HS 1 | Wednesday 11:30am - 12:00pm

PDEs on random hypersurafaces

Ana Djurdjevac[1], **Lewis Church**[2], **Charlie Elliott**[2], **Ralf Kornhuber**[3] **and Thomas Ranner**[4]

[1] *Technische Universität Berlin, Germany*
[2] *University of Warwick, UK*
[3] *FU Berlin, Germany*
[4] *University of Leeds, UK*

Most of the PDEs that appear in a mathematical modeling contain some uncertainty, which comes either from parameters or a domain. In particular, uncertainty in the geometry often appears in biological systems where PDEs are posed on an evolving curved domain.
We consider an abstract framework for PDEs posed on random hyepersur- faces. Utilizing the domain mapping method we transfer these problems into PDEs with random coefficients on a fixed domain. We present necessary geomet-ric analysis that is required for the pull-back analysis. For numerical analysis, we consider surface FEM coupled with a Monte Carlo sampling. The abstract results are applied to an elliptic problem on a random surface and a coupled elliptic bulk-surface system. Our theoretical convergence rates are confirmed by numerical experiments.
This work is supported by DFG through project AA1-3 of MATH^{+}.

Room: HS 1

Wednesday 12:00pm - 12:30pm

Space-Time Trace-FEM for Solving PDEs on Evolving Surfaces

Hauke Sass and Arnold Reusken

Rheinisch-Westfälische Technische Hochschule Aachen, Germany

We consider the parabolic equation

$$\begin{aligned} \dot{u} + (\mathrm{div}_{\Gamma(t)}\mathbf{w})u - \nu_d \Delta_\Gamma u = f \quad \text{on } \Gamma(t), \quad t \in (0,T], \\ u(x,0) = 0 \quad \text{on } \Gamma(0), \end{aligned}$$

posed on a smooth, closed and evolving surface $\Gamma(t)$, which is defined as the zero level of a level set function and is advected by a velocity field $\mathbf{w}$. Here, $\dot{u}$ denotes the material derivative. Based on a space-time weak formulation, we present a fully discrete Eulerian finite element method using DG in time and continuous in space finite elements. The zero level of the space-time linear approximation of the level set function defines a Lipschitz space-time manifold S_h, which approximates the evolving surface $\Gamma(t)$. Based on volumetric finite elements we use traces on S_h as trial and test surface FE-spaces for discretization.
In a setting with exact and smooth geometry first order error bounds in an energy norm are known to be valid. In recent work we analysed the effect of geometry approximation on the discretization error. A space-time volume normal stabilization is introduced that is crucial for optimal convergence and ensures better conditioning properties of the resulting discretization matrices. In the presentation we explain this space-time Trace-FEM and present results of numerical experiments. A few main results of the error analysis are also discussed.

MS 12: Part 1
Numerical methods for plasma physics

Room: UR 3

Tuesday 10:30am - 11:00am
Lukas Einkemmer
Algorithmic and computational advances for solving kinetic problems from plasma physics

Tuesday 11:00am - 11:30am
Matthias Wiesenberger
Reproducibility and elliptic grids – two numerical challenges for fusion plasma turbulence

Tuesday 11:30am - 12:00pm
Kaibo Hu
Structure-preserving finite element methods for MHD systems

Tuesday 12:00pm - 12:30pm
Katharina Kormann
Towards geometric particle-in-cell simulations of the Vlasov-Maxwell equations in curvilinear coordinates

Room: UR 3 | Tuesday 10:30am - 11:00am

Algorithmic and computational advances for solving kinetic problems from plasma physics

Lukas Einkemmer

University of Innsbruck, Austria

Plasma physics provides a number of challenging computational problems. This is, in particular, true for the kinetic equations considered in this talk. Kinetic equations are posed in an up to six-dimensional phase space. This poses a number of challenges, both for designing numerical methods and for implementing them efficiently on modern computer systems.
A deficiency of many of the commonly used numerical methods is that they are global in nature. As an alternative, we consider a conservative semi-Lagrangian discontinuous Galerkin method, which is competitive from an algorithmic standpoint. Moreover, it can be implemented with only local data accesses. This helps us to run these simulations on supercomputers as well as on graphic processing units (GPUs). One common theme of this talk will be to explore the interplay between designing algorithms and running them efficiently on modern computer hardware. In this context we also explore how we evaluate the performance of a numerical algorithm far away from the asymptotic regime, which is a fairly typical situation for the plasma physics simulations we have in mind.

Room: UR 3 | Tuesday 11:00am - 11:30am

Reproducibility and elliptic grids – two numerical challenges for fusion plasma turbulence

Matthias Wiesenberger[1], **Markus Held**[2], **Lukas Einkemmer**[3] **and Roman Iakymchuk**[4]

[1] *Department of Physics, Technical University of Denmark (DTU), Denmark*
[2] *Department of Space, Earth and Environment, Astronomy and Plasma Physics, Chalmers University of Technology, Gothenburg, Sweden*
[3] *Department of Mathematics, Universität Innsbruck, Austria*
[4] *Department of Computational Science and Technology, Royal Institute of Technology (KTH), Sweden*

In this contribution we present two of the main challenges we face in numerical simulations of plasma turbulence. First, we observe that our simulations are non-deterministic in a parallel computing environment. Even though we can restore reproducibility in code, point-wise convergence of our numerical algorithms is lost for longer simulation times. This raises the question how correct simulation behaviour can be ensured. We briefly discuss possible strategies like invariants of the system or reduced physical quantities of interest.
In a second part we investigate the numerical generation of elliptic structured grids that are aligned to the magnetic flux-function. We show that we can construct the coordinate transformation as well as its Jacobian up to machine precision with the help of streamline integration. The algorithm is derived from the underlying differential geometry formalism. Issues appear when the flux-function exhibits an X-point (a saddle point). We prove that orthogonal grids exist if and only if the Laplacian of the flux-function vanishes at the X-point. However, the solution to an elliptic equation converges with the correct order only if grid refinement is used around the X-point due to the diverging volume element.

Room: UR 3

Tuesday 11:30am - 12:00pm

Structure-preserving finite element methods for MHD systems

Kaibo Hu

University of Minnesota, United States of America

The magnetic Gauss law $\mathrm{div}B = 0$ plays an important role in the numerical simulation of magnetohydrodynamics (MHD) systems. We construct structure-preserving finite element methods which precisely preserve the magnetic Gauss law and the discrete energy law. Moreover, we discuss the discrete magnetic and cross helicity in the ideal limit. Continuous and discrete de Rham complexes and proper temporal discretization are crucial in the study of these schemes.

Room: UR 3

Tuesday 12:00pm - 12:30pm

Towards geometric particle-in-cell simulations of the Vlasov-Maxwell equations in curvilinear coordinates

Benedikt Perse[1,2], Katharina Kormann[1,2] and Eric Sonnendrücker[1,2]

[1] *Max Planck Institute for Plasma Physics, Germany*
[2] *Technical University of Munich, Germany*

A kinetic description of a plasma in external and self-consistent fields is given by the Vlasov equation for the particle distribution functions coupled to Maxwell's equation. Numerical schemes that preserve the structure of the kinetic equations can provide new insights into the long time behavior of fusion plasmas. An electromagnetic particle-in-cell solver for the Vlasov-Maxwell equations that preserves at the discrete level the non-canonical Hamiltonian structure of the Vlasov-Maxwell equations has been presented in [Kraus et al., J Plasma Phy 83, 2017]. While this original formulation has been obtained for Cartesian coordinates, we will explain in this talk how a coordinate transformation can be integrated into the semi-discrete Poisson structure. The final fully discrete scheme is obtained by applying an antisymmetric splitting of the Poisson matrix and by applying an average-vector-field discretization to the subsystems. Preliminary numerical results verify the conservation properties of the scheme for standard test cases.

MS 12: Part 2
Numerical methods for plasma physics

Room: UR 3

Tuesday 02:00pm - 02:30pm
Michael Kraus
Geometric Discontinuous Galerkin Methods for Fluids and Plasmas

Tuesday 02:30pm - 03:00pm
Nicolas Crouseilles
High order numerical methods for Vlasov-Maxwell equations

Tuesday 03:00pm - 03:30pm
Yajuan Sun
Particle in cell method for Vlasov-Poisson-Fokker-Planck system

Room: UR 3 | Tuesday 02:00pm - 02:30pm

Geometric Discontinuous Galerkin Methods for Fluids and Plasmas

Michael Kraus

Max Planck Institut for Plasma Physics, Germany

Most conservative problems in fluid dynamics, plasma physics as well as many other branches of science and engineering have the form of hyperbolic conservation laws that inhibit a Lagrangian and/or Hamiltonian structure. That is their dynamical equations can be obtained from an action principle or a Poisson bracket and a Hamiltonian functional, typically the total energy of the system. Non-conservative problems are usually composed of a conservative (Lagrangian or Hamiltonian) and a dissipative part. In both cases, it is important to preserve the structure of the conservative part in the course of discretisation in order to obtain stable numerical schemes that deliver accurate and reliable simulation results.

We discuss Lagrangian and Hamiltonian structure-preserving discretisation approaches based on high-order Discontinuous Galerkin Spectral Element Methods (DGSEM). We show how these approaches relate to and generalise known energy-stable schemes based on split-forms and summation-by-parts properties. The inviscid Burgers equation and the compressible Euler equations serve as main examples. Generalisations to other important fluid and plasma systems are sketched.

A remarkable property of the proposed approach is that exact mass, momentum and energy conservation can be achieved even if the system of equations is not cast in conservative form and momentum and energy do not explicitly appear as variables.

Room: UR 3 | Tuesday 02:30pm - 03:00pm

High order numerical methods for Vlasov-Maxwell equations

Nicolas Crouseilles

Inria, France

In this talk, high order splitting methods will be presented for the discretization of the Vlasov-Maxwell equations. In particular, the splitting enables to solve each subpart exactly in time (and with a spectral accuracy in phase space) and composition methods are used to design efficient fourth order method.

Room: UR 3 | Tuesday 03:00pm - 03:30pm

Particle in cell method for Vlasov-Poisson-Fokker-Planck system

Yajuan Sun

Academy of Mathematics and Systems Science, CAS, China, People's Republic of

Abstract:
In the plasma physics, it is important to study the problem on the effect of small-angle collisions on longitudinal plasma oscillations. To deal with the problem, it is required to solve the Vlasov-Poisson-Fokker-Planck (VPFP) system [1, 2]. In this talk, we study the corresponding Langevin equations in the framework of stochastic equivalence, and investigate its ergodicity. Combining particle-in-cell (PIC) technique, we verify the numerical ergodicity of numerical discretizations, and simulate the Landau damping and distribution function.

References.

[1] A. Lenard, I. B. Bernstein, Plasma Oscillations with Diffusion in Velocity Space, Phys. Rev. 112(5):1456-1459

[2] S. Jin, L. Wang, An asymptotic preserving scheme for the vlasov-poisson-fokker-planck system in the high field regime, Acta Math. Sci. 2011,31B(6):2219–2232

MS 13
Algebraic structures for numerical differential equations

Room: HS 2

Wednesday 10:30am - 11:00am
Nikolas E. Tapia M.
Algebraic aspects of signatures

Wednesday 11:00am - 11:30am
Fernando Casas
Continuous changes of variables and the Magnus expansion

Wednesday 11:30am - 12:00pm
Pranav Singh
Exploiting structure in the design of specialised splittings

Wednesday 12:00pm - 12:30pm
Charles Curry
Post-Lie Magnus expansion and Lie group integrators

Room: HS 2

Wednesday 10:30am - 11:00am

Algebraic aspects of signatures

Nikolas E. Tapia M.[1], **Kurusch Ebrahimi-Fard**[2] **and Joscha Diehl**[3]

[1] *TU Berlin/WIAS, Germany*
[2] *Norwegian University of Science and Technology, Norway*
[3] *Universität Greifswald, Germany*

Iterated-integrals signatures of smooth paths, introduced by K.T. Chen, and generalized by Lyons to finite p-variation paths for $p > 1$ (i.e. rough paths) are an important tool for studying solutions to a central class of controlled differential equations.
We present some of its combinatorial structures involved in practical computations, e.g. the BCH formula and the Magnus expansion. In a recent paper, together with J. Diehl and K. Ebrahimi-Fard, motivated by extraction of invariant features of time series, we introduced a discrete analogue of the Chen signature.
We review the similarities and differences between these two approaches, and describe the connection between the discrete-time approach and quasisymmetric functions.

Room: HS 2

Wednesday 11:00am - 11:30am

Continuous changes of variables and the Magnus expansion

Fernando Casas

Universitat Jaume I, Spain

The Magnus expansion constitutes nowadays a standard tool for obtaining both analytic and numerical approximations to the solution of non-autonomous linear differential equations. The generalization to arbitrary nonlinear differential equations requires typically as an intermediate stage the introduction of an operator equation, and so the procedure is different and more involved. In this talk we provide a unified framework to derive the Magnus expansion in a simpler way. This is possible by applying the continuous transformation theory developed by Dewar in 1976 in the context of perturbation theory of classical mechanics. In that setting, the Magnus series is shown to be just the generator of the continuous transformation sending the original differential equation to the trivial one.
This is a joint work with Philippe Chartier and Ander Murua.

Room: HS 2

Wednesday 11:30am - 12:00pm

Exploiting structure in the design of specialised splittings

Pranav Singh

University of Oxford, United Kingdom

Exponential splittings are Lie group methods where the flow under a vector field is approximated by a composition of flows under other vectors from the tangent bundle. In the context of autonomous linear (partial) differential equations, the flow is given by the matrix (operator) exponential. The most common examples of splittings for these equations are "classical splittings" where the exponential of A+B is approximated by various combinations of the exponentials of A and B. Computational advantages of splitting the exponential in this manner arise when the separate evaluation of the various exponentials of A and B is less expensive than the full exponential.
The computational ease of evaluating the exponential of a matrix, however, mostly depends on the structure and size of exponents. This raises the possibility of developing more efficient methods for approximating the exponential of A+B by utilising components in the tangent field other than A and B alone. In this talk, I will present concrete examples of such splittings for non-autonomous equations of quantum mechanics arising in laser-matter interaction and spin dynamics under the influence of external time-dependent controls. These splittings are specialised for the respective equations and are developed by exploiting the Lie algebraic and linear algebraic structures that arise therein.

Room: HS 2 | Wednesday 12:00pm - 12:30pm

Post-Lie Magnus expansion and Lie group integrators

Charles Curry

NTNU (Norwegian University of Science and Technology), Norway

We relate the classical and post-Lie Magnus expansions. Intertwining algebraic and geometric arguments allows us to place the classical Magnus expansion in the context of Lie group integrators. We then discuss the relevance of these results for numerical integration of differential equations on matrix Lie groups.

MS 14: Part 1
Numerical methods for rare events and applications

Room: HS 3

Monday 10:30am - 11:00am
Wei Zhang
Analysis of the first passage path ensemble of jump processes and connections with transition path theory

Monday 11:00am - 11:30am
Bo Lin
Computing committor functions for the study of rare events using deep learning

Monday 11:30am - 12:00pm
Samuel Francis Potter
Computing the quasipotential for nongradient SDEs in 3D

Monday 12:00pm - 12:30pm
Xiang Zhou
Generative Model based on Moving Mesh Method for Rare-event Simulation and Adaptivity in High Dim PDE

Room: HS 3 | Monday 10:30am - 11:00am

Analysis of the first passage path ensemble of jump processes and connections with transition path theory

Wei Zhang[1], **Max von Kleist**[2] **and Christof Schuette**[1,2]

[1] *Zuse Institute Berlin*
[2] *Free University Berlin*

The transition mechanism of jump processes between two different subsets in state space reveals important dynamical information of the processes and has attracted considerable attention in the past years. In this work, we study the first passage path ensemble of both discrete-time and continuous-time jump processes on a finite state space. The main approach is to divide each first passage path into nonreactive and reactive segments and to study them separately. The analysis can be applied to jump processes which are non-ergodic, as well as continuous-time jump processes where the waiting time distributions are non-exponential. In the particular case that the jump processes are both Markovian and ergodic, our analysis elucidates the relations between the study of the first passage paths and the study of the transition paths in transition path theory. This is a joint work with Max von Kleist and Christof Schuette.

Room: HS 3

Monday 11:00am - 11:30am

Computing committor functions for the study of rare events using deep learning

Qianxiao Li[2], **Bo Lin**[1] **and Weiqing Ren**[1]

[1]*National University of Singapore, Singapore*
[2]*Institute of High Performance Computing, A*STAR, Singapore*

The committor function is a central object in understanding transitions between metastable states in complex systems. It has a very simple mathematical description – it satisfies the backward Kolmogorov equation. However, computing the committor function for realistic systems at low temperatures is a challenging task, due to the curse of dimensionality and the scarcity of transition data. In this talk, I will present a computational approach that overcomes these issues and achieves good performance on complex benchmark problems with rough energy landscapes. The new approach combines deep learning, importance sampling and feature engineering techniques. This establishes an alternative practical method for studying rare transition events among metastable states of complex, high dimensional systems. The work was supported by Singapore MOE ACRF grants and NSF of China (No.11871365).

Room: HS 3 | Monday 11:30am - 12:00pm

Computing the quasipotential for nongradient SDEs in 3D

Samuel Francis Potter

University of Maryland Department of Computer Science

An ordered line integral method for computing the quasipotential in 3D is presented. The algorithm is based on a first-order Dijkstra-like semi-Lagrangian algorithm for solving the Hamilton-Jacobi equation. This work significantly enhances and promotes the previously developed 2D ordered line integral method to 3D by introducing a number of technical innovations. These include (i) a new hierarchical update strategy, (ii) a method of skipping updates based on constrained optimization theory, and (iii) pruning unnecessary updates by using a fast search. An extensive numerical study is conducted on linear and nonlinear examples where the quasipotential is available analytically or can be found by other methods. In particular, we apply the solver to Tao's examples in which transition states are hyperbolic periodic orbits, and to the genetic switch model of Lv et al.

Room: HS 3 | Monday 12:00pm - 12:30pm

Generative Model based on Moving Mesh Method for Rare-event Simulation and Adaptivity in High Dim PDE

Xiang Zhou and **Hongqiao Wang**

City University of Hong Kong, Hong Kong S.A.R. (China)

The generative model by transforming a simple distribution to a complicated target distribution is becoming popular and attractive due to the advance of deep neural network to represent the high dim map. In contrast to the traditional parametric mixture model as the linear combination of simple distributions, the generative model comprises a much richer family of candidate distributions. By learning the generative map from the data, with the aid of the neural network, this generative model has proven its power in various applications such as computer visions. Our work is to study the generative model in the context of applying to the importance sampling and the adaptivity in solving high dim PDE by using machine learning techniques. In contrast to the Monge-Ampere flow, our main approach is based on the harmonic map which is the foundation of many traditional moving mesh methods. We show how to design the monitor function so that the transformed random variable satisfies the target distribution in the importance sampling. Numerical examples are also included in the talk.

MS 14: Part 2
Numerical methods for rare events and applications

Room: HS 3

Monday 02:00pm - 02:30pm
Ling Lin
Quasi-Potential Calculation and Minimum Action Method for Limit Cycle

Monday 02:30pm - 03:00pm
Shuting Gu
Simplified Gentlest Ascent Dynamics for Saddle Points in Non-gradient systems

Monday 03:00pm - 03:30pm
Xiao-Ping Wang
Threshold dynamics for arbitrary anistropic surface energy

Room: HS 3 | Monday 02:00pm - 02:30pm

Quasi-Potential Calculation and Minimum Action Method for Limit Cycle

Ling Lin[1], **Haijun Yu**[2,3] **and Xiang Zhou**[4]

[1]*Sun Yat-sen University, China, People's Republic of*
[2]*University of Chinese Academy of Sciences, China, People's Republic of*
[3]*Academy of Mathematics and Systems Science, China, People's Republic of*
[4]*City University of Hong Kong, Hong Kong SAR*

We study the noise-induced escape from a stable limit cycle of a non-gradient dynamical system driven by a small additive noise. The fact that the optimal transition path in this case is infinitely long imposes a severe numerical challenge to resolve it in the minimum action method. We first consider the landscape of the quasi-potential near the limit cycle, which characterizes the minimal cost of the noise to drive the system far away form the limit cycle. We derive and compute the quadratic approximation of this quasi-potential near the limit cycle in the form of a positive definite solution to a matrix-valued periodic Riccati differential equation on the limit cycle. We then combine this local approximation in the neighborhood of the limit cycle with the minimum action method applied outside of the neighborhood. The neighborhood size is selected to be compatible with the path discretization error. By several numerical examples, we show that this strategy effectively improves the minimum action method to compute the spiral optimal escape path from limit cycles in various systems.

Room: HS 3 | Monday 02:30pm - 03:00pm

Simplified Gentlest Ascent Dynamics for Saddle Points in Non-gradient systems

Shuting Gu[1] **and Xiang Zhou**[2]

[1]*South China Normal University, China, People's Republic of*
[2]*City University of Hong Kong, Hong Kong, S.A.R.(China)*

The gentlest ascent dynamics (GAD) [W. E and X. Zhou, Nonlinearity 24, 1831 (2011)] is a time continuous dynamics to efficiently locate saddle points with a given index by coupling the position and direction variables together. These saddle points play important roles in the activated process of randomly perturbed dynamical systems. For index-1 saddle points in non-gradient systems, the GAD requires two direction variables to approximate, respectively, the eigenvectors of the Jacobian matrix and its transposed matrix. In the particular case of gradient systems, the two direction variables are equal to the single minimum mode of the Hessian matrix. In this note, we present a simplified GAD which only needs one direction variable even for non-gradient systems. This new method not only reduces the computational cost for the direction variable by half but also avoids inconvenient transpose operation of the Jacobian matrix. This is a joint work with Prof. Xiang Zhou.

Room: HS 3 | Monday 03:00pm - 03:30pm

Threshold dynamics for arbitrary anistropic surface energy

Xiao-Ping Wang

Hong Kong University of Science and Technology, Hong Kong S.A.R. (China)

The threshold dynamics (MBO) is an efficient algorithm to simulate mean curvature flow with isotropic surface tensions. It was also generalized to cases with anisotropic surface energy by replacing the Gaussian kernel with customized kernel.
We derive a threshold dynamics algorithm without changing the kernels. Unconditional stability and convergence are also established. Numerical examples are also presented.

Contributed Mini-Symposia

MS 21: Part 1
Numerical methods for stochastic (partial) differential equations

Room: HS 2

Thursday 10:30am - 11:00am
Michaela Szölgyenyi
Convergence order of the Euler-Maruyama scheme in dependence of the Sobolev regularity of the drift

Thursday 11:00am - 11:30am
Matthias Sachs
Hypercoercivity properties of adaptive Langevin dynamics

Thursday 11:30am - 12:00pm
Gabriel Stoltz
Hybrid Monte Carlo methods for sampling probability measures on submanifolds

Thursday 12:00pm - 12:30pm
Adrien Laurent
Multirevolution integrators for differential equations with fast stochastic oscillations

Room: HS 2

Thursday 10:30am - 11:00am

Convergence order of the Euler-Maruyama scheme in dependence of the Sobolev regularity of the drift

Andreas Neuenkirch[1], **Michaela Szölgyenyi**[2] **and Lukasz Szpruch**[3]

[1] *University of Mannheim, Germany*
[2] *University of Klagenfurt, Austria*
[3] *University of Edinburgh, Great Britain*

We study the strong convergence rate of the Euler-Maruyama scheme for scalar SDEs with additive noise and irregular drift. We provide a framework for the error analysis by reducing it to a weighted quadrature problem for irregular functions of Brownian motion. By analysing the quadrature problem we obtain for abitrarily small $\epsilon > 0$ a strong convergence order of $(1 + \kappa)/2 - \epsilon$ for a non-equidistant Euler-Maruyama scheme, if the drift has Sobolev-Slobodeckij-type regularity of order $\kappa \in (0, 1)$.

Room: HS 2

Thursday 11:00am - 11:30am

Hypercoercivity properties of adaptive Langevin dynamics

Matthias Sachs[1], **Gabriel Stoltz**[2] **and Benedict Leimkuhler**[3]

[1] *Duke University*
[2] *Université Paris-Est, CERMICS (ENPC)*
[3] *University of Edinburgh*

Adaptive Langevin dynamics is a method for sampling the Boltzmann–Gibbs distribution at prescribed temperature in cases where the potential gradient is subject to stochastic perturbation of unknown magnitude. The method replaces the friction in underdamped Langevin dynamics with a dynamical variable, updated according to a negative feedback loop control law as in the Nose–Hoover thermostat. Using a hypocoercivity analysis we show that the law of Adaptive Langevin dynamics converges exponentially rapidly to the stationary distribution, with a rate that can be quantified in terms of the key parameters of the dynamics. This allows us in particular to obtain a central limit theorem with respect to the time averages computed along a stochastic path. Our theoretical findings are illustrated by numerical simulations involving classification on the MNIST data set of handwritten digits using Bayesian logistic regression.

Room: HS 2 | Thursday 11:30am - 12:00pm

Hybrid Monte Carlo methods for sampling probability measures on submanifolds

Tony Lelievre[1], **Mathias Rousset**[2] **and** **Gabriel Stoltz**[1]

[1] *Ecole des Ponts and Inria, France*
[2] *Inria Rennes*

Probability measures supported on submanifolds can be sampled by adding an extra momentum variable to the state of the system, and discretizing the associated Hamiltonian dynamics with some stochastic perturbation in the extra variable. In order to avoid biases in the invariant probability measures sampled by discretizations of these stochastically perturbed Hamiltonian dynamics, a Metropolis rejection procedure can be considered. The so-obtained scheme belongs to the class of generalized Hybrid Monte Carlo (GHMC) algorithms. We show here how to generalize to GHMC a procedure suggested by Goodman, Holmes-Cerfon and Zappa for Metropolis random walks on submanifolds, where a reverse projection check is performed to enforce the reversibility of the algorithm for any timesteps and hence avoid biases in the invariant measure. We also provide a full mathematical analysis of such procedures, as well as numerical experiments demonstrating the importance of the reverse projection check on simple toy examples. We also illustrate the method in a high-dimensional case corresponding to computing the distribution of eigenvalues of random matrices with prescribed affine statistics on the empirical measure.

Room: HS 2 | Thursday 12:00pm - 12:30pm

Multirevolution integrators for differential equations with fast stochastic oscillations

Adrien Laurent and **Gilles Vilmart**

Université de Genève, Switzerland

We introduce a new methodology based on the multirevolution idea for constructing integrators for stochastic differential equations in the situation where the fast oscillations themselves are driven by a Stratonovich noise. Applications include in particular highly-oscillatory Kubo oscillators and spatial discretizations of the nonlinear Schrödinger equation with fast white noise dispersion. We construct a method of weak order two with computational cost and accuracy both independent of the stiffness of the oscillations. A geometric modification that conserves exactly quadratic invariants is also presented. Preprint available at: http://www.unige.ch/ alaurent

MS 21: Part 2
Numerical methods for stochastic (partial) differential equations

Room: HS 2

Thursday 02:00pm - 02:30pm
Andrea Barth
Solving elliptic equations with Levy-random-field coefficients

Thursday 02:30pm - 03:00pm
Erika Hausenblas
Coupled stochastic system for pattern formation

Thursday 03:00pm - 03:30pm
Ludovic Goudenège
Splitting scheme for stochastic partial differential equations

Thursday 03:30pm - 04:00pm
Andreas Petersson
Weak convergence of fully discrete finite element approximations of semilinear hyperbolic SPDE with additive noise

Room: HS 2

Thursday 02:00pm - 02:30pm

Solving elliptic equations with Levy-random-field coefficients

Andrea Barth

University of Stuttgart, Germany

Many phenomena in the Sciences and Engineering are modelled by dynamical systems with discontinuous parameters. If, moreover, the parameters are uncertain, a discontinuous random field or stochastic process should be used. The reduced regularity and the involved structure of these random fields lead to a more involved analysis, approximation and simulation of the stochastic dynamical system. When sampling-based methods are used to approximate statistical properties of the solution, the spacial (and/or temporal) discretization has to be adapted to the discontinuities, leading to a sample-adapted discretization. In this talk, I will give an introduction to the modelling of discontinuous random fields. For the approximation of moments of an elliptic problems with jump-diffusion coefficients, a sample-adapted multilevel Monte Carlo method is used. I will close the talk with some hints on how to solve the corresponding inverse problem involving deed neural networks.
This is based on joint work with Andreas Stein and Babak Maboudi Afkham.

Room: HS 2

Thursday 02:30pm - 03:00pm

Coupled stochastic system for pattern formation

Erika Hausenblas[1], **Mechthild Thalhammer**[2] **and Tsiry Avisoa Randrianasolo**[3]

[1] *Montanuniversitaet Leoben, Austria*
[2] *University of Innsbruck*
[3] *University of Bielefeld*

Mathematical models based on systems of reaction-diffusion equations provide fundamental tools for the description and investigation of various processes in biology, biochemistry, and chemistry; in a specific situation, an appealing characteristic of the arising nonlinear partial differential equations is the formation of patterns, reminiscent of those found in nature. The deterministic Gray–Scott equations constitute an elementary two-component system that describes autocatalytic reaction processes; depending on the choice of the specific parameters, complex patterns of spirals, waves, stripes, or spots appear.
In the derivation of a macroscopic model such as the deterministic Gray–Scott equations from basic physical principles, certain aspects of microscopic dynamics, e.g. fluctuations of molecules, are disregarded; an expedient mathematical approach that accounts for significant microscopic effects relies on the incorporation of stochastic processes and the consideration of stochastic partial differential equations.
In the talk, we present a theoretical and numerical study of the stochastic Gray–Scott equations driven by independent spatially time-homogeneous Wiener processes. Under suitable regularity assumptions on the prescribed initial states, existence, as well as the uniqueness of the solution processes, is proven. Numerical simulations based on the application of a time-adaptive first-order operator splitting method and the fast Fourier transform illustrate the formation of patterns in the deterministic case and their variation under the influence of stochastic noise.

Room: HS 2

Thursday 03:00pm - 03:30pm

Splitting scheme for stochastic partial differential equations

Ludovic Goudenège

CNRS, France

I will present a numerical method, based on splitting scheme, suitable for a special class of parabolic stochastic partial differential equations with non linearity. We will make the assumptions that we can prove moment estimates on the solution of SPDE with non-linear term, which is a classical result in case of globally Lipschitz non-linearity, and that we can solve explicitly the stochastic differential equation (without space differential operator) at a fixed space point. I will present the general idea to obtain strong and weak order and I will treat in particular the Allen-Cahn equation for which the weak order is 1/2 and the strong order 1/4.

Room: HS 2 | Thursday 03:30pm - 04:00pm

Weak convergence of fully discrete finite element approximations of semilinear hyperbolic SPDE with additive noise

Mihály Kovács[3], **Annika Lang**[1,2] and **Andreas Petersson**[1,2]

[1] *Chalmers University of Technology, Sweden*
[2] *University of Gothenburg, Sweden*
[3] *Pázmány Péter Catholic University, Hungary*

We consider the numerical approximation of the mild solution to a semilinear stochastic wave equation driven by additive noise. For the spatial approximation, we consider a standard finite element method and for the temporal approximation, a rational approximation of the semigroup of the mild solution. We first show strong convergence of this approximation in both a positive and a negative norm. With the help of Malliavin calculus techniques, this result is then used to deduce weak convergence rates for the class of twice continuously differentiable test functions with polynomially bounded derivatives. Under appropriate assumptions on the parameters of the equation, the weak rate is found to be essentially twice the strong rate. This extends earlier work by one of the authors to the semilinear setting. Numerical simulations illustrate the theoretical results.

MS 22: Part 1
Optimal control problems with ODEs and DAEs

Room: UR 1

Monday 10:30am - 11:00am
Roland Pulch
Sensitivity Analysis of Random Linear Dynamical Systems using Galerkin-Projections

Monday 11:00am - 11:30am
Christopher Schneider
Duality for Optimal Control Problems with Bang-Bang Solutions

Monday 12:00pm - 12:30pm
Simon Pirkelmann
Multi-sensor moving horizon estimation for autonomous ground vehicles

Room: UR 1 | Monday 10:30am - 11:00am

Sensitivity Analysis of Random Linear Dynamical Systems using Galerkin-Projections

Roland Pulch

Universität Greifswald, Germany

We consider linear systems of ordinary differential equations (ODEs), where parameters are substituted by random variables for uncertainty quantification. Our objective is a variance-based sensitivity analysis of the random output. The stochastic Galerkin-projection generates a larger linear system of ODEs with multiple outputs. Norms are associated to the system like the Hankel norm and Hardy norms, for example. We apply the system norms for different subsets of the outputs to define sensitivity coefficients, which are independent of the controls in the ODEs. We investigate the properties of these sensitivity measures. Furthermore, model order reduction by the balanced truncation technique allows for an efficient computation of the system norms with guaranteed a priori error bounds. We present results of numerical computations for a test example.

Room: UR 1 | Monday 11:00am - 11:30am

Duality for Optimal Control Problems with Bang-Bang Solutions

Christopher Schneider

Ernst-Abbe-Hochschule Jena, Germany

We consider the class of linear-quadratic optimal control problems, where the control variable appears linearly and is box-constrained. It is well-known that these problems typically have bang-bang or singular solutions. We assume that the solution is of bang-bang type and obtain the dual problem—which turns out to be non-smooth—guided by the methodology of Fenchel duality. Then we prove that strong duality and a saddle point property hold, which together ensure that the primal solution can be recovered from the dual solution. It will be shown that applying L^2-regularization to the primal problem translates to a smooth approximation of the cost functional for the dual problem. We also propose a discretization scheme for the dual problem and prove its convergence. Numerical experiments conclude the talk, where we demonstrate that significant computational savings can be achieved by solving the dual rather than the primal problem.

Room: UR 1 | Monday 12:00pm - 12:30pm

Multi-sensor moving horizon estimation for autonomous ground vehicles

Simon Pirkelmann

University of Bayreuth, Germany

In this talk we present an optimization based approach for estimating the position and velocity of a ground vehicle.
The vehicle has several on-board sensors available: a camera, an inertial measurement unit and wheel encoder discs. By its own none of these sensors is able to determine the full state of the vehicle, but by combining the measurements from all of the sensors a reliable estimation of the vehicles' trajectory becomes possible. To achieve this we apply moving horizon estimation (MHE) which takes into account the last N measurements of the sensors. The measurements are combined with the predicted movements of the vehicle described by a dynamical model in order to estimate the trajectory of the car that both fits the measurements and the model.
Our approach is tested on a real 1:10 scale RC car based on the Berkeley Autonomous Car Project (see: Gonzales, J., Zhang, F., Li, K., and Borrelli, F. (2016). Autonomous drifting using onboard sensors. In 13th International Symposium on Advanced Vehicle Control. (AVEC).)

MS 22: Part 2
Optimal control problems with ODEs and DAEs

Room: UR 1

Monday 02:00pm - 02:30pm
Gaby Albrecht
Optimal control of a two serotype dengue fever model with vaccination of seropositive humans

Monday 02:30pm - 03:00pm
Enrico Bertolazzi
PINS and indirect solver for Optimal Control Problems

Monday 03:00pm - 03:30pm
Kathrin Flaßkamp
Solving Optimal Control Problems by Structure-Exploiting Motion Planning

Monday 03:30pm - 04:00pm
Andreas Huber
Structure exploitation for fully discretized optimal control problems with simple vehicle models

Room: UR 1 | Monday 02:00pm - 02:30pm

Optimal control of a two serotype dengue fever model with vaccination of seropositive humans

Gaby Albrecht[1,2] **and Kurt Chudej**[1,2]

[1] *Lehrstuhl für Wissenschaftliches Rechnen, Universität Bayreuth, Germany*
[2] *MODUS- Forschungszentrum Modellierung und Simulation, Universität Bayreuth, Germany*

Dengue fever is a disease with about 390 Mio. cases per year (WHO, 2016). It is a vector borne disease which is transmitted by tiger mosquitoes. Though dengue fever is originally a tropical and subtropical disease the asian tiger mosquitoes spread across south Europe. In the Mediterranean area the tiger mosquito is already established and unfortunately self-preservative populations are already observed from Freiburg im Breisgau, Sinsheim and Heidelberg (in 2018). With the spread of the asian tiger mosquito is also an increasing danger of the Dengue fever associated. Due to the fact that a second infection can cause Dengue shock Syndrom (DSS), a severe form of the disease, we consider a new dengue fever model with a vaccination of seropositive humans. With adapted parameters to Europe we present numerical simulations and optimal control strategies in order to predict possible outbreak scenarios.

Room: UR 1 | Monday 02:30pm - 03:00pm

PINS and indirect solver for Optimal Control Problems

Enrico Bertolazzi and **Francesco Biral**

Department Of Industrial Engineering, University of Trento, Italy

PINS (Pins Is Not a Solver) is a software library for the fast prototype of Optimal Control Problem (OCP) solved by using the indirect method. PINS generates standalone C++ library that solves the optimal control problem you have defined. Then you can use this library from Matlab (via mex interface already provided), Octave, mruby, ruby, Lua, and of course C++. To generate the problem you need Maple from 2015 and XOptima a Maple Package that comes with PINS to define the OCP. The standard work flow is the following:

- In Maple you define the dynamic model and formulate the OCP, parameters values, guess (which can be symbolic), link with external library and so on.
- The problem so far defined is automatically coded in C++ and compiled and link to the solver. At the same time are generated, the interfaces for all the languages above cited and the data file to run and solve the problem.

Thus the problem formulation and setup is pretty automatic and you can use the language that you like to run it. It can be used both for off-line solution of optimal control problem and in MPC framework.

Room: UR 1 | Monday 03:00pm - 03:30pm

Solving Optimal Control Problems by Structure-Exploiting Motion Planning

Kathrin Flaßkamp and Christof Büskens

University of Bremen, Germany

Optimization problems for nonlinear control systems which are modeled by systems of ODEs or DAEs arise in many fields of applications, e.g. in robotics, automotive, or biomechanics. In nonlinear model predictive control (NMPC), numerical solutions have to be perpetually provided to adjust the control to current conditions; thus, computational efficiency plays an important role as well as practical relevance of a solution does. This talk presents a planning approach by motion primitives that goes back to Frazzoli et al., see [1].

Motion primitives, in particular trim primitives, are symmetry-induced motions that are chosen to quantize the system dynamics by a motion planning graph. Optimal solutions are approximated by motion primitive sequences. In practice, NMPC suffers from the locality of numerical solvers. Here, solution sequences can be used as an initial guess to overcome this issue. Recent results from [2] on the asymptotic stability of the MPC closed-loop of a mobile robot system are presented. Moreover, we discuss the optimality of trim primitives in terms of turnpike properties of ODE control systems (see [3]). The proposed approach is key to autonomous navigation systems, as we demonstrate via an example of autonomous ship navigation in harbors.

[1] Frazzoli, E., Dahleh, M., Feron, E.: Maneuver-based motion planning for nonlinear systems with symmetries. IEEE Transactions on Robotics 21(6), 1077–1091 (2005)

[2] Flaßkamp, K., Ober-Blöbaum, S., and Worthmann, K.: Symmetry and Motion Primitives in Model Predictive Control. ArXiv: 1906.09134. (2019)

[3] Faulwasser, T., Flaßkamp, K., Ober-Blöbaum, S., Worthmann, K.: Towards velocity turnpikes in optimal control of mechanical systems. In: Proc. 11th IFAC Symp. Nonlinear Control Systems (NOLCOS) (2019)

Room: UR 1

Monday 03:30pm - 04:00pm

Structure exploitation for fully discretized optimal control problems with simple vehicle models

Andreas Huber[1], **Matthias Gerdts**[1] **and Enrico Bertolazzi**[2]

[1] *Universität der Bundeswehr München, Germany*
[2] *University of Trento, Italy*

We investigate the structure of saddle-point matrices that are produced by fully discretized optimal control problems in an interior-point method. In particular we define a linear algebra solver to solve a reordered saddle-point matrix and compare the performance to the linear algebra solver MA57.
In a second step we apply the optimizer to simple vehicle models. The objective here is the calculation of an optimal raceline on a racetrack. In particular, this is achieved by the use of an MPC method on a moving horizon. The results are then analyzed in terms of online capability and compared to an online shooting method.

MS 23
Optimality conditions given by differential equations

Room: HS 3

Wednesday 10:30am - 11:00am
Natália da Costa Martins
A generalization of the variational problem of Herglotz: optimality conditions and conservation laws

Wednesday 11:00am - 11:30am
Luis Machado
A variational approach to generate interpolating curves in fluid environments

Wednesday 11:30am - 12:00pm
Ricardo Almeida
Calculus of variations with distributed-order fractional derivatives: analytical and numerical solutions

Wednesday 12:00pm - 12:30pm
Maria Isabel Cacao
Multidimensional orthogonal polynomials via Clifford algebras and some of their properties

Room: HS 3

Wednesday 10:30am - 11:00am

A generalization of the variational problem of Herglotz: optimality conditions and conservation laws

Natália da Costa Martins, Simão Pedro Silva Santos and Delfim Fernando Marado Torres

University of Aveiro, Portugal

We study, from an optimal control perspective, higher-order variational problems of Herglotz type with time delay. Main results are higher-order Euler-Lagrange and Dubois-Reymond necessary optimality conditions as well as higher-order first and second Noether theorems for delayed variational problems of Herglotz type.

References:

S. P. S. Santos, N. Martins and D. F. M. Torres, Noether's theorem for higher-order variational problems of Herglotz type, 10th AIMS Conference on Dynamical Systems, Dynamical Systems, Differential Equations and Applications, Vol. 2015, AIMS Proceedings, 2015, 990–999.

S. P. S. Santos, N. Martins and D. F. M. Torres, Higher-order variational problems of Herglotz with time delay, Pure and Applied Functional Analysis, 1 (2016), no. 2, 291–307.

S. P. S. Santos, N. Martins and D. F. M. Torres, Noether currents for higher-order variational problems of Herglotz type with time delay, Discrete and Continuous Dynamical Systems - Series S, (2018), 11(1): 91-102.

Room: HS 3

Wednesday 11:00am - 11:30am

A variational approach to generate interpolating curves in fluid environments

Luis Machado

University of Trás-os-Montes e Alto Douro & Institute of Systems and Robotics - Coimbra, Portugal

Dynamics of autonomous underwater or aerial vehicles are substantially affected by the vehicle's velocity and acceleration as well as by the resistance offered by the fluid environment to the moving vehicle. This resistance is characterized by a mechanical force called drag.
Our purpose here is to formulate trajectory planning on fluid environments as an optimization problem responsible for driving a vehicle from an initial position to a final target while minimizing acceleration and drag. The corresponding Euler-Lagrange equations will be derived. As we will see, the presence of the drag term increases substantially the complexity of the problem even when the problem is only posed on a Euclidean setting.
To tackle these hurdles, a numerical optimization approach based on the discretization of the cost functional will be proposed and some of the numerical illustrations for some special curved spaces will be provided.

Room: HS 3 | Wednesday 11:30am - 12:00pm

Calculus of variations with distributed-order fractional derivatives: analytical and numerical solutions

Ricardo Almeida

University of Aveiro, Portugal

In this work, we extend some fractional calculus of variations results by considering functionals depending on distributed-order fractional derivatives. Using variational techniques, we deduce optimal necessary conditions of Euler-Lagrange type. We also study the case where integral and holonomic constraints are imposed. Finally, a numerical procedure is given to solve some proposed problems.

Room: HS 3

Wednesday 12:00pm - 12:30pm

Multidimensional orthogonal polynomials via Clifford algebras and some of their properties

Maria Isabel Cacao

University of Aveiro, Portugal

Clifford algebras (or geometric algebras) unite the scalar and exterior product into a single invertible geometric product, which allows to deal in arbitrary dimensions with metric relations in Euclidean and non-Euclidean spaces. Simple examples are the complex numbers and the quaternions. Clifford algebras are widely applied in several areas of mathematics, physics and engineering, such as differential geometry, PDE, dynamical systems, control theory, computer vision and robotics. During the last decades some studies were concerned with orthogonal Clifford algebra-valued polynomials that can play an important role in several of those areas. In particular, we consider the work of R. Lavicka, where he constructed an orthogonal basis of polynomials with values in a Clifford algebra and we provide a three-term recursion formula and a second order differential equation for that orthogonal polynomial system, generalizing the classical case. Moreover, we show how the entire process of construction relies only on one and the same basic Appell sequence of polynomials, furnishing a more compact and easy computation process.

MS 24: Part 1
Theory and computation of nonlinear waves

Room: HS 3

Thursday 10:30am - 11:00am
Baofeng Feng
An integrable self-adaptive moving mesh method

Thursday 11:00am - 11:30am
Yong Chen
Constructing two-dimensional optimal system of the group invariant solutions

Thursday 11:30am - 12:00pm
Xiangke Chang
Integrable algorithms

Thursday 12:00pm - 12:30pm
Shun Sato
Linear gradient structures and discrete gradient methods for conservative/dissipative differential-algebraic equations

Room: HS 3

Thursday 10:30am - 11:00am

An integrable self-adaptive moving mesh method

Baofeng Feng

University of Texas RGV, United States of America

In this talk, we will firstly report our recent work on integrable discretizations for a class of soliton equations with hodograph transformations. Based on Hirota's bilinear method and reductions from the Kadomtsev-Petviashvili (KP) hierarchy, integrable discretizations are constructed for many soliton equations such as the Camassa-Holm equation, the short pulse equation and the reduced Ostrovsky equation. In the second part of the talk, we will show how these integrable discretizations can be successfully used as a self-adaptive moving mesh method for the numerical simulation of these PDEs.

Room: HS 3

Thursday 11:00am - 11:30am

Constructing two-dimensional optimal system of the group invariant solutions

Yong Chen

East China Normal University, China, People's Republic of

To search for inequivalent group invariant solutions of two-dimensional optimal system, a direct and systematic approach is established, which is based on commutator relations, adjoint matrix, and the invariants. The details of computing all the invariants for two-dimensional algebra are presented, which is shown more complex than that of one-dimensional algebra. The optimality of two-dimensional optimal systems is shown clearly for each step of the algorithm, with no further proof. To leave the algorithm clear, each stage is illustrated with a couple of examples: the heat equation and the Novikov equation. Finally, two-dimensional optimal system of the (2+1) dimensional Navier-Stokes (NS) equation is found and used to generate intrinsically different reduced ordinary differential equations. Some interesting explicit solutions of the NS equation are provided.

Room: HS 3

Thursday 11:30am - 12:00pm

Integrable algorithms

Xiangke Chang

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

Some intimate relations between certain numerical algorithms and integrable systems have been revealed in recent years. On the one hand, many algorithms in numerical analysis when considered as dynamical systems, have a variety of interesting dynamical behavior, such as integrability. On the other hand, some integrable equations can lead to new algorithms. In this talk, I will introduce some recent results on "Integrable algorithms".

Room: HS 3

Thursday 12:00pm - 12:30pm

Linear gradient structures and discrete gradient methods for conservative/dissipative differential-algebraic equations

Shun Sato

The University of Tokyo, Japan

As one of the most popular numerical methods for conservative/dissipative ordinary differential equations, the framework of the discrete gradient method has been intensively developed over recent decades. Although discrete gradients have been applied to several specific differential-algebraic equations (DAEs), no unified framework has yet been constructed. The class of such DAEs involves mechanical systems with some constraints and the spatial discretization of the evolutionary equations with a mixed derivative which often appear as models of the propagation of various waves. In this talk, we move toward the establishment of a framework for discrete gradient methods for DAEs, and introduces concepts including an appropriate linear gradient structure for DAEs. Then, we reveal that the simple use of discrete gradients does not imply the discrete conservation/dissipation laws. Fortunately, however, for the case of index-1 DAEs, an appropriate reformulation and a new discrete gradient enable us to successfully construct a novel scheme, which satisfies both of the discrete conservation/dissipation law and the constraint. This first attempt may provide an indispensable basis for constructing a unified framework of discrete gradient methods for DAEs.

MS 24: Part 2
Theory and computation of nonlinear waves

Room: HS 3

Thursday 02:00pm - 02:30pm
Zuonong Zhu
On discrete Hirota equation

Thursday 02:30pm - 03:00pm
Ji Lin
Soliton and periodic wave interaction solutions for sine-Gordon-type equations

Thursday 03:00pm - 03:30pm
Ruoxia Yao
Soliton solutions and n-fold Darboux transformations for a new nonlocal Alice-Bob system

Thursday 03:30pm - 04:00pm
Changzheng Qu
Stability of Peakons to Novikov-type equations

Room: HS 3

Thursday 02:00pm - 02:30pm

On discrete Hirota equation

Zuonong Zhu

Shanghai Jiao Tong University, People's Republic of China

In this talk, we will address the topic that how to get the integrability of the Hirota equation from the integrability of a space discrete Hirota equation. This is a joint work with A. Pickering and H.Q. Zhao.

Room: HS 3

Thursday 02:30pm - 03:00pm

Soliton and periodic wave interaction solutions for sine-Gordon-type equations

Ji Lin

Zhejiang Normal University, China, People's Republic of

The Backlund transformation(BT) of the mKdV-sG equation is constructed by introducing a new transformation. Many nonlocal symmetries are obtained in terms of its BT. The soliton-periodic wave interaction solutions are explicitly derived by the classical Lie-group reduction method. Particularly, some special concrete soliton and periodic wave interaction solutions and their behaviours are discussed both in analytical and graphical ways., We also investigated soliton- periodic wave solutions of (2+1)-dimensional Sine-Gordon type equations

Room: HS 3

Thursday 03:00pm - 03:30pm

Soliton solutions and n-fold Darboux transformations for a new nonlocal Alice-Bob system

Ruoxia Yao[1], **Yali Shen**[1] **and Zhibin Li**[2]

[1] *Shaanxi Normal University, Xi'an, Shaanxi, China, People's Republic of*
[2] *Eash China Normal University, Shanghai, China, PR China*

Motivated by the increasing desire to understand many events happened at different space-times in natural and social sciences and usually entangled or correlated closely can be described by using nonlocal Alice and Bob systems. In this paper, a new such kind of nonlinear Schrödinger equation (AB-NLS) derived from the well-known AKNS system is investigated, which is a new real integrable two-place system. We investigate not only the bilinear Bäcklund transformation for the unreduced AB-NLS by the bilinear method, but also the n-fold Darboux transformation for the reduced AB-NLS. Armed with them we present several kinds of nonlinear waves for the nonlocal AB-NLS, which are quite different from that of the NLS equation.

Room: HS 3

Thursday 03:30pm - 04:00pm

Stability of Peakons to Novikov-type equations

Changzheng Qu

Ningbo University, China, People's Republic of

In this talk, orbital stability of peaked solitons for the Novikov equation and its multi-component generalizations are investigated. First, the integrability and conservation laws to these equations are studied. Second, it is shown that these equations admit single and multi-peaked solitons on the real line $\mathbb{R}$, and multi-periodic peaked solitons on $\mathbb{S}$. Finally, we verify that these solitons are orbitally stable under small perturbations in the energy space.

MS 25
Rosenbrock-Wanner-type methods: theory and applications

Room: HS 2

Friday 10:30am - 11:00am
Paul Tranquilli
Adaptive Rosenbrock-Krylov Methods

Friday 11:00am - 11:30am
Domingo Hernández-Abreu
Convergence of one-stage AMF-W-methods for parabolic problems.

Friday 11:30am - 12:00pm
Soledad Perez-Rodriguez
Refined AMF-W-methods on multidimensional problems with applications to SABR/LIBOR market models

Room: HS 2

Friday 10:30am - 11:00am

Adaptive Rosenbrock-Krylov Methods

Paul Tranquilli

Lawrence Livermore National Laboratory, United States of America

The Rosenbrock-Krylov family of time integrators is an extension of Rosenbrock-W methods which employ a specific Krylov based approximation of the linear systems present within each stage of the integrator. Here we will briefly introduce Rosenbrock-Krylov methods, and discuss recent developments towards fully adaptive schemes. These adaptive Rosenbrock-Krylov methods show substantial improvements in computational efficiency relative to prior implementations.

Room: HS 2

Friday 11:00am - 11:30am

Convergence of one-stage AMF-W-methods for parabolic problems.

Severiano González-Pinto[1]**, Ernst Hairer**[2] **and Domingo Hernández-Abreu**[1]

[1] *Universidad de La Laguna, Spain*
[2] *Université de Genève, Switzerland*

In this talk we shall consider a convergence analysis for one-stage W-methods, endowed with the splitting provided by the Approximate Matrix Factorization (AMF), when they are applied to parabolic problems with linear diffusion terms on a rectangular domain in an arbitrary number of spatial dimensions $m \geq 2$ discretized in space by means of Finite Differences.
The global error analysis is carried out both for the Euclidean ℓ_2 norm and the maximum ℓ_∞ norm, and optimal bounds are obtained under a mild and realistic assumption on the time stepsize and the spatial grid size. In particular, for the second order one-stage W-method, order two (in time and space) in both norms is proved in case of time-independent Dirichlet boundary conditions. For time-dependent boundary conditions, the order of convergence is nearly two in the ℓ_2-norm when $m \geq 2$, whereas an order reduction to order one in the ℓ_∞ norm occurs for $m \geq 3$. Numerical experiments illustrating these theoretical results will be presented.

Room: HS 2 | Friday 11:30am - 12:00pm

Refined AMF-W-methods on multidimensional problems with applications to SABR/LIBOR market models

Soledad Perez-Rodriguez[1], Jose German Lopez-Salas[2] and Carlos Vazquez[2]

[1] *Universidad de La Laguna, Spain*
[2] *Universidade da Coruña, Spain*

In [3] the authors proposed a new approach based a PDE formulation for the pricing of interest rate derivatives with SABR/LIBOR market models. These stochastic volatility models describe interest rate dynamics and are intended for pricing interest rate derivatives after their calibration to real market data. In particular, the work [3] focus on the multi-dimensional Mercurio & Morini model that was shown to perform better than other alternative ones in terms of the balance between pricing computational cost and market fitting [1]. In order to solve numerically the resulting PDE and to reduce the high computational cost involved when more than two underlying forward LIBOR rates are considered, they applied a space-time discretization by using standard finite differences schemes on sparse grids with the so-called combination technique.
In this work, we propose an alternative Method of Lines (MoL) approximation to the solution of the Mercurio & Morini PDE model, where firstly a spatial semi-discretization with finite differences is carried out on the same spatial grid as in [3] and then a Refined AMF-W-method (AMF-R-W-method) [2] for the time-integration of the resulting initial value problem is applied. As can be seen in [2], AMF-R-W-methods are a particular type of W-methods that can be selected to be unconditionally stable on linear problems with constant coefficients regardless of the spatial dimension of the PDE. Moreover, AMF-R-W-methods reduce severely the computational cost due to their efficient approximation of the mixed derivative terms in the PDE. Furthermore, in order to tackle high dimensional problems a merging with a sparse grid combination technique will be studied as well.
Finally, we present examples to illustrate the convergence order and efficiency tests of this new sparse AMF-type W-method to be compared with the ones given in [3] and the alternative classical costly Monte Carlo simulations, when the payoff of the derivative depends on a moderate number of LIBOR forward rates.

References

[1] A.M. Ferreiro, J.A. García, J.G. López-Salas, C. Vázquez, *SABR/LIBOR market models: Pricing and calibration for some interest rate derivatives*, Appl. Math. Comput. 242 (2014) 65–89.
[2] S. González-Pinto, E. Hairer, D. Hernández-Abreu, S. Perez-Rodríguez, *AMF-type W-methods for parabolic problems with mixed derivatives*, SIAM J. Sci. Comput., 40 (5) (2018), A2905- A2929.
[3] J.G. López-Salas, C. Vázquez. *PDE formulation of some SABR/LIBOR market models and its numerical solution with a sparse grid combination technique.* Comput. Math. Appl., 75 (2018), 1616-1634.

MS 26: Part 1
Numerical approximation of stochastic systems

Room: SR 3

Tuesday 10:30am - 11:00am
Carlos Mora
A stable numerical scheme for stochastic differential equations with multiplicative noise

Tuesday 11:00am - 11:30am
Gilles Vilmart
Accelerated convergence to equilibrium and reduced asymptotic variance for Langevin dynamics using Stratonovich perturbations

Tuesday 11:30am - 12:00pm
Juan Carlos Cortés
Approximating the probability density function of random differential equations using numerical schemes:

Tuesday 12:00pm - 12:30pm
David Cohen
Drift-preserving numerical integrators for stochastic Hamiltonian systems

Room: SR 3

Tuesday 10:30am - 11:00am

A stable numerical scheme for stochastic differential equations with multiplicative noise

Carlos Mora

Universidad de Concepción, Chile

We present the direction and norm decomposition method, a new approach for designing numerical schemes for stochastic differential equations (SDEs). We approximate the solution X_t, of the SDE under study, by solving numerically the system of coupled SDEs that describes the evolution of the norm of X_t and its projection on the unit sphere. This yields an explicit scheme for stiff SDEs with multiplicative noise that shows a very good performance in various numerical experiments. Under general hypotheses, the new numerical scheme preserves the almost sure stability of the solutions for any step-size, as well as the property of being distant from 0. The talk is based on the paper " C. M. Mora, H. A. Mardones, J.C. Jimenez, M. Selva, R. Biscay (2017) A stable numerical scheme for stochastic differential equations with multiplicative noise. SIAM Journal on Numerical Analysis Vol. 55, 1614–1649".

Room: SR 3

Tuesday 11:00am - 11:30am

Accelerated convergence to equilibrium and reduced asymptotic variance for Langevin dynamics using Stratonovich perturbations

Assyr Abdulle[1], Grigorios A. Pavliotis[2] and Gilles Vilmart[3]

[1] *Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland*
[2] *Imperial College London, UK*
[3] *University of Geneva, Switzerland*

We propose a new approach for sampling from probability measures in, possibly, high dimensional spaces. By perturbing the standard overdamped Langevin dynamics by a suitable Stratonovich perturbation that preserves the invariant measure of the original system, we show that accelerated convergence to equilibrium and reduced asymptotic variance can be achieved, leading, thus, to a computationally advantageous sampling algorithm. The new perturbed Langevin dynamics is reversible with respect to the target probability measure and, consequently, does not suffer from the drawbacks of the nonreversible Langevin samplers that were introduced in [C.-R. Hwang, S.-Y. Hwang-Ma, and S.-J. Sheu, Ann. Appl. Probab. 1993] and studied in, e.g. [T. Lelievre, F. Nier, and G. A. Pavliotis J. Stat. Phys., 2013] and [A. B. Duncan, T. Lelievre, and G. A. Pavliotis J. Stat. Phys., 2016], while retaining all of their advantages in terms of accelerated convergence and reduced asymptotic variance. In particular, the reversibility of the dynamics ensures that there is no oscillatory transient behaviour.
Preprints available at: http://www.unige.ch/ vilmart

Room: SR 3 | Tuesday 11:30am - 12:00pm

Approximating the probability density function of random differential equations using numerical schemes:

Julia Calatayud, Juan Carlos Cortés and Marc Jornet

Universitat Politècncia de València, Spain

In this contribution, we will present a computational approach to approximate the probability density function of random di fferential equations. The technique is based on the combination of the so called Random Variable Transformation technique and random finite di fference schemes. We will illustrate how to obtain reliable approximations of the first probability density function of the solution stochastic process to Poisson-type random differential equation whose reaction coefficient and boundary conditions are random variables. The theoretical results will be illustrated via several numerical experiments.

Room: SR 3 | Tuesday 12:00pm - 12:30pm

Drift-preserving numerical integrators for stochastic Hamiltonian systems

David Cohen

Umeå University, Sweden

The subject of the presentation is the study of numerical discretisations for separable Hamiltonian systems with additive noise. For such problems, the expected value of the total energy, along the exact solution, drifts linearly with time. We present and analyze a time integrator having the very same property for all times.
This is an ongoing work with Chuchu Chen (CAS), Raffaele D'Ambrosio (UNIVAQ), Annika Lang (Chalmers).

MS 26: Part 2
Numerical approximation of stochastic systems

Room: SR 3

Tuesday 02:00pm - 02:30pm
Xiaoying Han
Explicit schemes for stiff chemical Langevin equations via computational singular perturbation

Tuesday 02:30pm - 03:00pm
Ibrahim Almuslimani
Explicit stabilized integrators for stiff and ergodic SDEs, and stiff optimal control problems

Tuesday 03:00pm - 03:30pm
Raffaele D'Ambrosio
Nonlinear stability issues for stochastic multistep methods

Tuesday 03:30pm - 04:00pm
Hugo de la Cruz
Numerical schemes for the integration of stochastic advection equations

Room: SR 3

Tuesday 02:00pm - 02:30pm

Explicit schemes for stiff chemical Langevin equations via computational singular perturbation

Xiaoying Han[1], **Mauro Valorani**[2] **and Habib Najm**[3]

[1] *Auburn University, United States of America*
[2] *Sapienza University Rome, Italy*
[3] *Sandia National Laboratories, United States of America*

An explicit time-scale splitting algorithm for stiff chemical Langevin equations (CLEs) is developed, based on computational singular perturbation. The drift term of the CLE is projected onto basis vectors that span the fast and slow subspaces. The corresponding fast modes exhaust quickly, in the mean sense, and the system state then evolves, with a mean drift controlled by slow modes, on a random manifold. The drift-driven time evolution of the state due to fast exhausted modes is modeled algebraically as an exponential decay process, while that due to slow drift modes and diffusional processes is integrated explicitly. This allows stable explicit time integration step sizes larger than those required by typical explicit numerical methods for stiff stochastic differential equations. The algorithm is highlighted, and is illustrated on a model system.

Room: SR 3 | Tuesday 02:30pm - 03:00pm

Explicit stabilized integrators for stiff and ergodic SDEs, and stiff optimal control problems

Assyr Abdulle[1], **Ibrahim Almuslimani**[2] **and Gilles Vilmart**[2]

[1] *École polytechnique fédérale de Lausanne (EPFL)*
[2] *University of Geneva, Switzerland*

Explicit stabilized Runge-Kutta methods are efficient for solving stiff (deterministic or stochastic) differential equations in large dimensions.
In the first part of the talk, we present a new explicit stabilized scheme of weak order one for stiff and ergodic stochastic differential equations (SDEs). In the absence of noise, the new method coincides with the classical deterministic stabilized scheme (or Chebyshev method) for diffusion dominated advection-diffusion problems and it inherits its optimal stability domain size, in contrast to known existing methods for mean-square stable stiff SDEs. In addition, the new method can be used to sample the invariant measure of a class of ergodic SDEs, and combined with postprocessing techniques of geometric numerical integration originally from the deterministic literature, it achieves a convergence rate of order two at a negligible overcost.
In the second part of the talk, we show how an explicit stabilized method for deterministic optimal control can be derived inspired by these results.

[1] A. Abdulle, I. Almuslimani, and G. Vilmart, Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations, SIAM/ASA J. Uncertain. Quantif. 6 (2018), no. 2, 937–964.
[2] I. Almuslimani and G. Vilmart, Explicit stabilized methods for stiff optimal control problems, in preparation.

Room: SR 3 | Tuesday 03:00pm - 03:30pm

Nonlinear stability issues for stochastic multistep methods

Raffaele D'Ambrosio[1] **and Evelyn Buckwar**[2]

[1] *University of L'Aquila, Italy*
[2] *Johannes Kepler University of Linz*

We analyze conservation properties of numerical methods for nonlinear stochastic differential equations (SDEs), hidden behind proper conditional stability issues. We study the numerical approximation of nonlinear SDEs of Ito type with an exponential mean-square contractive behaviour by stochastic linear multistep methods, in order to provide stepsize restrictions ensuring similar exponential mean-square properties also numerically, without adding further constraints on the numerical method itself. A selection of numerical experiments confirms the sharpness of the estimates.

Room: SR 3

Tuesday 03:30pm - 04:00pm

Numerical schemes for the integration of stochastic advection equations

Hugo de la Cruz[1] **and Christian Olivera**[2]

[1] *School of Applied Mathematics. FGV/EMAp, Brazil*
[2] *University of campinas. IMECC, Brazil*

The integration of stochastic advection equation is considered. We propose numerical schemes for the effective simulation of trajectories of the solution of this equation in the case of regular and irregular coefficients. Results on the convergence of the suggested schemes and details on their efficient implementation are presented. The performance of the introduced methods is illustrated through computer simulations.

MS 27: Part 1
Stability issues for stochastic, implicit-explicit, and parallel initial value problem solvers

Room: UR 3

Monday 10:30am - 11:00am
Evelyn Buckwar
A numerical investigation of the stochastic FitzHugh-Nagumo model

Monday 11:00am - 11:30am
Severiano González-Pinto
About the power-boundedness of stability mappings appearing in the time integration of parabolic PDEs

Monday 11:30am - 12:00pm
Gabriel; Campbell Lord
Adapting for stability of the numerical solution of SPDEs

Monday 12:00pm - 12:30pm
Catalin Trenchea
BOundary update via resolvent for fluid-structure interaction

Room: UR 3 | Monday 10:30am - 11:00am

A numerical investigation of the stochastic FitzHugh-Nagumo model

Evelyn Buckwar

Johannes Kepler University Linz, Austria

The stochastic FitzHugh Nagumo model is a two-dimensional nonlinear stochastic differential equation with additive noise. It models the firing activity of a single neuron in the brain, where its first component describes the membrane potential of the neuron at time t and the second component corresponds to a recovery variable modeling the channel kinetics. The driving noise is a standard Wiener process only acting on the second component The model includes a parameter corresponding to a time scale separation. We first discuss several properties and issues arising with standard numerical methods, such as the Euler-Maruyama method and an order 1.5 Taylor scheme and then present a reliable splitting approach. This is joint work with Adeline Samson, Irene Tubikanec and Massimiliano Tamborrino.

Room: UR 3 | Monday 11:00am - 11:30am

About the power-boundedness of stability mappings appearing in the time integration of parabolic PDEs

Severiano González-Pinto[1], **Ernst Hairer**[2] **and Domingo Hernández-Abreu**[1]

[1] *University of La Laguna, Spain*
[2] *University of Geneve, Switzerland*

When splitting methods are applied to the time integration of ODEs $\dot{U}(t) = (\sum_{j=1}^{m} A_j)U(t) + g(t)$, stemming from the space semi-discretization of m-dimensional linear parabolic PDE problems, the uniform boundedness of the stability mapping $\|R(\tau A_1, \ldots, \tau A_m)^n\|$, $n = 1, 2, \ldots$, independent of the dimensions of the matrices A_j and of the time step-size $\tau > 0$, plays an essential role to get convergence results in PDE sense. In this talk, we address the study of those uniform bounds in case of the ℓ_2-norm and the uniform norm. This meets direct applications in the PDE convergence analysis of Douglas-type methods, Stabilizing correction methods or AMF-W-methods. Uniform bounds for the ℓ_2-norm have been known since the sixties but that is not the case of the uniform norm.

Room: UR 3 | Monday 11:30am - 12:00pm

Adapting for stability of the numerical solution of SPDEs

Gabriel Lord[1,2] **and Stuart Campbell**[1]

[1] *Heriot-Watt University, Edinburgh, UK*
[2] *Radboud University, Nijmegen, NL*

We consider a stochastically forced PDE with a nonlinear term that only satisfies a one-sided Lipschitz condition. The standard fixed uniform step methods for this case are known not to converge strongly in general. However, we show that by adapting the time step we can obtain strong convergence of Euler-Maruyama type integrators and that adapting the time step leads to more efficient methods.

Room: UR 3

Monday 12:00pm - 12:30pm

BOundary update via resolvent for fluid-structure interaction

Catalin Trenchea[1] and **Martina Bukac**[2]

[1] *University of Pittsburgh, United States of America*
[2] *University of Notre Dame, United States of America*

We propose a *BOundary Update using Resolvent* (BOUR) partitioned method, second-order accurate in time, unconditionally stable, for the interaction between a viscous, incompressible fluid and a thin structure. The method is algorithmically similar to the sequential Backward Euler - Forward Euler implementation of the midpoint discretization scheme. (i) The structure and fluid sub-problems are first solved using a Backward Euler scheme, (ii) the velocities of fluid and structure are updated on the boundary via a second-order consistent resolvent operator, and then (iii) the structure and fluid sub-problems are solved again, using a Forward Euler scheme. The stability analysis based on energy estimates shows that the scheme is unconditionally stable. Error analysis of the semi-discrete problem yields second-order convergence in time. The two numerical examples confirm the theoretical convergence analysis results and show an excellent agreement of the proposed partitioned scheme with the monolithic scheme.

MS 27: Part 2
Stability issues for stochastic, implicit-explicit, and parallel initial value problem solvers

Room: UR 3

Monday 02:00pm - 02:30pm
Andrew Steyer
HEVI time-stepping with the IMKG family of IMEX Runge-Kutta methods

Monday 02:30pm - 03:00pm
Conall Kelly
Pathwise stability for the explicit discretisation of nonlinear SDEs with stochastically stabilising diffusion

Monday 03:00pm - 03:30pm
Fandi Sun
Strong convergence of an adaptive time-stepping Milstein method for SDEs with one-sided Lipschitz drift

Monday 03:30pm - 04:00pm
David Shirokoff
Unconditional stability theory for multistep ImEx schemes, and implications for fluid solvers

Room: UR 3

Monday 02:00pm - 02:30pm

HEVI time-stepping with the IMKG family of IMEX Runge-Kutta methods

Andrew Steyer[1], **Christopher Vogl**[2], **Mark Taylor**[1] **and Oksana Guba**[1]

[1]*Sandia National Laboratories, USA*
[2]*Lawrence Livermore National Laboratory, USA*

We derive and analyze the IMKG family of implicit-explicit (IMEX) Runge-Kutta methods for horizontally explicit vertically implicit (HEVI) time-stepping in nonhydrostatic atmosphere models. In HEVI time-stepping, the governing equations for atmospheric flow are partitioned into a stiff term corresponding to vertical acoustic wave propagation, and a nonstiff term corresponding to advection and horizontal acoustic wave propagation. We employ a specialized 3D stability function to characterize the stability of IMEX methods for HEVI time-stepping. Based on this characterization, the IMKG methods we derive are empirically shown to have superior stability properties in the HOMME-NH atmsophere model compared to other IMEX Runge-Kutta methods from the literature.

Room: UR 3

Monday 02:30pm - 03:00pm

Pathwise stability for the explicit discretisation of nonlinear SDEs with stochastically stabilising diffusion

Conall Kelly[1], **Alexandra Rodkina**[2] **and Eeva Maria Rapoo**[3]

[1] *University College Cork, Ireland*
[2] *The University of the West Indies, Mona, Kingston, Jamaica*
[3] *The University of South Africa, Johannesburg, South Africa*

We consider the use of adaptive timestepping to allow a strong explicit Euler-Maruyama discretisation to reproduce dynamical properties of a class of nonlinear stochastic differential equations with a unique equilibrium solution and non-negative, non-globally Lipschitz coefficients. Solutions of such equations may display a tendency towards explosive growth, countered by a sufficiently intense and nonlinear diffusion. We construct an adaptive timestepping strategy which closely reproduces the almost sure (a.s.) asymptotic stability and instability of the equilibrium, and which can ensure the positivity of solutions with arbitrarily high probability.

Room: UR 3

Monday 03:00pm - 03:30pm

Strong convergence of an adaptive time-stepping Milstein method for SDEs with one-sided Lipschitz drift

Conall Kelly[1], **Gabriel Lord**[2,3] and **Fandi Sun**[3]

[1]*School of Mathematical Sciences, University College Cork, Ireland*
[2]*Department of Mathematics, IMAPP, Radboud University, Netherlands*
[3]*Department of Mathematics, MACS, Heriot-Watt University, United Kingdom.*

Traditional methods for the numerical solution of SDEs rely on a global Lipschitz condition on the drift and/or diffusion term. This restriction can be overcome by using adaptive time step based methods. With no commutativity condition, we investigated the strong convergence rate of the adaptive Milstein with non-globally Lipschitz drift to be 1 with certain computational efficiency. Typical applications are from computational neuroscience or from mathematical finance.

Room: UR 3

Monday 03:30pm - 04:00pm

Unconditional stability theory for multistep ImEx schemes, and implications for fluid solvers

David Shirokoff[1], **Benjamin Seibold**[2], **Rodolfo Ruben Rosales**[3] **and Dong Zhou**[4]

[1]*New Jersey Institute of Tech, United States of America*
[2]*Temple University, United States of America*
[3]*Massachusetts Institute of Technology, United States of America*
[4]*California State University, Los Angeles, United States of America*

We present rigorous details for a new unconditional stability theory developed for multistep ImEx schemes. The new theory involves an unconditional stability region, which plays a role analogous to that of the absolute stability region in conventional time stepping methods; combined with computable quantities (such as a numerical range) that play the role of eigenvalues in absolute stability theory. The new theory characterizes what is (and what is not possible) in the way of devising unconditionally stable ImEx schemes. We then turn our attention to the implications (and limitations) for devising high order semi-implicit schemes for two models in fluids: i) the incompressible Navier-Stokes equations, and (time permitting) ii) the dispersive shallow water equations.

MS 28: Part 1
Selected topics in computation and dynamics: machine learning and multiscale methods

Room: SR 3

Monday 10:30am - 11:00am
Hannes Vandecasteele
Efficiency and statistical properties of a micro-macro acceleration particle method

Monday 11:00am - 11:30am
Gene Ryan Yoo
Kernel Flows: from learning kernels from data into the abyss

Monday 11:30am - 12:00pm
Johan Warnegard
Conservative numerical schemes for nonlinear Schrödinger equations in complex physical setups

Room: SR 3

Monday 10:30am - 11:00am

Efficiency and statistical properties of a micro-macro acceleration particle method

Hannes Vandecasteele, **Przemysław Zieliński and Giovanni Samaey**

KU Leuven, Belgium

Many stochastic processes in nature have an inherent time-scale separation. On the other hand, we are typically only interested in the evolution of some well-chosen macroscopic state variables on long time scales. Here, we investigate a new micro-macro acceleration algorithm for such multiscale systems when the microscopic model is a stiff stochastic differential equation (SDE).
The proposed algorithm interleaves short bursts of stochastic microscopic simulation with extrapolation of the macroscopic states over a larger time interval. The matching operator then constructs a new microscopic state that is consistent with the given macroscopic state, while minimally perturbing the last known microscopic state. Since the extrapolation step is larger than the small step size of the explicit inner microscopic time integrator, the method is expected to provide a gain in computational efficiency. The drawback is an increased time discretization error and a larger statistical error.
In this talk, we will introduce the micro-macro acceleration algorithm and show that our method can attain a lower error than an approximate macroscopic model for the slow components, while gaining in efficiency compared to the microscopic time stepper. We will also quantify the statistical error of micro-macro acceleration and give some pointers on how matching can be used for data assimilation.

Room: SR 3

Monday 11:00am - 11:30am

Kernel Flows: from learning kernels from data into the abyss

Gene Ryan Yoo

California Institute of Technology, United States of America

Learning can be seen as approximating an unknown function by interpolating the training data. Kriging offers a solution to this problem based on the prior specification of a kernel. We explore a numerical approximation approach to kernel selection/construction based on the simple premise that a kernel must be good if the number of interpolation points can be halved without significant loss in accuracy (measured using the intrinsic RKHS norm $\|\cdot\|$ associated with the kernel). We first test and motivate this idea on a simple problem of recovering the Green's function of an elliptic PDE (with inhomogeneous coefficients) from the sparse observation of one of its solutions. Next we consider the problem of learning non-parametric families of deep kernels of the form $K_1(F_n(x), F_n(x'))$ with $F_{n+1} = (I_d + \epsilon G_{n+1}) \circ F_n$ and $G_{n+1} \in \text{Span}\{K_1(F_n(x_i), \cdot)\}$. With the proposed approach constructing the kernel becomes equivalent to integrating a stochastic data driven dynamical system, which allows for the training of very deep (bottomless) networks and the exploration of their properties. These networks learn by constructing flow maps in the kernel and input spaces via incremental data-dependent deformations/perturbations (appearing as the cooperative counterpart of adversarial examples) and, at profound depths, they (1) can achieve accurate classification from only one data point per class (2) appear to learn archetypes of each class (3) expand distances between points that are in different classes and contract distances between points in the same class. This is a joint work with Houman Owhadi. A preprint is available at arXiv:1808.04475.

Room: SR 3

Monday 11:30am - 12:00pm

Conservative numerical schemes for nonlinear Schrödinger equations in complex physical setups

Johan Warnegard and **Patrick Henning**

KTH Royal Institute of Technology, Sweden

In this talk we compare various mass-conservative time-integrators for the Gross-Pitaevskii equation in physically relevant setups. The comparison contains methods that are purely mass-conservative, methods that are additionally symplectic and methods that preserve the energy exactly. Our finding is that in particular in low-regularity regimes, e.g. in the context of rapidly oscillating potentials or close to quantum phase transitions, the numerical approximations are very sensitive to small variations in the discrete energy. Consequently, mass conservation alone will not lead to a competitive method in complex settings. Interesting are the differences between symplectic and energy-conservative discretizations, which turn out to be stronger than expected if the regularity of the solution is low. The talk concludes with a simulation of the phase transition from a (pseudo) Mott insulator to a superfluid.

MS 28: Part 2
Selected topics in computation and dynamics: machine learning and multiscale methods

Room: SR 3

Monday 02:00pm - 02:30pm
Kevin Lin
Data-driven modeling of chaotic dynamics: a model reduction perspective

Monday 02:30pm - 03:00pm
Giulio Trigila
Characterization and simulation of conditional probability densities

Monday 03:00pm - 03:30pm
Jeremy Heng
Gibbs flow transport for Bayesian inference

Monday 03:30pm - 04:00pm
Florian Schaefer
A probabilistic view on sparse Cholesky factorizations

Room: SR 3

Monday 02:00pm - 02:30pm

Data-driven modeling of chaotic dynamics: a model reduction perspective

Kevin Lin[1], **Fei Lu**[2] **and Alexandre Chorin**[3]

[1] *University of Arizona, United States of America*
[2] *Johns Hopkins University, United States of America*
[3] *University of California at Berkeley, United States of America*

Nonlinear dynamic phenomena often require a large number of dynamical variables for their description, only a small fraction of which are of direct interest. Reduced models using only these relevant variables can be very useful in such situations, both for computational efficiency and insights into the underlying dynamics. Unfortunately, except in special cases, deriving reduced models from first principles can be quite challenging. This has motivated interest in both parametric and nonparametric data-driven modeling in the model reduction community. In this talk, I will review a discrete-time version of the Mori-Zwanzig (MZ) projection operator formalism from nonequilibrium statistical mechanics, which provides a simple and general framework for model reduction. I will discuss data-driven modeling and model reduction for chaotic / stochastic dynamical systems within the MZ framework, highlighting some of the theoretical and practical issues that arise.

Room: SR 3

Monday 02:30pm - 03:00pm

Characterization and simulation of conditional probability densities

Giulio Trigila

Baruch College, United States of America

Conditional probability estimation provides data-based answers to critical questions, such as the expected response of specific patients to different medical treatments, weather forecasts and the effect of political measures on the economy. In the complex systems behind these examples, the outcome x of a process depends on many and diverse factors z. In addition, x is probabilistic in nature due in part to our ignorance of other relevant factors and to the chaotic nature of the underlying dynamics.
This talk will describe a general procedure for the characterization, estimation and simulation of the conditional probability density $\rho(x|z)$ underlying a sample set $\{x_i, z_i\}$. The methodology relies on a data-driven formulation of the Wasserstein barycenter problem, posed as a minimax problem in terms of two adversarial flows.

Room: SR 3

Monday 03:00pm - 03:30pm

Gibbs flow transport for Bayesian inference

Jeremy Heng[1], **Arnaud Doucet**[2] **and Yvo Pokern**[3]

[1] *ESSEC Business School, Singapore*
[2] *Oxford University*
[3] *University College London*

In this work, we consider the construction of transport maps between two distributions using flows. In the Bayesian formalism, this ordinary differential equation approach is natural when one introduces a curve of distributions that connects the prior to posterior by tempering the likelihood. We present a novel approximation of the resulting partial differential equation which yields an ordinary differential equation whose drift depends on the full conditional distributions of the posterior. We discuss properties of the Gibbs flow and efficient implementation in practical settings when employing the flow as proposals within sequential Monte Carlo samplers. Gains over state-of-the-art methods at a fixed computational complexity will be illustrated on a variety of applications.

Room: SR 3 | Monday 03:30pm - 04:00pm

A probabilistic view on sparse Cholesky factorizations

Florian Schaefer[1], **Tim Sullivan**[2], **Matthias Katzfuss**[3] **and Houman Owhadi**[1]

[1] *Caltech, United States of America*
[2] *Free University of Berlin and Zuse Institute Berlin, Germany*
[3] *Texas A&M University*

In this talk we will explore how probabilistic interpretations of the well-known Cholesky factorization motivate novel, fast, and simple algorithms for classical problems in numerical analysis.
In the first part of the talk we show that many dense kernel matrices arising in statistics, machine learning, and scientific computing have almost sparse Cholesky factors, under a suitable elimination ordering that is motivated by the conditional near-independence of the associated Gaussian process. By using recent results on operator adapted wavelets, we can prove rigorously that kernel matrices obtained from evaluations of Green's functions of elliptic boundary value problems at pairs of N points in a domain $\Omega \subset \mathbb{R}^d$ have ϵ-approximate Cholesky factors with $O(N \log(N) \log^d(N/\epsilon))$ nonzero entries, that can be computed in complexity $O(N \log^2(N) \log^{2d}(N/\epsilon))$ by standard zero fill-in incomplete Cholesky factorization.
In the second part of the talk we show that the problem of finding the best sparse approximate (in KL-divergence) inverse-Cholesky factor of a given positive definite matrix has a simple closed form solution, recovering algorithms that were used previously (without knowledge of their KL-optimality) in the fields of spatial statistics and sparse approximate inverses. This allows us to compute ϵ-approximate inverse-Cholesky factors of Green's matrices of elliptic boundary value problems in computational complexity $O(N \log^d(N/\epsilon))$ in space, and $O(N \log^{2d}(N/\epsilon))$ in time. To the best of our knowledge, this is the best asymptotic complexity for this problem. We conclude with a discussion of the practical advantages of the resulting algorithm, including its almost embarrassing parallelism

MS 29: Part 1
Implicit-explicit methods for differential systems

Room: UR 1

Thursday 10:30am - 11:00am
Adrian Sandu
Implicit-explicit GARK methods

Thursday 11:00am - 11:30am
Raymond John Spiteri
Gating-enhanced IMEX splitting methods for cardiac monodomain simulation

Thursday 11:30am - 12:00pm
Teo Roldan
Low-Storage Additive Semi-Implicit Runge-Kutta methods

Thursday 12:00pm - 12:30pm
Giuseppe Izzo
Variable stepsize implicit-explicit general linear methods

Room: UR 1 | Thursday 10:30am - 11:00am

Implicit-explicit GARK methods

Adrian Sandu, Steven Roberts and Arash Sarshar

Virginia Tech, United States of America

The GARK framework reveals the underlying structure of partitioned Runge-Kutta methods, and consequently it opens fresh opportunities for the construction of new schemes and the analysis of old ones. This talk presents new developments in the field of implicit-explicit time integration methods in the General-structure Additive Runge-Kutta family.

Room: UR 1 Thursday 11:00am - 11:30am

Gating-enhanced IMEX splitting methods for cardiac monodomain simulation

Raymond John Spiteri

University of Saskatchewan, Canada

The electrical activity in excitable cardiac tissue can be simulated using the monodomain model. The monodomain model is a continuum-based multi-scale model that consists of non-linear ordinary differential equations describing the electrical activity at the cellular scale along with a quasi-linear parabolic partial differential equation describing electrical propagation at the tissue scale. The standard "scale-based" splitting method for simulating the monodomain model is to split the tissue and cell models, applying different integrators to each. Typically, the tissue model is simulated with an implicit time integration method, and the cell model is simulated with an explicit or explicit-exponential one. We demonstrate that the application of implicit-explicit (IMEX) linear multistep or Runge–Kutta methods to this splitting can have poor stability properties when the cell model is stiff. We propose a novel "gating-enhanced" IMEX splitting that treats the tissue variable and the (typically stiff) cell model gating variables together implicitly. The performance of fourteen different IMEX methods using both splittings is measured in a variety of one- and two-dimensional experiments. The low incremental overhead combined with the substantially improved stability of the gating-enhanced splitting is shown to result in a performance increase of approximately a factor of four for simulations of the monodomain model with the stiff ten Tusscher–Panfilov model of human endocardial cells.

Room: UR 1 | Thursday 11:30am - 12:00pm

Low-Storage Additive Semi-Implicit Runge-Kutta methods

Teo Roldan and **Inmaculada Higueras**

Universidad Publica de Navarra, Spain

In [1] we considered a class of implicit-explicit Runge-Kutta methods for additive differential systems whose terms had different stiffness properties. This class of schemes were constructed having in mind high dimension systems coming from the space semi-discretization of some time-dependent partial differential equations. In this way some Additive Semi-Implicit Runge-Kutta methods with low-storage requirements were constructed. The special structure of the Butcher matrices of these schemes restricts the number of free parameters of the method and some order barriers appear for methods with positive coefficients [2].

[1] Construction of additive semi-implicit Runge-Kutta methods with low-storage requirements. Journal of Scientific Computing (2016) 67:1019–1042.
[2] Order Barrier for Low-Storage DIRK Methods with Positive Weights. Journal of Scientific Computing (2018) 75: 395-404.
Supported by Ministerio de Economía y Competividad (Spain), Project MTM2016-77735-C3-2-P.

Room: UR 1 | Thursday 12:00pm - 12:30pm

Variable stepsize implicit-explicit general linear methods

Angelamaria Cardone[1], **Giuseppe Izzo**[2] **and Zdzislaw Jackiewicz**[3]

[1] *University of Salerno, Italy*
[2] *University of Napoli Federico II, Italy*
[3] *Arizona State University, United States of America*

Many practical problems in science and engineering are modeled by large systems of ordinary differential equations (ODEs) with additive vector field, whose terms have different stiffness properties. Such a systems can often be written in the form

$$\begin{cases} y'(t) = f\big(y(t)\big) + g\big(y(t)\big), & t \in [t_0, T], \\ y(t_0) = y_0, \end{cases}$$

$y_0 \in \mathbb{R}^m$, $f : \mathbb{R}^m \to \mathbb{R}^m$, $g : \mathbb{R}^m \to \mathbb{R}^m$, where $f(y)$ represents the non-stiff processes and $g(y)$ represents stiff processes. For efficient integration of this kind of initial value problems we consider implicit-explicit (IMEX) methods, where the non-stiff part $f(y)$ is integrated by an explicit numerical scheme, and the stiff part $g(y)$ is integrated by an implicit numerical scheme.
After the investigation of IMEX Runge-Kutta (RK) methods [1], and IMEX General Linear Methods (GLMs) [2,3] in a fixed stepsize formulation, we focus on estimation of local discretization errors and rescaling stepsize techniques for high stage order IMEX GLMs in fixed and variable stepsize environments. We also describe the construction of such methods with desirable accuracy and stability properties.
References
[1] G. Izzo and Z. Jackiewicz, Highly stable implicit-explicit Runge-Kutta methods, Appl. Numer. Math., Vol. 113, 2017, 71–92.
[2] M. Bras, G. Izzo and Z. Jackiewicz, Accurate Implicit–Explicit General Linear Methods with Inherent Runge–Kutta Stability, J. Sci. Comput., Vol. 70(3), 2017, 1105–1143.
[3] G. Izzo and Z. Jackiewicz, Transformed implicit-explicit DIMSIMs with strong stability preserving explicit part, Numer. Algorithms, 2019 (in press).

MS 29: Part 2
Implicit-explicit methods for differential systems

Room: UR 1

Thursday 02:00pm - 02:30pm
Jens Lang
Super-Convergent IMEX-Peer Methods with Variable Time Steps

Thursday 02:30pm - 03:00pm
Benjamin Seibold
Unconditionally stable ImEx methods: How to solve complex problems without having to do complex solves

Thursday 03:00pm - 03:30pm
Michał Braś
Search for implicit-explicit general linear methods with inherent Runge-Kutta stability

Thursday 03:30pm - 04:00pm
Angela Martiradonna
Numerical approximation of optimal control models for invasive species by symplectic Lawson IMEX schemes

Room: UR 1 | Thursday 02:00pm - 02:30pm

Super-Convergent IMEX-Peer Methods with Variable Time Steps

Jens Lang[1], **Moritz Schneider**[1] **and Rüdiger Weiner**[2]

[1] *Technische Universität Darmstadt, Germany*
[2] *Martin-Luther Universität Halle-Wittenberg, Germany*

Dynamical systems with sub-processes evolving on many different time scales are ubiquitous in applications. Their efficient solution is greatly enhanced by automatic time step variation. In this talk, I will present the theory, construction and application of IMEX-Peer methods that are super-convergent for variable step sizes and A-stable in the implicit part [5]. IMEX-Peer schemes – like other IMEX-methods as well – combine the necessary stability of implicit and low computational costs of explicit methods to efficiently solve systems of ordinary differential equations with both stiff and non-stiff parts included in the source term [1,2,3,4]. To construct super-convergent IMEX-Peer methods which keep their higher order for variable step sizes and exhibit favourable linear stability properties, we derive necessary and sufficient conditions on the nodes and coefficient matrices and apply an extrapolation approach based on already computed stage values. New super-convergent IMEX-Peer methods of order $s+1$ for $s=2,3,4$ stages are given as result of additional order conditions which maintain the super-convergence property independent of step size changes. Numerical experiments and a comparison to other super-convergent IMEX-Peer methods show the potential of the new methods when applied with local error control.

[1] Lang and Hundsdorfer: Extrapolation-based implicit-explicit Peer methods with optimised stability regions, J. Comp. Phys. 337 (2017), 203-215.
[2] Soleimani, Knoth and Weiner: IMEX Peer methods for fast-wave-slow-wave problems, Appl. Numer. Math. 118 (2017), 221-237.
[3] Soleimani and Weiner: Superconvergent IMEX Peer methods, Appl. Numer. Math. 130 (2018), 70-85.
[4] Schneider, Lang and Hundsdorfer: Extrapolation-based superconvergent implicit-explicit Peer methods with A-stable implicit part, J. Comp. Phys. 367 (2018), 121-133.
[5] Schneider, Lang and Weiner: Super-convergent implicit-explicit Peer methods with variable step sizes, arXiv:1902.01161 (2019)

Room: UR 1 | Thursday 02:30pm - 03:00pm

Unconditionally stable ImEx methods: How to solve complex problems without having to do complex solves

Benjamin Seibold[1], **David Shirokoff**[2] **and Dong Zhou**[3]

[1] *Temple University, United States of America*
[2] *New Jersey Institute of Technology*
[3] *California State University Los Angeles*

A common paradigm in ImEx time-stepping is that the problem's stiff parts should be treated implicitly, and the time step is then restricted by the explicit components. However, it is in fact possible to design schemes and ImEx splittings in a way that unconditional stability is achieved. Such approaches admit an efficient treatment of problems in which the explicit part is stiff. Based on the notion of an unconditional ImEx stability region, we present a class of ImEx linear multistep methods that generalizes SBDF formulas to allow for arbitrarily large stability regions. We then argue how the ImEx splitting and the time-stepping scheme can be co-designed to optimize efficiency (accuracy over cost). The resulting methods allow one to efficiently time-step complex problems (such as nonlinear diffusion), without having to conduct any implicit solves of the complex operator.

Room: UR 1 | Thursday 03:00pm - 03:30pm

Search for implicit-explicit general linear methods with inherent Runge-Kutta stability

Michał Braś[1], **Angelamaria Cardone**[2], **Zdzislaw Jackiewicz**[1,3] **and Paulina Pierzchała**[1]

[1] *AGH University of Sience and Technology, Poland*
[2] *Università di Salerno, Italy*
[3] *Arizona State University, USA*

Many practical problems in science and engineering are modeled by large systems of ordinary differential equations (ODEs) which arise from discretization in space of partial differential equations (PDEs) by finite difference methods, finite elements or finite volume methods, or pseudospectral methods. For such systems there are often natural splittings of the right hand sides of the differential systems into two parts, one of which is non-stiff or mildly stiff, and suitable for explicit time integration, and the other part is stiff, and suitable for implicit time integration. The efficient solution can be provided by implicit-explicit (IMEX) schemes.
In present research we consider the class of general linear methods (GLMs) for ordinary differential equations. We construct IMEX GLMs of order $p = 1, 2, \ldots, 4$ with desired stability properties. We assume that the explicit and implicit parts of the IMEX scheme have the same abscissa vector $\mathbf{c}$ and coefficient matrices $\mathbf{U}$ and $\mathbf{B}$. We look for implicit methods of order p and stage order $q = p$, which have the property of so-called inherent Runge–Kutta stability (IRKS), and which are A-stable and if possible, also L-stable. We also require that the vector of external approximation is of Nordsieck form. Next, we attempt to maximize the combined region of absolute stability. Finally, we apply constructed methods to a series of test problems.
This is a joint work with A. Cardone, Z. Jackiewicz and P. Pierzchała.

Room: UR 1 | Thursday 03:30pm - 04:00pm

Numerical approximation of optimal control models for invasive species by symplectic Lawson IMEX schemes

Angela Martiradonna

Institute for Applied Mathematics M. Picone, CNR, Bari, Italy

We focus on some optimal control models for invasive species, where we search for the lowest cost strategy to reduce a given population to a desired level. We show how the phase-space analysis of the state-control optimality system allows to provide a qualitative description of the optimal solution. For some classes of optimal control problems, we find the optimal value of the time horizon corresponding to the minimal management effort and we give the analytic expressions of both the minimum control effort and the corresponding density [1]. We account for a reaction-diffusion equation for modeling the spatiotemporal dynamics of the controlled population [2].
For the numerical solution, we rely on methods based on finite difference/element spatial discretization and forward-backward procedure for the approximation in time. Implicit-Explicit schemes are applied to the diffusion flow and the nonlinear reaction term [3,4]. We make use of Runge-Kutta schemes and their exponential-Lawson symplectic counterpart. This choice arises from our description of the optimality state-costate system in a Hamiltonian dynamical setting.
This is a joint work with F. Diele (CNR-IAC), C. Marangi (CNR-IAC) and S. Ragni (University of Ferrara).

[1] Baker, C. M., Diele, F., Lacitignola, D., Marangi, C., and Martiradonna, A. (2019). Optimal control of invasive species through a dynamical systems approach. Nonlinear Analysis: Real World Applications, 49, 45-70.
[2] Baker, C. M., Diele, F., Marangi, C., Martiradonna, A., and Ragni, S. (2018). Optimal spatiotemporal effort allocation for invasive species removal incorporating a removal handling time and budget. Natural Resource Modeling, 31(4), e12190.
[3] Diele, F., Garvie, M., and Trenchea, C. (2017). Numerical analysis of a first-order in time implicit-symplectic scheme for predator-prey systems. Computers & Mathematics with Applications, 74(5), 948-961.
[4] Diele, F., Marangi, C., and Ragni, S. (2014). IMSP schemes for spatially explicit models of cyclic populations and metapopulation dynamics. Mathematics and Computers in Simulation, 100, 41-53.

MS 30: Part 1
Spectral deferred correction methods for time integration

Room: UR 3

Thursday 10:30am - 11:00am
Martin Weiser
Inexact Spectral Deferred Correction Methods for Long-Time Integration

Thursday 11:00am - 11:30am
Lisa Fischer
SDC-based methods for stochastic differential equations

Thursday 11:30am - 12:00pm
Daniel Ruprecht
GMRES-accelerated SDC for second order problems motivated by fast ion tracking in nuclear fusion reactors

Thursday 12:00pm - 12:30pm
Jörg Stiller
A spectral deferred correction method for incompressible flows with variable viscosity

Room: UR 3

Thursday 10:30am - 11:00am

Inexact Spectral Deferred Correction Methods for Long-Time Integration

Martin Weiser and Felix Binkowski

Zuse Institute Berlin, Germany

Simulating wear testing of implants under cyclic loading requires a multi-scale approach in time. Simple cycle jumping realizes an explicit Euler scheme for the averaged evolution of the shape. In this talk, we consider spectral deferred correction methods for higher order integration, and exploit the accuracy-effort trade-off available in finite element based simulations. This leads to inexact SDC methods, which can be much more efficient than standard SDC approaches. Based on work and accuracy models, a theoretically optimal choice of inexactness is derived. The efficiency of the resultingmethod is illustrated at some numerical examples.

Room: UR 3 | Thursday 11:00am - 11:30am

SDC-based methods for stochastic differential equations

Matthew R. Christian[3], **Lisa Fischer**[1], **Sebastian Götschel**[1] **and Michael L. Minion**[2]

[1] *Zuse Institut Berlin, Germany*
[2] *Lawrence Berkeley National Laboratory*
[3] *University of North Carolina - Chapel Hill*

Many biological processes such as gene expression are intrinsically stochastic in nature, and can be modelled by stochastic differential equations. Typically, model parameters like reaction propensities are unknown, and have to be estimated, e.g., using Bayesian inference. Also, often it is of interest to compute expectation values using (multilevel) Monte Carlo sampling, thus requiring the computation of many realizations by numerically approximating the involved SDEs. The discretization error of the numerical scheme induces bias in the computed Monte Carlo estimator. As the usually used numerical schemes, like Euler-Maruyama or Milstein, are low order, even reasonably coarse error bounds for the simulation are costly to achieve. In this talk we develop efficient higher order methods based on a Wong-Zakai approximation of Brownian motion combined with spectral deferred correction methods well known for the numerical solution of ordinary differential equations. We investigate the convergence order of the proposed method, and show numerical examples.

Room: UR 3

Thursday 11:30am - 12:00pm

GMRES-accelerated SDC for second order problems motivated by fast ion tracking in nuclear fusion reactors

Krasymyr Tretiak[1], Daniel Ruprecht[1], Rob Akers[2] and James Buchanan[2]

[1] *University of Leeds, United Kingdom*
[2] *Culham Centre For Fusion Energy, United Kingdom*

The talk will present Boris-SDC, a variant of spectral deferred corrections (SDC) for the second order Lorentz equations. These equations model movement of electrically charged particles in electromagnetic fields and are widely used in plasma physics. Boris-SDC is an arbitrary order time stepping method for the Lorentz equations based on the popular Boris algorithm, introduced by Boris in 1970. It is based on a combination of the Velocity-Verlet method as a sweeper within SDC and a trick to avoid the need for an implicit solver. A convergence acceleration strategy applying GMRES to SDC, developed by Huang et al. in 2006, will be adopted for inhomogeneous magnetic fields. Performance results will be shown for various test cased related to modelling fast ion trajectories in the DIIID, JET and ITER fusion reactors.

Room: UR 3

Thursday 12:00pm - 12:30pm

A spectral deferred correction method for incompressible flows with variable viscosity

Jörg Stiller

TU Dresden, Germany

The present work adopts the spectral deferred correction method for incompressible flows, including the effect of time-dependent boundary conditions and variable viscosity. An extended version of the dual splitting scheme serves as the propagator, combined with the discontinuous Galerkin method for space discretization. Multigrid-preconditioned Krylov methods are used for solving the elliptic subsystems. The contribution considers the influence of various aspects on robustness and efficiency, including the splitting error and pressure robustness. Different scenarios of variable viscosity will be studied: 1) variation in space, 2) variation in space and time, and 3) solution dependent viscosity.

MS 30: Part 2
Spectral deferred correction methods for time integration

Room: UR 3

Thursday 02:00pm - 02:30pm
Michael L. Minion
Exponential Integrators, SDC, and PFASST

Thursday 02:30pm - 03:00pm
Gitte Kremling
Convergence analysis for multi-level spectral deferred corrections

Thursday 03:00pm - 03:30pm
Ruth Schoebel
Parallel Newton-multigrid and PFASST for nonlinear differential equations

Room: UR 3 | Thursday 02:00pm - 02:30pm

Exponential Integrators, SDC, and PFASST

Michael L. Minion and **Tommaso Buvoli**

Lawrence Berkeley National Lab, United States of America

Exponential integrators are an approach to the temporal integration of ODEs wherein one uses the matrix exponential operator to integrate a linear part of the equation exactly. Nonlinear terms are typically included using an operator splitting approach. I will describe the serial approach of Buvoli to construct exponential integrators where the nonlinear terms are treated to arbitrarily high order by an extension of Spectral Deferred Corrections (SDC). I will then discuss the extension of these methods to multi-level SDC. Finally I will present some preliminary results on the parallel performance of the PFASST algorithm using exponential SDC sweepers.

Room: UR 3

Thursday 02:30pm - 03:00pm

Convergence analysis for multi-level spectral deferred corrections

Gitte Kremling and Robert Speck

Forschungszentrum Jülich, Germany

The spectral deferred correction (SDC) method is an iterative solver for ordinary differential equations (ODEs). It can be interpreted as a preconditioned Picard iteration for the collocation problem. The convergence of this method is well-known, it gains one order per iteration up to the order of the quadrature method of the collocation problem. This appealing feature enables an easy creation of flexible, high-order accurate methods for ODEs. A variation of SDC are multi-level spectral deferred corrections (MLSDC). Here, sweeps are performed on a hierarchy of levels and an FAS correction term, as in nonlinear multigrid methods, couples solutions on different levels. While there are several numerical examples which show its correctness and efficiency, a theoretical convergence proof is still missing. This talk addresses this issue. A proof of the convergence of MLSDC, including the determination of the convergence order, will be outlined and the results of the theoretical analysis will be numerically demonstrated. It turns out that there are restrictions for the superiority of this method over SDC regarding the convergence order.

Room: UR 3 | Thursday 03:00pm - 03:30pm

Parallel Newton-multigrid and PFASST for nonlinear differential equations

Ruth Schoebel and **Robert Speck**

Forschungszentrum Jülich GmbH, Germany

To overcome scaling limits arising from spatial parallelism, it has become a promising approach to expand traditional parallelization techniques to the temporal dimension. The "parallel full approximation scheme in space and time" (PFASST) is based on the iterative spectral deferred correction (SDC) method. While SDC solves the so called collocation problem on one time step, PFASST can integrate multiple time steps simultaneously. SDC iterations with different costs are coupled in a multigrid way, using a multilevel hierarchy in space and time for the so-called composite collocation problem. While numerical experiments and scaling studies show promising results, the theoretical analysis of PFASST is quite at the beginning. In practice, the nonlinear PFASST algorithm results in local nonlinear systems, which are often solved by Newton's method. However, it is also possible to exchange the order of PFASST and Newton by creating a parallel Newton multigrid for the composite collocation problem. There, the Newton is used as the outer solver and PFASST, now applied to linear problems, as the inner one. In this talk, we will analyze both approaches and show local convergence under suitable conditions. In addition, we will support the results with numerical examples and examine the impact of inexact inner solvers and different numbers of processors.

MS 31
Structural approaches for differential-algebraic systems

Room: HS 3

Friday 10:30am - 11:00am
Caren Tischendorf
An introduction to differential algebraic equations with network structure

Friday 11:00am - 11:30am
Victoria Wieloch
BLieDF- a k-step BDF Lie group time integrator for constrained mechanical systems

Friday 11:30am - 12:00pm
Idoia Cortes Garcia
Parallel-in-time methods for field/circuit coupled differential algebraic equations

Friday 12:00pm - 12:30pm
Christian Strohm
The influence of circuit-field-coupling structures onto simulation using waveform relaxation

Room: HS 3 | Friday 10:30am - 11:00am

An introduction to differential algebraic equations with network structure

Caren Tischendorf

Humboldt University of Berlin, Germany

The simulation of dynamic flows on networks is of interest in various applications. Using differential equation models for describing the flow on the edges of the network yields in systems of differential equations and algebraic constraints with a certain structure. We demonstrate that they result (after spatial discretisation for distributed models) in differential algebraic equation (DAE) systems with a particular structure reflecting the network topology. We present several properties of such DAEs and show that they are closely related to (generalised) port Hamiltonian DAEs. Finally, we demonstrate how numerical simulation methods preserve the structural properties.

Room: HS 3

Friday 11:00am - 11:30am

BLieDF- a k-step BDF Lie group time integrator for constrained mechanical systems

Victoria Wieloch and **Martin Arnold**

Martin Luther University Halle-Wittenberg, Germany

BDF multistep methods are frequently applied to constrained mechanical systems in industrial multibody system simulation. Some applications of these multibody systems include large rotations that can be described without singularities by using matrix Lie groups. In this framework, BLieDF is a k-step Lie group integrator for DAEs of index 3, that avoids order reduction by a slightly perturbed argument of the exponential map for representing the nonlinearity of the numerical flow in the configuration space without any time-consuming re-parametrization. For $2 \leq k \leq 6$, local truncation errors and convergence of order $p = k$ can be proven in all solution components. The convergence analysis combines classical BDF multistep concepts with aspects of DAE and Lie group theory. Numerical tests for the Heavy top benchmark in the Lie group formulation $\mathbb{R}^3 \times SO(3)$ will confirm the theoretical investigations.

Room: HS 3

Friday 11:30am - 12:00pm

Parallel-in-time methods for field/circuit coupled differential algebraic equations

Idoia Cortes Garcia[1,2], **Iryna Kulchytska-Ruchka**[1,2] **and Sebastian Schöps**[1,2]

[1] *Graduate School of Computational Engineering (GSCE), Technische Universität Darmstadt*
[2] *Institut für Teilchenbeschleunigung und Elektromagnetische Felder (TEMF), Technische Universität Darmstadt*

The analysis of complex systems requires simulations with high abstraction level but sometimes also a detailed insight into the spatially distributed phenomena of individual devices is necessary. In those cases, so-called refined modelling is performed. In the context of electrotechnical applications the spatially discretised system of partial differential equations describing the electromagnetic field inside the elements may be coupled to the system of differential algebraic equations describing the circuit surrounding it [1]. Each refined model can have hundreds of thousands of degrees of freedom arising from, e.g. a finite element discretisation. Therefore, such coupled systems often lead to computationally heavy simulations that need to be sped up.
One way to do so is to use parallel-in-time algorithms such as Parareal [2] that allow to parallelise time-domain simulations. These algorithms have mainly been studied for ordinary differential equations. When considering differential algebraic equations, new difficulties may arise that need to be taken into account, e.g. with respect to consistent initial conditions or convergence.
This contribution discusses the usage of the Parareal algorithm for systems of differential algebraic equations, with the motivation of speeding up the simulation of field/circuit coupled systems.

[1] I. A. Tsukerman, A. Konrad, G. Meunier, and J. C. Sabonnadière. Coupled Field-Circuit Problems: Trends and Accomplishments. IEEE Transactions on Magnetics 29.2, pp. 1701–1704, 1993.
[2] J.-L. Lions, Y. Maday, and G. Turinici. A parareal in time discretization of PDEs. Comptes Rendus de l'Académie des Sciences – Series I – Mathematics, vol. 332, no. 7, pp.661-668, 2001.

Room: HS 3 | Friday 12:00pm - 12:30pm

The influence of circuit-field-coupling structures onto simulation using waveform relaxation

Christian Strohm

Humboldt Universität zu Berlin, Germany

We consider coupled dynamical systems, arising from lumped circuit modeling coupled to distributed modeling of electromagnetic devices. The corresponding subsystems form an ordinary differential equation system, reflecting the spatially discretized electromagnetic field equations, see e. g. [4], and a system of differential-algebraic equations (DAEs), describing the circuit obtained by modified nodal analysis (MNA), see e. g. [2]. The different nature of the subsystems motivates us to solve the coupled systems by co-simulation in form of waveform relaxation methods, see e. g. [3]. It allows the use of sophisticated solvers for each subsystem. Furthermore, one can easily exploit the different structural properties of the subsystems. This becomes even more important due to the fact that the systems dimension may easily reach millions of unknowns. However, convergence of waveform relaxation methods is not always guaranteed as soon as DAEs are involved, see e. g. [1]. As one prototype of waveform relaxation methods we analyze the convergence behavior of the Gauss-Seidel approach. We present a criterion that guarantees convergence and discuss the influence of three different coupling formulations onto the convergence behavior. In particular, tests show that the number of needed iterations can be very small but also drastically high, depending on the coupling formulation.

[1] Arnold, M., Günther, M.: Preconditioned dynamic iteration for coupled differential-algebraic systems. BIT Numerical Mathematics 41(1), 1–25 (2001).
[2] Lamour, R., März, R., Tischendorf, C.: Differential-Algebraic Equations: A Projector Based Analysis: Springer, Heidelberg (2013).
[3] Lelarasmee, E.: The waveform relaxation method for time domain analysis of large scale integrated circuits: Theory and applications. Electronics Research Laboratory, College of Engineering, Universityof California (1982).
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MS 32
Numerical methods for pattern formation in PDEs and applications

Room: SR 3

Thursday 10:30am - 11:00am
Ivonne Sgura
Matrix-oriented discretization methods for reaction-diffusion PDEs: comparisons and applications

Thursday 11:00am - 11:30am
Deborah Lacitignola
Spatio-temporal dynamics on the sphere for a PDE morphochemical electrodeposition model

Thursday 11:30am - 12:00pm
Giuseppina Settanni
Numerical Modellig for Crypt Fission in the Colonic Ephitelium

Thursday 12:00pm - 12:30pm
Fasma Diele
Positive techniques for lake ecosystem dynamics

Room: SR 3

Thursday 10:30am - 11:00am

Matrix-oriented discretization methods for reaction-diffusion PDEs: comparisons and applications

Maria Chiara D'Autilia[1], **Ivonne Sgura**[1] **and Valeria Simoncini**[2]

[1] *Dipartimento di Matematica e Fisica "E. De Giorgi', Università del Salento, Lecce, Italy*
[2] *Dipartimento di Matematica, Alma Mater Studiorum Università di Bologna, Italy*

Systems of reaction-diffusion partial differential equations (RD-PDEs) are widely applied for modelling life science and physico-chemical phenomena. In particular, the coupling between diffusion and nonlinear kinetics can lead to the so-called Turing instability, giving rise to a variety of spatial patterns (like labyrinths, spots, stripes, etc.) attained as steady state solutions for large time intervals. To capture the morphological peculiarities of the pattern itself, a very fine space discretization may be required, limiting the use of standard (vector-based) ODE solvers in time because of excessive computational costs.

We show that the structure of the diffusion matrix can be exploited in order to use matrix-based versions of time integrators, such as Implicit-Explicit (IMEX) and exponential schemes. This implementation entails the solution of a sequence of discrete matrix problems of significantly smaller dimensions than in the vector case, thus allowing for a much finer space discretization. We illustrate our findings for the Schnackenberg model, prototype of RD-PDE systems with Turing pattern solutions, and for the morphochemical electrodeposition model describing metal growth during battery charging processes.

Room: SR 3

Thursday 11:00am - 11:30am

Spatio-temporal dynamics on the sphere for a PDE morphochemical electrodeposition model

Deborah Lacitignola[1], **Benedetto Bozzini**[2] **and Ivonne Sgura**[2]

[1] *University of Cassino and Southern Lazio, Italy*
[2] *University of Salento, Italy*

In the framework of the morphological control of electrodeposit materials, the spherical geometry for the electrode surface has a great practical importance since spheres are the shape of choice for flow batteries and metal-air devices. Inspired by these experimental motivations, we consider a morpho-electrochemical reaction-diffusion model on a sphere and investigate its spatio-temporal dynamics specifically focussing on the system capabilities to support Turing patterns and spiral waves. On this line, we derive conditions for the occurrence of the Turing instability phenomenon and provide an example of pattern selection. As far as the spiral wave phenomenology is concerned, we show that spiral waves can emerge because of the interplay between two specific model parameters: one regulating the oscillatory dynamics in the kinetics and the other one related to the domain size. Interestingly, the model also supports a mechanism of spirals break up leading to a complex spatio-temporal phenomenology. To support theoretical results, we provide systematic numerical simulations based on the finite element method LSFEM and accompanied by the computation of suitable indicators that allow to characterize and compare the diffent spatio-temporal features emerging from the model. Finally, we present two experimental validations of the obtained results: zinc electrodeposition onto cupper spheres for Turing pattern formation and Ag-In and Ag-Co electrodeposition for the emergence of spiral waves.

References

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[4] Lacitignola, D., Bozzini, B., Frittelli, M., Sgura, I., 2017. Turing pattern formation on the sphere for a morphochemical reaction-diffusion model for electrodeposition. Communications in Nonlinear Science and Numerical Simulation 48, 484 – 508.

[5] Lacitignola, D., Sgura I., Bozzini, B., Dobrovolska Ts., Krastev I., Spiral waves on the sphere for an alloy electrodeposition model, (submitted).

Room: SR 3

Thursday 11:30am - 12:00pm

Numerical Modellig for Crypt Fission in the Colonic Ephitelium

Giuseppina Settanni[1] **and Giuseppe Romanazzi**[2]

[1] *University of Bari Aldo Moro, Italy*
[2] *Universidade Estadual de Campinas (Unicamp)*

The aim of this talk will be to present a mathematical model describing crypt deformation and fission, coupled with a continuous spatial differential model in a hexagonal cluster of seven initial crypts. The model is used to predict formation of an Aberrant Crypt Foci (ACF), which are characterized by clusters of abnormal crypts, generated by crypt fission originated by cell mutations. In particular, the model considers the activation of Wnt signaling and the block of differentiation as cause of mutations. We use a differential convective and diffusive model considering two cell families, transit and fully differentiated. Each abnormal crypt is characterized by three steps: initiation, deformation and fission. Deformation can occur in three different directions depending on the concentration of abnormal cells and Wnt at the top of the crypt. Numerical results will show how the model, numerically solved by using a Galerkin finite element method, leads to abnormal crypt fission in a set of seven adjacent crypts.

Room: SR 3 | Thursday 12:00pm - 12:30pm

Positive techniques for lake ecosystem dynamics

Fasma Diele

CNR, Istituto per Applicazioni del Calcolo M.Picone, Bari, Italy

Motivated by the research activities carried out within the H2020 project 'ECOPOTENTIAL: Improving Future Ecosystem Benefits Through Earth Observation', some (simplified versions) of lake ecosystems models that describe the dynamical behaviour of trophic chains, will be presented [3],[5]. The population dynamics is modelled by reaction-advection-diffusion equations where the diffusive term represents the eddy diffusivity and the advection term is related to the autonomous motion (e.g. sinking or active swimming) of each ecosystem component. For their numerical approximation a splitting approach is adopted, where reaction, diffusion and advection are solved separately. To assure the positivity of the state variables, the reaction term is approximated by some positive schemes recently introduced in literature [2],[4]. Whenever the solutions are featured by some conservation properties, the integration schemes preserve both positivity and conservation [1]. The benefits of adopting the proposed approach will be illustrated on the formation of spatial patterns for some examples taken from literature.
This activities have many different aspects that have been study studied together with the collaborators C.Marangi and A.Martiradonna (IAC-CNR), S.Giamberini , A.Provenzale (IGG-CNR), G.Colonna (IMIP-CNR).
References:
[1] Burchard, H., K. Bolding, W. Kuhn, A. Meister, T. Neumann, L. Umlauf, Description of a flexible and extendable physical-giogeochemical model system for the water column, J.Marine Systems 61 (2006) 180-211.
[2] Diele, F., C. Marangi, Positive symplectic integrators for predator-prey dynamics, Discrete and Continuous Dynamical Systems, Series B, 23 (2018) 2661-2678.
[3] Huisman, J., NNP Thi, D.M. Karl, B. Sommeijer, Reduced mixing generates oscillations and chaos in the oceanic deep chlorophyll maximum, NATURE 439 (2006) 322-325.
[4] Martiradonna A., G. Colonna, F. Diele, GeCo: Geometric Conservative nonstandard schemes for biochemical systems, Applied Numerical Mathematics (submitted).
[5] Provenzale A. , J. von Hardenberg, A model ecosystem for small mesotrophic and eutrophic subalpine lakes, SILMAS project (Sustainable Instruments for Lake Management in the Alpine Space), technical report. Project co-financed by the European Regional Development Fund through the Interreg Alpine Space programme, 2009-2012.

MS 33
Probabilistic numerics for differential equations

Room: UR 1

Friday 10:30am - 11:00am
Jonathan Cockayne
Probabilistic Meshless Methods for Partial Differential Equations

Friday 11:00am - 11:30am
Takeru Matsuda
Estimation of ODE models with quantifying discretization error

Friday 11:30am - 12:00pm
Han Cheng Lie
Probabilistic integration of ordinary differential equations

Friday 12:00pm - 12:30pm
Motonobu Kanagawa
Convergence Guarantees for Adaptive Bayesian Quadrature Methods

Room: UR 1

Friday 10:30am - 11:00am

Probabilistic Meshless Methods for Partial Differential Equations

Jonathan Cockayne

University of Warwick, United Kingdom

In this talk we will present a probabilistic numerical method for solution of partial differential equations (PDEs) and study application of that method to PDE-constrained inverse problems. This approach enables the solution of challenging inverse problems whilst accounting, in a statistically principled way, for the impact of discretisation error due to numerical solution of the PDE. In particular, the approach confers robustness to failure of the numerical PDE solver, with statistical inferences driven to be more conservative in the presence of substantial discretisation error.

Room: UR 1 | Friday 11:00am - 11:30am

Estimation of ODE models with quantifying discretization error

Takeru Matsuda[1,2] **and Yuto Miyatake**[3]

[1] *The University of Tokyo, Japan*
[2] *RIKEN Center for Brain Science, Japan*
[3] *Osaka University, Japan*

We consider estimation of ODE models from noisy observations. For this problem, it is common to fit numerical solutions of ODEs to data. However, such a method does not account for the discretization error in numerical solutions and has limited estimation accuracy. In this study, we propose an estimation method that quantifies the discretization error based on data. The key idea is to model the discretization error by random variables and then apply the iteratively reweighted least squares method. Experimental results demonstrate that the proposed method improves estimation accuracy by accounting for the discretization error.

Room: UR 1 | Friday 11:30am - 12:00pm

Probabilistic integration of ordinary differential equations

Han Cheng Lie[1], **Andrew Stuart**[2] **and T. J. Sullivan**[3,4]

[1] *Universität Potsdam, Germany*
[2] *California Institute of Technology*
[3] *Zuse Institut Berlin*
[4] *Freie Universität Berlin*

Probabilistic integration of ordinary differential equations (ODEs) is an approach for quantifying uncertainty in trajectories, such as the uncertainty induced by discretisation errors. Such uncertainty quantification is important in problems where it is not computationally feasible to use arbitrarily fine discretisations and when the result of numerical integration step is part of a computational pipeline, for example in numerical weather prediction. As a proxy for the uncertainty in each numerical integration step, Conrad et al. (Stat. Comput. 2017) proposed to use independent, identically distributed (i.i.d) Gaussian random variables; this proposal leads to ensembles of randomly perturbed solutions of the ODE of interest. In this paradigm, Conrad et al. established mean square convergence of the resulting random solutions for globally Lipschitz vector fields. We build on these pioneering results by considering a more general paradigm that uses non-Gaussian, not necessarily i.i.d. random variables as proxies for the uncertainty. We establish a convergence result that yields better control over the random solutions via a stronger metric on solution space, and establish a tighter connection between the rate of convergence of the random solutions and the integrability of the random variables used in the randomisation steps.

Room: UR 1 | Friday 12:00pm - 12:30pm

Convergence Guarantees for Adaptive Bayesian Quadrature Methods

Motonobu Kanagawa[1] and **Philipp Hennig**[1,2]

[1] *University of Tuebingen, Germany*
[2] *Max Planck Institute for Intelligent Systems, Germany*

Adaptive Bayesian quadrature (ABQ) is a powerful approach to numerical integration that empirically compares favorably with Monte Carlo integration on problems of medium dimensionality (where non-adaptive quadrature is not competitive). Its key ingredient is an acquisition function that changes as a function of previously collected values of the integrand. While this adaptivity appears to be empirically powerful, it complicates analysis. Consequently, there are no theoretical guarantees so far for this class of methods. In this work, for a broad class of adaptive Bayesian quadrature methods, we prove consistency, deriving non-tight but informative convergence rates. To do so we introduce a new concept we call weak adaptivity. In guaranteeing consistency of ABQ, weak adaptivity is notionally similar to the ideas of detailed balance and ergodicity in Markov Chain Monte Carlo methods, which allow sufficient conditions for consistency of MCMC. Likewise, our results identify a large and flexible class of adaptive Bayesian quadrature rules as consistent, within which practitioners can develop empirically efficient methods.

MS 34
Models and simulations of cellular systems: from single-cells to population dynamics

Room: UR 1

Wednesday 10:30am - 11:00am
Martina Prugger
A Python-based modeling framework for mechanistic models of cell-decision processes

Wednesday 11:00am - 11:30am
Linda Petzold
The Master Clock: Structure and Function

Wednesday 11:30am - 12:00pm
Kathrin Thedieck
Systems approaches to metabolic signaling

Wednesday 12:00pm - 12:30pm
James R. Faeder
Identifying biochemical mechanisms that give rise to heterogeneity in single-cell responses

Room: UR 1

Wednesday 10:30am - 11:00am

A Python-based modeling framework for mechanistic models of cell-decision processes

Carlos Lopez and Martina Prugger

Vanderbilt University, United States of America

The complexity of biological models increases as we learn more details about the biochemical interactions that give rise to cellular commitment to fate decisions. These models can range from a few reactions, which can be managed using traditional methods, to highly complex systems comprising hundreds or thousands of chemical species that must be represented using numerical methods. Here we show how we leverage the power of the Python programming ecosystem to build a robust and reliable modeling framework for model-building, simulation, visualization and analysis. We highlight how we can use High Performance Computing architectures to tackle the problems of mechanistic hypothesis exploration, parameter fitting, and dynamic network analysis. Our work presents an open-source, easily accessible approach for model dissemination.

Room: UR 1

Wednesday 11:00am - 11:30am

The Master Clock: Structure and Function

Linda Petzold

University of California Santa Barbara, United States of America

In the mammalian suprachiasmatic nucleus (SCN), noisy cellular oscillators communicate within a neuronal network to generate precise system-wide circadian rhythms. In past work we have inferred the functional network for synchronization of the SCN. In recent work we have inferred the directionality of the network connections. We discuss the network structure and its advantages for function.

Room: UR 1

Wednesday 11:30am - 12:00pm

Systems approaches to metabolic signaling

Kathrin Thedieck

University of Innsbruck, Austria

mTOR (mammalian/mechanistic target of rapamycin) is at the center of a multiply intertwined, highly dynamic kinase network that is key for metabolic control. mTOR controls the cellular response to nutrients, growth factors and stress and promotes growth and survival. mTOR dysregulation has been reported for most cancers, and compounds which target the mTOR network are in the clinics and many clinical trials. Yet, the success of targeted treatments remains limited due to currently unpredictable initial resistance or relapse in a significant proportion of patients. Toward the development of disease mechanism-driven personalized therapies, we develop systems approaches to kinase and metabolic networks. This talk will focus on mTOR's drug response and cover our latest advances toward a systems understanding of metabolic signaling in tumor cells.

Room: UR 1 | Wednesday 12:00pm - 12:30pm

Identifying biochemical mechanisms that give rise to heterogeneity in single-cell responses

Sanjana Gupta[1], **Caleb C. Reagor**[1,2], **Robin E. C. Lee**[1] and **James R. Faeder**[1]

[1] *Department of Computational and Systems Biology, University of Pittsburgh, Pittsburgh, Pennsylvania, United States of America*
[2] *Department of Biology, Lipscomb University, Nashville, Tennessee, United States of America*

Individual cells within an isogenic population may exhibit widely varying responses to the same stimuli and identifying the biochemical mechanisms that account for heterogeneity is one of the major challenges in systems biology. I will talk about several computational approaches we have been developing to determine the mechanistic basis for individuality at the single-cell level using Bayesian parameter estimation (BPE) and related Monte Carlo approaches for sensitivity analysis. BPE is widely-used to learn models from data, but standard algorithms, such as Markov Chain Monte Carlo (MCMC), suffer from slow convergence when applied to complex models, particularly with sparse data as is the usual case for biological systems. We have used an accelerated sampling method called parallel tempering, which uses multiple Markov Chains run in parallel at different temperatures, to improve the performance of BPE for complex models. In addition, we have applied a sparsity-promoting penalty called Lasso, which is widely-used in machine learning, to reduce model complexity and to identify in a systematic fashion the mechanisms within a model that are required to reproduce key features of the data. Finally, we have applied a variant of Principal Component Analysis that we call "Last Component Analysis" (LCA) to identify the model variables that contribute maximally to a given property of interest. We show with several examples that LCA can identify combinations of parameters whose variation correlates strongly to a given property of interest, thus establishing potential mechanisms that can account for observed heterogeneity.

MS 35
Time-integration of partial differential equations

Room: UR 3

Friday 10:30am - 11:00am
Marlis Hochbruck
An FEM-IMEX scheme for semilinear wave equations with dynamic boundary conditions

Friday 11:00am - 11:30am
Eskil Hansen
Domain decomposition based time integrators for parabolic problems

Friday 11:30am - 12:00pm
Benny Stein
Strang splitting for PDEs with random parameters and random initial data

Friday 12:00pm - 12:30pm
Sergio Blanes
Exponential propagators for the Schrödinger equation with a time-dependent potential

Room: UR 3

Friday 10:30am - 11:00am

An FEM-IMEX scheme for semilinear wave equations with dynamic boundary conditions

Marlis Hochbruck and **Jan Leibold**

Karlsruhe Institute of Technology, Germany

In this talk we consider semilinear acoustic wave equations with dynamic boundary conditions. In contrast to standard boundary conditions, as of Dirichlet or Neumann type, dynamic boundary conditions do not neglect the momentum of the wave on the boundary. The mathematical modeling of such effects leads to an evolution equation in the interior domain coupled to an evolution equation on the smooth boundary. A typical example are kinetic boundary conditions [4].
We are interested in full discretizations of such equations comprising finite element discretizations in space and implicit-explicit (IMEX) time integration schemes [1].
Boundary conditions which involve tangential derivatives, as, e.g., the Laplace–Beltrami operator, are intrinsically posed on domains with (piecewise) smooth, possibly curved boundaries. Hence, numerical methods have to approximate the domain first. This renders the approximation non-conforming and makes the error analysis much more involved. These difficulties are addressed in [2,3], where a unified error analysis is presented that allows to derive space discretization error bounds. We show how this analysis can be combined with an analysis of the IMEX scheme and finally provide a rigorous error analysis of the full discretization.

[1] U. M. Ascher, S. J. Ruuth, R. J. Spiteri, Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations, Appl. Numer. Math. 25 (1997), 151-167.
[2] D. Hipp, M. Hochbruck, C. Stohrer, Unified error analysis for nonconforming space discretizations of wave-type equations, IMA Journal of Numerical Analysis (2018), online first, dry036.
[3] J. Leibold, Semilineare Wellengleichungen mit dynamischen Randbedingungen, Master's Thesis, Karlsruhe Institue of Technology (2017).
[4] E. Vitillaro, Strong solutions for the wave equation with a kinetic boundary condition, Contemp. Math. 594 (2013), 295-307.

Room: UR 3 | Friday 11:00am - 11:30am

Domain decomposition based time integrators for parabolic problems

Eskil Hansen

Lund University, Sweden

Domain decomposition based schemes allow the usage of parallel and distributed hardware, making them well-suited for discretization of time dependent PDEs in general and parabolic equations in particular. In this talk, we will review the somewhat overlooked possibility of introducing the domain decomposition approach directly into the temporal discretization. We will outline a convergence analysis for these domain decomposition based time integrators for two standard families of nonlinear parabolic equations, namely, the parabolic p-Laplace and the porous medium type equations.
The analysis is conducted by first casting the domain decomposition procedure into a new variational framework. The time integration of a nonlinear parabolic equation can then be interpreted as an operator splitting scheme applied to an abstract evolution equation governed by a maximal dissipative vector field. By utilizing this abstract setting, we prove temporal convergence for the most common choices of domain decomposition based integrators. We conclude with a few numerical experiments.
This is joint work with Monika Eisenmann (TU Berlin).

Room: UR 3 | Friday 11:30am - 12:00pm

Strang splitting for PDEs with random parameters and random initial data

Benny Stein and **Tobias Jahnke**

Karlsruhe Institute of Technology, Germany

Partial differential equations provide well-established models for many processes and phenomena in science and technology. In many real-life applications, however, some part of the information that is required to solve the mathematical problem is not available or cannot be measured with the desired accuracy. In this talk, we present a splitting method for time-dependent, semilinear partial differential equations with a number of random parameters and with random initial data. The main idea is to switch between two different discretizations of the stochastic variable, namely a stochastic Galerkin method on sparse grids for the linear parts of the right-hand side, and a stochastic collocation method for the nonlinear part. With this strategy each subproblem can be propagated very efficiently. The new method is computationally much cheaper than standard stochastic Galerkin methods, and numerical tests show that it outperforms standard stochastic collocation methods, too.

Room: UR 3 | Friday 12:00pm - 12:30pm

Exponential propagators for the Schrödinger equation with a time-dependent potential

Sergio Blanes

Universitat Politècnica de València, Spain

We consider the numerical integration of the Schrödinger equation with a time-dependent Hamiltonian given as the sum of the kinetic energy and a time-dependent potential usign commutator-free (CF) propagators. They are exponential propagators that have shown to be highly efficient for general time-dependent Hamiltonians. We propose new CF propagators that are tailored for Hamiltonians of particular structure, showing a considerably improved performance. We obtain new fourth- and sixth-order CF propagators as well as a novel sixth-order propagator that incorporates a double commutator that only depends on coordinates, so this term can be considered as cost-free. The algorithms require the computation of the action of exponentials on a vector similarly to the well known exponential midpoint propagator. We illustrate the performance of the new methods on several numerical examples.

MS 36
Low-rank methods for matrix- and operator-valued differential equations

Room: UR 3

Wednesday 10:30am - 11:00am
Tony Stillfjord
Singular value decay of operator-valued differential Lyapunov and Riccati equations

Wednesday 11:00am - 11:30am
Lena-Maria Pfurtscheller
An operator-valued differential equation approach for El Niño

Wednesday 11:30am - 12:00pm
Björn Baran
Recent Advances in Riccati-Feedback Stabilization of a Two-Phase Stefan Problem

Wednesday 12:00pm - 12:30pm
Chiara Piazzola
Dynamical low-rank integrators for PDEs

Room: UR 3 | Wednesday 10:30am - 11:00am

Singular value decay of operator-valued differential Lyapunov and Riccati equations

Tony Stillfjord

Max Planck Institute Magdeburg, Germany

It is frequently observed in practice that the singular values of the solutions to differential Lyapunov equations (DLEs) or differential Riccati equations (DREs) decay very quickly. This is the basis for the low-rank approach which is often used in numerical methods for such equations: if a fast decay is not present, the solution approximant is either no longer of low rank or no longer a good approximant. In the former case, the computational cost and memory requirements become infeasible, and in the latter case the result is worthless. In spite of this, the literature contains very few, or any, theoretical results on when such decay is to be expected. The situation is better understood for algebraic Lyapunov and Riccati equations, but these results are not directly applicable to the differential case.
In this talk I will discuss recent results [1] on extending the algebraic results to the differential case. The main result is that one should not expect exponential decay, but exponential in the negative square root. We consider the operator-valued setting, with the standard assumption that the state operator A generates an analytic semigroup and the input and output operators B and C are not too unbounded. This corresponds, e.g., to the control of abstract parabolic problems where the control may act either in a distributed fashion or through the boundary conditions. In the commonly considered matrix-valued case, which corresponds to a spatial discretization of the operator-valued equation, exponential decay has been demonstrated. I will show by an example that this is only relevant for small-scale problems; as the discretization is refined this decay deteriorates and becomes exponential in the negative square-root.

[1] T. Stillfjord, Singular value decay of operator-valued differential Lyapunov and Riccati equations, SIAM J. Control Optim. 56(5) (2018), pp. 3598–3618.

Room: UR 3 | Wednesday 11:00am - 11:30am

An operator-valued differential equation approach for El Niño

Hermann Mena[1,2] **and** **Lena-Maria Pfurtscheller**[1]

[1] *University of Innsbruck, Austria*
[2] *Yachay Tech University, Ecuador*

In this talk, we consider the numerical approximation of stochastic partial differential equations based models for a quasi-periodic climate pattern in the tropical Pacific Ocean known as El Niño phenomenon. We show that for these models the mean and the covariance are given by a deterministic partial differential equation and by an operator-valued differential equation, respectively. In this context, we provide a numerical framework based on low-rank splitting methods to approximate these parameters directly. Numerical results for different scenarios taking as a reference measured data of the years 2014 and 2015 (last Niño event) validate the efficiency of our approach.

Room: UR 3 | Wednesday 11:30am - 12:00pm

Recent Advances in Riccati-Feedback Stabilization of a Two-Phase Stefan Problem

Björn Baran, Peter Benner and Jens Saak

Max Planck Institute for Dynamics of Complex Technical Systems, Germany

Our goal is the linear-quadratic feedback stabilization of a two-dimensional two-phase Stefan problem. The Stefan problem can model solidification and melting of pure materials and gets its name from the purely algebraic Stefan condition which describes the coupling between the temperature of the material and its melting process.
After linearization and discretization, the stabilization problem results in a non-autonomous differential Riccati equation (DRE) with differential-algebraic structure. The two phases in the domain evolve, which causes all coefficients of the resulting DRE to be time-varying. The problem specific collocation of Dirichlet conditions and outputs require special techniques for the finite element discretization.
Since all coefficients are time-varying, existing DRE solvers have to be adapted to this highly non-autonomous case which has significantly increased computational costs and memory requirements.
We present the most recent techniques to tackle the difficulties and show first results of the application of our feedback stabilization.

Room: UR 3 | Wednesday 12:00pm - 12:30pm

Dynamical low-rank integrators for PDEs

Chiara Piazzola

University of Innsbruck, Austria

In this talk we exploit the dynamical low-rank approximation (Koch, Lubich, 2007) for the solution of PDEs. The approach consists of constraining the evolution of the system to a low-rank manifold, such that the time integration is performed on a lower dimensional space. We employ this strategy for the solution of matrix differential equations arising after the space discretization of PDEs. Furthermore, we propose a low-rank integrator for the solution of the Vlasov–Maxwell equations, which are kinetic equations posed in an up to six dimensional space.
This talk is based on joint work with L. Einkemmer, A. Ostermann, and H. Walach.

MS 37
Simulation and sensitivity analysis of nonsmooth dynamical systems

Room: SR 3

Wednesday 10:30am - 11:00am
Kamil Khan
Advances in generalized derivative evaluation methods for nonsmooth ODEs

Wednesday 11:00am - 11:30am
Alexandre Rocca
Complementarity systems approach to switched ODEs and DAEs

Wednesday 11:30am - 12:00pm
Tom Streubel
Implicit Event Treatment for Numerical Integration of Continuous Piecewise Smooth ODEs using Piecewise Smooth Taylor Expansion

Wednesday 12:00pm - 12:30pm
Peter Stechlinski
Theory of nonsmooth DAEs with generalized differentiation index one

Room: SR 3

Wednesday 10:30am - 11:00am

Advances in generalized derivative evaluation methods for nonsmooth ODEs

Kamil Khan

McMaster University, Canada

Several numerical methods for nonsmooth systems require generalized derivatives at each iteration to gain local intuition. Such methods include semismooth Newton methods for equation-solving and bundle methods for local optimization. However, generalized derivatives can be difficult to furnish in practice, since they typically satisfy calculus rules only as inclusions. This presentation describes several recent advances in evaluating generalized derivatives for solutions of nonsmooth parametric ODEs with respect to parameters. These new methods leverage automatic differentiation techniques in new ways.

Room: SR 3

Wednesday 11:00am - 11:30am

Complementarity systems approach to switched ODEs and DAEs

Alexandre Rocca, Vincent Acary and Bernard Brogliato

Inria Grenoble-Alpes, France

In this work, we study differential algebraic equations with constraints defined in a piece-wise manner using conditional statement. Such models classically appear in systems where constraints can evolve in a very small time frame compared to the observed time scale.
The use of conditional statements or hybrid automata are a powerful way to describe such systems and are, in general, well suited to simulation with event driven numerical scheme. However, such methods are often subject to chattering at mode switch in presence of sliding modes, and can result in Zeno behaviours.
In contrast, the representation of such systems using differential inclusions and method from non-smooth dynamics are often closer to the physical theory but may be harder to interpret. Associated time-stepping numerical methods have been extensively used in mechanical modelling with success and then extended to other fields such as electronics and system biology.
In a similar manner to the previous application of non-smooth methods to the simulation of piece-wise linear ODEs we want to apply non-smooth numerical scheme to piece-wise linear DAEs. In particular, we will present the study of a 2-D dynamical system of index-2 with a switching constraint represented using set-valued operators.

Room: SR 3

Wednesday 11:30am - 12:00pm

Implicit Event Treatment for Numerical Integration of Continuous Piecewise Smooth ODEs using Piecewise Smooth Taylor Expansion

Tom Streubel[1,3], **Andreas Griewank**[2] **and Caren Tischendorf**[3]

[1] *Zuse Institute Berlin, Germany*
[2] *School of Mathematical Sciences and Information Technology, Yachaytech, Ecuador*
[3] *Humboldt University of Berlin, Germany*

In recent months we were able to prove that the concept of Taylor polynomial expansion can be enhanced into a piecewise polynomial expansion for piecewise smooth functions. The computation of this expansions can be realized efficiently by slight modifications to standard algorithmic differentiation tools. With this generalized Version of Taylor expansion at hand an explicit and implicit ODE integrator with consistency error of order 3 can be developed, ultimately allowing PEC or PECE integration schemes. We will discuss the expansion process, the two integrators and consider some numerical experiments.

Room: SR 3 | Wednesday 12:00pm - 12:30pm

Theory of nonsmooth DAEs with generalized differentiation index one

Peter Stechlinski[1], **Paul I. Barton**[2] **and Matthew R. Billingsley**[2]

[1] *Department of Mathematics and Statistics, University of Maine, USA*
[2] *Process Systems Engineering Laboratory, MIT, USA*

Nonsmooth DAEs naturally model the dynamics of a wide range of physical problems encountered in, for example, multibody mechanical systems, electrical circuits, atmospheric chemistry and process systems engineering. Traditionally such problems have been viewed as having continuous/discrete behavior, and thus modeled using various hybrid systems formalisms. However, a suitable foundational theory for nonsmooth DAEs is now available, including well-posedness, sensitivity and open-loop optimal control theory that mirrors classical theory for smooth DAEs. This theory is applicable to nonsmooth DAEs of generalized differentiation index one, which is implied by matrix-theoretic conditions involving generalized derivatives. Moreover, this theoretical toolkit is computationally relevant, allowing for simulations and dynamic optimization of large-scale problems. The new nonsmooth DAEs modeling paradigm advocated here applies to classes of optimization-constrained differential equations, complementarity systems and differential variational inequalities. Using the new approach outlined here, connections between nonsmooth DAEs and underlying discontinuous ODEs have been made, which is promising for sensitivity analysis of discontinuous dynamical systems.

MS 38
Spatially-adapted time discretizations for PDEs

Room: SR 3

Friday 10:30am - 11:00am
Chris Kees
A partition of unity approach to time and space adaptivity and limiting in continuous finite element methods

Friday 11:00am - 11:30am
Ludovica Delpopolo Carciopolo
Conservative multirate multiscale simulation of multiphase flow in heterogeneous porous media

Friday 11:30am - 12:00pm
Giacomo Rosilho de Souza
Multirate explicit stabilized integrators for stiff differential equations

Friday 12:00pm - 12:30pm
David I. Ketcheson
Relaxation Runge-Kutta methods: fully-discrete entropy-stability for hyperbolic PDEs

Room: SR 3

Friday 10:30am - 11:00am

A partition of unity approach to time and space adaptivity and limiting in continuous finite element methods

Chris Kees[1], **Manuel Quezada de Luna**[2] **and Dmitri Kuzmin**[3]

[1] *ERDC, United States of America*
[2] *KAUST, Saudi Arabia*
[3] *TU Dortmund, Germany*

The partition of unity finite element method provides a convenient but rigorous framework for blending space and time discretizations of different orders. In this work we consider the application of the method as an alternative to traditional hp-adaptivity for finite elements by using the convenient correspondence of nodes for Lagrange finite elements of different orders. We also consider continuous blending of time discretization methods across different regions of space, to take advantage of the different regularity and wave speeds in different spatial regions. These methods can be combined with traditional h-adaptivity and time adaptivity to yield methods with significant improvements in accuracy while still preserving fundamental properties such as conservation and discrete maximum principles. A range of numerical examples are given for standard model problems.

Room: SR 3 | Friday 11:00am - 11:30am

Conservative multirate multiscale simulation of multiphase flow in heterogeneous porous media

Ludovica Delpopolo Carciopolo[1], **Luca Formaggia**[1], **Anna Scotti**[1] **and Hadi Hajibeygi**[2]

[1] *Politecnico di Milano, Italy*
[2] *Tu Delft, Netherlands*

Accurate and efficient simulation of multiphase flow in heterogeneous porous media motivates the development of space-time multiscale strategies for the coupled nonlinear flow (pressure) and saturation transport equations. The flow equation entails heterogeneous high-resolution (fine-scale) coefficients and is global (elliptic or parabolic). The time-dependent saturation profile, on the other hand, has local sharp gradients (fronts) where the accuracy of the solution demands for tight time-step sizes. Therefore, accurate flow solvers need to resolve the spatial multiscale challenge, while advanced transport solvers need to also resolve the challenge related to time-step size. In this work, we develop the first integrated multirate multiscale method which implements a space-time conservative multiscale framework for sequentially coupled flow and transport equations. The method solves the pressure equation with a multiscale finite volume method at the spatial coarse scale, the transport equation is solved by taking different time-step sizes at different locations of the domain. At each time step, a coarse time step is taken, and then based on an adaptive recursive strategy, the front region is sharpened through a local-fine-scale time-stepping strategy. The accuracy and efficiency of the method are investigated for a wide range of heterogeneous test cases. The results demonstrate that the proposed method provides a promising strategy to minimise the accuracy-efficiency tradeoff by developing an integrated space-time multiscale simulation strategy.

Room: SR 3 | Friday 11:30am - 12:00pm

Multirate explicit stabilized integrators for stiff differential equations

Giacomo Rosilho de Souza[1], **Assyr Abdulle**[1] **and Marcus Grote**[2]

[1] *EPFL, Switzerland*
[2] *University of Basel, Switzerland*

We develop a new class of multirate explicit stabilized methods for stiff ordinary differential equations (ODE) involving different time scales. The method is based on a modified damped right hand side approximating the original equation and obtained via a stiffness reduction procedure. The modified equation is integrated employing an “outer” Runge–Kutta–Chebyshev (RKC) method. The stabilization procedure requires the solution of an auxiliary ODE, which depends only on the fast components of the original dynamics and is integrated with an “inner” RKC scheme.
Unlike other methods in the literature, our new scheme is fully explicit, does not exploit any clustering assumptions on the eigenvalues and does not need extrapolations. The global scheme is first order accurate and is stable in a large region along the negative real axis, whose width grows quadratically with the number of function evaluations. The method is particularly efficient for systems arising from spatially discretized parabolic differential equations on locally refined meshes. Numerical experiments confirm our theoretical findings, on accuracy, stability and efficiency.

References

A. Abdulle, M. Grote, G. Rosilho de Souza. Multirate explicit stabilized integrators for stiff differential equations (preprint).

Room: SR 3 | Friday 12:00pm - 12:30pm

Relaxation Runge-Kutta methods: fully-discrete entropy-stability for hyperbolic PDEs

David I. Ketcheson

King Abdullah University of Science & Technology, Saudi Arabia

Recent advances have enabled the development of efficient high-order entropy-stable discretizations for the Euler and Navier-Stokes equations. However, the strict entropy-stability property is destroyed by standard explicit time discretizations. I will present a class of Runge–Kutta-like methods, related to projection methods, that guarantee conservation or stability with respect to any inner-product norm, and thus provide fully-discrete entropy stability for symmetric hyperbolic systems at the same cost as standard explicit Runge-Kutta time stepping. Because of the methods' special form, they retain many desirable properties (including order of accuracy, approximate linear stability, and strong stability preservation) of the original Runge–Kutta method. I will show several numerical examples, including an extension to preservation of stability for arbitrary convex entropies such as the standard entropy for the Euler equations. This is joint work with H. Ranocha, M. Alsayyari, M. Parsani, and L. Dalcin.

MS 39: Part 1
Recent developments in multirate and related numerical methods for multiscale problems

Room: SR 2

Tuesday 11:00am - 11:30am
Mayya Tokman
On the construction of efficient hybrid time integrators for stiff systems

Tuesday 11:30am - 12:00pm
Carol Woodward
Evaluation of Implicit-Explicit Runge-Kutta Integrators for the HOMME-NH Dynamical Core

Tuesday 12:00pm - 12:30pm
Steven Roberts
Implicit Multirate GARK Methods

Room: SR 2

Tuesday 11:00am - 11:30am

On the construction of efficient hybrid time integrators for stiff systems

Mayya Tokman

University of California, Merced, USA

In this talk we discuss construction of efficient partitioned integrators that combine explicit, implicit or exponential integration approaches. We discuss why such integrators are of interest in applications and present several classes of new methods such as implicit-exponential, explicit-exponential and hybrid methods. Several concrete schemes and their performance on test problems will be presented. In addition, important issues will be considered in making these methods practical such as efficient calculation of exponential functions and parallelization of certain parts of an integrator.

Room: SR 2

Tuesday 11:30am - 12:00pm

Evaluation of Implicit-Explicit Runge-Kutta Integrators for the HOMME-NH Dynamical Core

Christopher Vogl[1], **Andrew Steyer**[2], **Daniel R. Reynolds**[3], **Paul Ullrich**[4] **and** **Carol Woodward**[1]

[1] *Lawrence Livermore National Laboratory, United States of America*
[2] *Sandia National Laboratories, United States of America*
[3] *Southern Methodist University, United States of America*
[4] *University of California at Davis, United States of America*

The nonhydrostatic High Order Method Modeling Environment (HOMME-NH) atmospheric dynamical core supports acoustic waves that propagate significantly faster than the advective wind speed, thus greatly limiting the timestep size that can be used with standard explicit time-integration methods. Resolving acoustic waves is unnecessary for accurate climate and weather prediction. This numerical stiffness is addressed by considering implicit-explicit additive Runge-Kutta (ARK IMEX) methods that can treat the acoustic waves in a stable manner without requiring implicit treatment of non-stiff modes. In this talk we discuss our work toward next-generation algorithms for non-hydrostatic simulations in global climate modeling. We focus on both modern, high-order methods for mixed implicit-explicit time discretizations, and customized nonlinear and linear solvers for solution of the resulting implicit algebraic systems. This talk will overview performance comparisons of various ARK IMEX methods evaluating for efficiency in producing accurate solutions, ability to take large timestep sizes, and sensitivity to grid cell length ratio. Both the Gravity Wave test and Baroclinic Instability test from the 2012 Dynamical Core Model Intercomparison Project (DCMIP) are used to recommend 5 of the 22 ARK IMEX methods for use in HOMME-NH.

Room: SR 2

Tuesday 12:00pm - 12:30pm

Implicit Multirate GARK Methods

Steven Roberts[1], **John Loffeld**[2], **Arash Sarshar**[1], **Adrian Sandu**[1] **and Carol Woodward**[2]

[1] *Virginia Tech, United States of America*
[2] *Lawrence Livermore National Laboratory*

This talk considers Multirate General-structure Additive Runge–Kutta (MrGARK) methods for solving stiff systems of ordinary differential equations (ODEs) with multiple time scales. These methods treat different partitions of the system with different timesteps for a more targeted and efficient solution compared to monolithic singlerate approaches. With implicit methods used across all partitions, methods must find a balance between stability and the cost of solving nonlinear equations for the stages. In order to characterize this important trade-off, we explore multirate coupling strategies, problems for assessing linear stability, and techniques to efficiently implement Newton iterations. Unlike much of the existing multirate stability analysis which is limited in scope to particular methods, we present general statements on stability and describe fundamental limitations for certain types of multirate schemes. New implicit multirate methods up to fourth order are derived, and there accuracy and efficiency properties are validated with numerical tests.

MS 39: Part 2
Recent developments in multirate and related numerical methods for multiscale problems

Room: SR 2

Tuesday 02:00pm - 02:30pm
Michael Günther
Interpolation/extrapolation based multilateral schemes for DAEs - a dynamic iteration perspective

Tuesday 02:30pm - 03:00pm
Vu Thai Luan
A new class of high-order methods for multirate differential equations

Tuesday 03:00pm - 03:30pm
John Loffeld
Experiences applying multirate methods to problem codes

Tuesday 03:30pm - 04:00pm
David Gardner
Multirate Integrators in SUNDIALS

Room: SR 2

Tuesday 02:00pm - 02:30pm

Interpolation/extrapolation based multilateral schemes for DAEs - a dynamic iteration perspective

Michael Günther, Andreas Bartel and Christoph Hachtel

Bergische Universität Wuppertal, Germany

Multilate scheme aim at exploiting different dynamics of subsystems by using different time steps adapted to the time scales of the subsystems. So far, multi step approaches for ODEs and DAEs are mainly based on two strategies: compound-step and interpolation/extrapolation based strategies, introduced first by Rice and Gear&Wells.
Whereas compound-step approaches have gained much intention in the last years, interpolation/extrapolation based ideas had been discussed mainly in the 80s and 90s of the last century. In this presentation we will interpret interpolation/extrapolation based multi rate schemes in the framework of dynamic iteration schemes, allowing an easy way to construct multi rate schemes for ODEs and index-1 DAEs.

Room: SR 2

Tuesday 02:30pm - 03:00pm

A new class of high-order methods for multirate differential equations

Vu Thai Luan, Rujeko Chinomona and Daniel R. Reynolds

Southern Methodist University (SMU), United States of America

This talk focuses on the development of a new class of high-order accurate methods for multirate time integration of systems of ordinary differential equations. More precisely, starting from an explicit exponential Runge–Kutta method of the appropriate form, we derive a multirate algorithm to approximate the action of the matrix exponential through the definition of modified" fast" initial-value problems. These fast problems may be solved using any viable solver, enabling multirate simulations through use of a subcycled method. Due to this structure, we name these as Multirate Exponential Runge–Kutta (MERK) methods. In addition to showing how MERK methods may be derived, we provide rigorous convergence analysis, showing that for an overall method of order p, the fast problems corresponding to internal stages may be solved using a method of order $p-1$, while the final fast problem corresponding to the time-evolved solution must use a method of order p. Numerical simulations are then provided to demonstrate the convergence and efficiency of MERK methods with orders three through five on a series of multirate test problems.

Room: SR 2 | Tuesday 03:00pm - 03:30pm

Experiences applying multirate methods to problem codes

John Loffeld[1], **Steven Roberts**[2], **David Gardner**[1], **Rujeko Chinomona**[3], **Carol Woodward**[1] **and Adrian Sandu**[2]

[1]*Lawrence Livermore National Laboratory, United States of America*
[2]*Virginia Polytechnic Institute and State University*
[3]*Souther Methodist University*

In recent years there has been a surge of attention in developing new multirate methods. So far these new schemes have mostly been studied on simpler test problems and not application problems. In this talk we present our experience in applying newer multirate schemes to a microphysics climate code and an unsteady flame problem. The former problem is non-stiff and can be solved using explicit methods while the latter is highly stiff and requires implicit schemes. We discuss how a high degree of stiffness in problems continues to be a challenge for implicit multirate methods.
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-774275.

Room: SR 2 | Tuesday 03:30pm - 04:00pm

Multirate Integrators in SUNDIALS

David Gardner[1], **Carol Woodward**[1], **Daniel R. Reynolds**[2], **Alan Hindmarsh**[1] **and Cody Balos**[1]

[1]*Lawrence Livermore National Laboratory*
[2]*Southern Methodist University*

SUNDIALS is a suite of robust and scalable solvers for systems of ordinary differential equations, differential-algebraic equations, and nonlinear equations designed for use on computing systems ranging from desktop machines to super computers. Originally developed in SUNDIALS as a library for additive Runge-Kutta methods, the ARKode package was recently refactored to serve as an infrastructure for general, adaptive, one-step time integration methods. Leveraging SUNDIALS' modular design, this new infrastructure enables the rapid development of time integration algorithms for the parallel solution of large-scale ODE systems arising from multi-physics applications. In particular, we will discuss the addition of MIS-type multi-rate methods in ARKode utilizing this updated infrastructure.
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-774275.

Contributed Sessions

CS 01
Monte Carlo methods, SDEs

Room: SR 16

Friday 10:30am - 11:00am
Leila Taghizadeh
Bayesian inference for two inverse problems in tomography and biofilms

Friday 11:00am - 11:30am
Ujjwal Koley
A finite difference scheme for conservation laws with noise

Friday 11:30am - 12:00pm
Zhaocheng Xuan
A finite elements based probabilistic numerical method for the solution of contact forces in elastic contact problems

Friday 12:00pm - 12:30pm
Alexander Steinicke
QMC rates for backward SDEs with smooth Hermite terminal conditions

Room: SR 16 | Friday 10:30am - 11:00am

Bayesian inference for two inverse problems in tomography and biofilms

Leila Taghizadeh and Clemens Heitzinger

TU Vienna, Austria

Real-world simulation and optimization problems usually include equations with unknown parameters, which cannot be determined directly from the experiments or the computational models. We apply Bayesian estimation to two real-world problems in life sciences and healthcare, namely electrical-impedance tomography (EIT) and biofilms, as this approach is capable of dealing with the ill-posedness and nonlinearity of the inverse problems naturally and successfully. The applications include for instance, body composition and detection of diseases in the case of EIT, as well as biofilms on teeth, on medical implants, and in food processing in the case of biofilms.

In an EIT sensor, which can be modeled by the nonlinear Poisson-Boltzmann equation, small voltages or currents are applied to the object of study through the electrodes which are attached to its surface and the resulting currents or voltages are measured at the contacts. The goal is to extract the quantities of interest in the model, such as permittivities, charges, and sizes of inclusions or material layers in the main body.

In the case of biofilms, we propose a model based on a system of PDEs which describes the time dependent evolution of growth and degradation of biofilms, as well as quorum sensing. The goal here is to recover important parameters of the model such as the growth rate and the diffusion parameter.

In these two inverse problems, we use an adaptive Metropolis-Hastings algorithm to extract the unknown quantities. The numerical results show good convergence of the Markov chains and accurate extraction of confidence intervals.

Furthermore, we study the Bayesian analysis in the measure-theoretic framework for the EIT model and prove well-definedness of the posterior measure and and well-posedness of the Bayesian-estimation problem.

Room: SR 16 | Friday 11:00am - 11:30am

A finite difference scheme for conservation laws with noise

Ujjwal Koley

TIFR CAM, India

In this talk, we discuss a semi-discrete finite difference scheme for a conservation laws driven by noise. Thanks to BV estimates, we show a compact sequence of approximate solutions, generated by the finite difference scheme, converges to the unique entropy solution of the underlying problem, as the spatial mesh size goes to zero. Moreover, we show that the expected value of the L^1-difference between the approximate solution and the unique entropy solution converges at an expected rate.

Room: SR 16

Friday 11:30am - 12:00pm

A finite elements based probabilistic numerical method for the solution of contact forces in elastic contact problems

Zhaocheng Xuan

Tianjin University of Technology and Education, China, People's Republic of

When the elastic bodies in contact mechanics are discretized by finite elements, we can select the nodes on the potential contact interface as objects to which the probability numerical method can be applied. Each potential contact node along with its normalized contact force is considered as a system, and all potential contact nodes together with their normalized contact forces are considered as a canonical ensemble with the normalized contact force of each node representing the microstate of the node, then entropy and its use in statistical analysis are extended to evaluate the contact forces. The product of non-penetration conditions for potential contact nodes and the normalized nodal contact forces may act as an expectation that its value will be zero, and maximizing the entropy under the constraints of the expectation and the minimum potential energy principle results in an explicit probability distribution for the normalized contact forces that shows the relation between contact forces and displacements in a formulation similar to the formulation for particles occupying microstates in statistical mechanics. Moreover, an iterative procedure that solves a series of isolated systems to find the contact forces is presented. Finally, some examples are examined to verify the correctness and efficiency of the method.

Room: SR 16 | Friday 12:00pm - 12:30pm

QMC rates for backward SDEs with smooth Hermite terminal conditions

Alexander Steinicke[1], **Gunther Leobacher**[2] **and Stefan Kremsner**[2]

[1] *Montanuniversitaet Leoben, Austria*
[2] *Karl-Franzens Universität Graz, Austria*

Solving backward stochastic differential equations (BSDEs) numerically is a difficult task. For the non-Markovian case, where Feynman-Kac approaches via PDEs are not feasible in an easy way anymore, there are several schemes available to approximate the BSDE's solution directly. However, all these schemes demand high numbers of path simulations for the computation of appearing conditional expectations (by regression methods or by computation of the Wiener chaos decomposition of random variables). We considered the Picard iteration scheme for BSDEs of Briand & Labart (2014), which is based on chaos decomposition techniques, and we replaced the original Monte Carlo (MC) methods by Quasi-Monte Carlo (QMC) methods. Numerical experiments confirmed the usual rate improvement (MC to QMC): convergence of order 1 in place of $\frac{1}{2}$. With the BSDE's terminal condition in a weighted Hermite space and for a suitable class of generators, we prove that the QMC-techniques lead to the mentioned rate enhancement for computing chaos decompositions of random variables and of the Picard iteration scheme.

CS 02
Plasma physics

Room: SR 16

Monday 02:00pm - 02:30pm
Yingzhe Li
Numerical simulations of Vlasov-Maxwell equations for laser plasma based on Poisson structure

Monday 02:30pm - 03:00pm
Yanyan Shi
Study of adaptive symplectic methods for simulating charged particle dynamics

Monday 03:00pm - 03:30pm
Markus Gasteiger
Numerical algorithms for kinetic simulations of the plasma edge

Monday 03:30pm - 04:00pm
Timm Treskatis
The Elastoviscoplastic Navier-Stokes Equations: Mimetic Discretisation and Preconditioned Defect Correction

Room: SR 16 | Monday 02:00pm - 02:30pm

Numerical simulations of Vlasov-Maxwell equations for laser plasma based on Poisson structure

Yingzhe Li[1,2,3], **Yajuan Sun**[1,2] **and Nicolas Crouseilles**[3,4]

[1] *LSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences*
[2] *University of Chinese Academy of Sciences*
[3] *University of Rennes 1*
[4] *MINGuS, Inria Bretagne Atlantique, ENS Rennes*

In this talk, Poisson bracket for a reduced Vlasov model describing laser plasma interaction is proposed, which can be derived from the the Poisson bracket of Vlasov-Maxwell system by a coordinate transformation. Then a splitting method is proposed based on the decomposition (into three parts) of the Hamiltonian; in the quasi-relativistic case, the solutions of these three subsystems can be written out explicitly. Fourier spectral method and finite volume method are used in phase space discretization. The splitting is extended to the fully relativistic case combined with conservative splitting method. Finally, some numerical experiments are conducted to confirm good long time behavior of our schemes.

Room: SR 16 | Monday 02:30pm - 03:00pm

Study of adaptive symplectic methods for simulating charged particle dynamics

Yanyan Shi[1,2], **Yajuan Sun**[1,2], **Yang He**[3], **Hong Qin**[4,5] **and Jian Liu**[5,6]

[1] *LSEC, ICMESEC, Academy of Mathematics and Systems Science, CAS, China*
[2] *School of Mathematical Sciences, University of Chinese Academy of Sciences, China*
[3] *School of Mathematics and Physics, University of Science and Technology, Beijing, China*
[4] *Plasma Physics Laboratory, Princeton University, Princeton, USA*
[5] *Department of Engineering and Applied Physics, USTC, Hefei*
[6] *Key Laboratory of Geospace Environment, CAS, China*

In this talk, the symplectic methods with adaptive time step strategy are introduced and analyzed for the study of the motion of charged particles in electromagnetic field. By presenting two kinds of step size functions, we simulate the motion of charged particles confined in a Penning trap under three different magnetic fields, and also investigate the dynamics of runaway electrons in tokamak. The numerical experiments illustrate the good performance of the new derived step size functions.

Room: SR 16 | Monday 03:00pm - 03:30pm

Numerical algorithms for kinetic simulations of the plasma edge

Markus Gasteiger

University of Innsbruck, Austria

The inhomogeneous Vlasov equation, a non-linear partial differential equation, is used in plasma physics to simulate the time-dependent distribution of particles in real and velocity space. There the particle interactions are modeled with collisions. The presented plasmas contain multiple species and various collision operators. Consequently, there are also quantities, e.g. the electric field, that must be determined self-consistently. Solvers for the ensuing systems of Vlasov and additional closure equations, e.g. Poisson's equation, are computationally expensive. Therefore, simulations of physically interesting problems require immense resources.
We reduce the computational effort by splitting the computation of the electric field, i.e. the closures, and also the species-specific Vlasov equations. Furthermore, we investigate how to optimally handle the specific collision operators. For the resulting equations a range of optimized numerical methods can be used (such as semi-Lagrangian schemes, preconditioned Krylov methods, ...). Most of these algorithms can be formulated in the framework of stencil computations. This means that we are able to achieve an efficient implementation, while still providing a high level interface to the user of the software.
In this talk we consider numerical experiments with parameters relevant to edge plasmas. These simulations are time-dependent and conducted in one space and two velocity dimensions. In particular, we will consider quantities like particle density or energy flux and how they are modified by different collision models. These quantities are relevant when designing the divertor targets in fusion devices.

Room: SR 16

Monday 03:30pm - 04:00pm

The Elastoviscoplastic Navier-Stokes Equations: Mimetic Discretisation and Preconditioned Defect Correction

Timm Treskatis

The University of British Columbia, Canada

Realistic models of complex fluids include viscous dissipation, but also an elastoplastic response to stresses. Flows of such gels or pastes can be described by the incompressible Navier-Stokes equations, complemented with a nonlinear and nonsmooth transport equation for the non-Newtonian stress contribution.

To solve this system numerically, we propose a pressure robust, mass and momentum conservative discontinuous Galerkin scheme, and a fully coupled, genuinely nonsmooth yet efficient nonlinear solver. Numerical results shall complement this presentation.

CS 03
Wave equations

Room: SR 16

Wednesday 10:30am - 11:00am
Constantin Carle
On Leapfrog-Chebyshev schemes

Wednesday 11:00am - 11:30am
Bernhard Maier
Space discretization of quasilinear wave-type equations

Wednesday 11:30am - 12:00pm
Mirko Residori
A splitting integrator for third order problems with transparent boundary conditions

Room: SR 16 | Wednesday 10:30am - 11:00am

On Leapfrog-Chebyshev schemes

Constantin Carle, Marlis Hochbruck and Andreas Sturm

Karlsruhe Institute of Technology, Germany

In this talk we consider variants of the leapfrog method for second order differential equations. In numerous situations the strict CFL condition of the standard leapfrog method is the main bottleneck that thwarts its performance. Based on Chebyshev polynomials new methods have been constructed that exhibit a much weaker CFL condition than the leapfrog method.
We will analyze the stability and the long-time behavior of leapfrog-Chebyshev methods in two-step formulation. This analysis indicates that one should modify the schemes proposed in the literature in two ways to improve their qualitative behavior.
For linear problems, we propose to use special starting values required for a two-step method instead of the standard choice obtained from Taylor approximation. For semilinear problems, we propose to introduce a stabilization parameter as it has been done for Runge-Kutta-Chebyshev methods before. For the stabilized methods we prove that they guarantee stability for a large class of problems.
While these results hold for quite general polynomials, we show that the polynomials used in the stabilized leapfrog Chebyshev methods satisfy all the necessary conditions. In fact, all constants in the stability and error analysis can be given explicitly.
The talk concludes with numerical examples illustrating our theoretical findings.
This is joint work with Marlis Hochbruck and Andreas Sturm, Karlsruhe Institute of Technology, funded by CRC 1173.

Room: SR 16 | Wednesday 11:00am - 11:30am

Space discretization of quasilinear wave-type equations

Marlis Hochbruck and Bernhard Maier

Karlsruhe Institute of Technology, Germany

We consider the numerical approximation of solutions to quasilinear wave-type equations of the form

$$\Lambda(y(t))y'(t) = Ay(t) + Q(y(t))y(t)$$

subject to homogeneous Dirichlet boundary conditions on a bounded domain with smooth boundary. Here, A is a linear skew-adjoint operator and the nonlinearities Λ and Q model for example nonlinear material laws such as the Kerr nonlinearity. Although the problem is well understood analytically, to the best of our knowledge, the full discretization of this general class of PDEs has not been studied so far.

As a first step to close this gap, we present an error analysis for general nonconforming space discretizations of quasilinear wave-type equations with finite elements. This includes a well-posedness result for the semi-discrete quasilinear wave-type equation, where we show that the solution to the semi-discrete problem exists at least as long as the solution to the continuous problem. As our main result, we provide an error bound in the energy norm with the same order of convergence as it is known for linear problems.

We conclude with a brief outlook towards the full discretization of quasilinear wave-type equations.

Room: SR 16 | Wednesday 11:30am - 12:00pm

A splitting integrator for third order problems with transparent boundary conditions

Mirko Residori

University of Innsbruck, Austria

The goal of the present work is to solve a linear dispersive equation with variable coefficient advection on an unbounded domain. Numerical simulations, however, are typically performed on a finite computational domain. This truncation of the unbounded domain introduces boundary conditions which must be carefully design in order to obtain a numerical solution that retains the same properties as the solution over the unbounded domain. Such boundary conditions are known as transparent boundary conditions (TBCs).
Designing numerical schemes with TBCs presents some difficulties since these boundary conditions are non-homogeneous and non-local in time and space. We choose to discretize space using a spectral method. This allows us to drastically reduce the number of grid points required for a given accuracy. Applying a fully implicit time integrator, however, would require us to invert full matrices. To overcome this problem an operator splitting scheme is applied so that the third order differential operator and the advection part are treated separately. This approach can also be interpreted as an IMEX scheme. We show how to design the numerical scheme and perform a number of numerical simulations.

CS 04
Maxwell - electromagnetism

Room: SR 16

Thursday 10:30am - 11:00am
Hayley Wragg
A generalised ray-launching approach to modeling high frequency electromagnetic wave propagation.

Thursday 11:00am - 11:30am
Jan Philip Freese
Numerical Homogenization of the Maxwell-Debye system

Thursday 11:30am - 12:00pm
Konstantin Zerulla
Error analysis of an ADI splitting scheme for Maxwell equations in heterogeneous media

Thursday 12:00pm - 12:30pm
Jonas Köhler
Error analysis of an ADI splitting for discontinuous Galerkin discretizations of linear wave-type problems

Room: SR 16 | Thursday 10:30am - 11:00am

A generalised ray-launching approach to modeling high frequency electromagnetic wave propagation.

Hayley Wragg

University of Bath, United Kingdom

Wireless communication has become a significant part of society with recent developments to the internet of things increasing the number of devices connecting in one home. This has increased user demand for bandwidth and lead to developments in new transmitter types. One of these developments is ultra-high frequency transmitters.
In this talk I will look at propagation models for high frequency electromagnetic waves with a particular focus of developing highly efficient ray-launching methods appropriate in cluttered unknown environments.
As well as developing models we are also developing a systematic computational tool to implement them with the aim of improving the quality and speed of optimisation.
The adapted ray-launching method uses the same assumptions as standard ray-tracing methods but the implementation allows us to output an expression for the value at a point without inputting all environment parameters.

Room: SR 16

Thursday 11:00am - 11:30am

Numerical Homogenization of the Maxwell-Debye system

Jan Philip Freese[1], Christian Wieners[1] and Dietmar Gallistl[2]

[1] *Karlsruhe Institute of Technology, Germany*
[2] *University of Twente, The Netherlands*

In this talk we investigate time-dependent Maxwell's equations coupled with the Debye polarization model in a medium with highly oscillatory parameters and thus with oscillating solutions.

$$\begin{aligned} \varepsilon^\delta \partial_t \mathbf{E}^\delta(t) + (\tau^\delta)^{-1}\nu^\delta \mathbf{E}^\delta(t) - (\tau^\delta)^{-1}\mathbf{P}^\delta(t) + \operatorname{curl} \mathbf{H}^\delta(t) &= -\mathbf{J}^\delta(t) \\ \mu^\delta \partial_t \mathbf{H}^\delta(t) - \operatorname{curl} \mathbf{E}^\delta(t) &= \mathbf{0} \\ \tau^\delta \partial_t \mathbf{P}^\delta(t) + \mathbf{P}^\delta(t) - \nu^\delta \mathbf{E}^\delta(t) &= \mathbf{0} \end{aligned}$$

We use analytical homogenization results to derive the effective Maxwell-Debye system with the corresponding cell problems. The solution of this effective system is the macroscopic part of the oscillating solution in which we are interested. Due to homogenization the system includes a convolution with a new time-dependent parameter whose corresponding cell corrector is also time-dependent. This time-dependence is the challenge, both in the implementation and in the analysis of the numerical scheme. We apply the Finite Element Heterogeneous Multiscale Method (FE-HMM) to solve the effective Maxwell-Debye system since the HMM is suitable in the context of locally periodic parameters. Finally, we present our semi-discrete error analysis and show numerical results that we have realized in the finite element library deal.II.

Room: SR 16

Thursday 11:30am - 12:00pm

Error analysis of an ADI splitting scheme for Maxwell equations in heterogeneous media

Konstantin Zerulla

Karlsruhe Institute of Technology (KIT), Germany

Alternating direction implicit (ADI) schemes are very attractive for the time integration of linear Maxwell equations on cuboids since they are unconditionally stable and have only linear complexity.
We here investigate the inhomogeneous linear isotropic Maxwell equations involving nontrivial conductivity, currents and charges. The considered domain is a cuboid which is divided into two smaller subcuboids. Each subdomain is further made of a homogeneous medium, but the two media may be different. This means that the corresponding material parameters are allowed to have a discontinuity at the interface between the two subcuboids.
Based on a regularity analysis for the Maxwell system, we provide a rigorous error analysis for the Peaceman-Rachford ADI scheme in the abstract time-discrete setting. The error result implies convergence of the method in L^2 to the exact solution of the Maxwell equations, and it involves only reasonable assumptions on the initial data but none on the exact solution.

Room: SR 16 | Thursday 12:00pm - 12:30pm

Error analysis of an ADI splitting for discontinuous Galerkin discretizations of linear wave-type problems

Marlis Hochbruck and Jonas Köhler

Karlsruhe Institute of Technology, Germany

We consider an alternating direction implicit (ADI) scheme for the approximation of a class of linear wave-type problems of the form

$$u' = Lu$$

on product domains. This class comprises important examples such as the 2D advection and wave equations as well as the 3D Maxwell's equations.

To discretize the equation in time, we split $L = A+B$, where the flows of A and B essentially decouple into one-dimensional flows. This allows for computationally cheap, yet unconditionally stable time integration via the Peaceman–Rachford (PR) scheme

$$u^{n+1} = (I - \tfrac{\tau}{2}B)^{-1}(I + \tfrac{\tau}{2}A)(I - \tfrac{\tau}{2}A)^{-1}(I + \tfrac{\tau}{2}B)u^n.$$

In order to obtain a fully discretized scheme, we use a central fluxes discontinuous Galerkin scheme for the discretization of the (split) operators. Efficiency of the resulting fully discrete scheme was investigated in [1].

In this talk, we investigate the convergence of the aforementioned ADI scheme. We derive error bounds that are robust under mesh refinement and exhibit optimal order in time and space. The proof exploits the fact that the PR scheme can be interpreted as a perturbation of the Crank–Nicolson scheme. This enables us to employ techniques developed in [2] for a locally implicit scheme. However, because of the splitting nature of the PR scheme, additional error terms arise, which have to be treated in a different manner. We tackle these terms by using the approximation properties of the discrete operators.

[1] Hochbruck, Köhler: On the efficiency of the Peaceman–Rachford ADI-dG method for wave-type problems (2019). Numerical Mathematics and Advanced Applications ENUMATH 2017.

[2] Hochbruck, Sturm: Error analysis of a second-order locally implicit method for linear Maxwell's equations (2016). SIAM J. Numer. Anal., 54(5):pp. 3167–3191.

CS 05
Monte Carlo, SDEs

Room: SR 17

Wednesday 10:30am - 11:00am
Grégoire Ferré
Error estimates on ergodic properties of Feynman-Kac semigroups

Wednesday 11:00am - 11:30am
Nada Cvetkovic
A convergent discretisation scheme for diffusion process transition path theory

Wednesday 11:30am - 12:00pm
Tsiry Avisoa Randrianasolo
Time-discretization of stochastic 2-D Navier–Stokes equations with a penalty-projection method

Wednesday 12:00pm - 12:30pm
Qian Guo
The truncated method for highly nonlinear stochastic differential equations

Room: SR 17 | Wednesday 10:30am - 11:00am

Error estimates on ergodic properties of Feynman-Kac semigroups

Grégoire Ferré and Stoltz Gabriel

CERMICS - Ecole des Ponts ParisTech, France

Feynman-Kac dynamics appear in several areas of mathematics, including large deviations theory, diffusion Monte Carlo methods and nonlinear filtering. Loosely speaking, they can be though of as a probabilistic representation for the principal eigenvalue and eigenvector of a second order linear operator. In particular, the dynamics is run for a long time until it converges to equilibrium, a standard procedure for Monte Carlo Markov Chain (MCMC) methods (similarly to sampling from a probability distribution).

In practice, like other MCMC approaches, the stochastic process at hand has to be discretized with a finite time step to be implemented in a numerical method. This discretization procedure induces a systematic bias which remains even when statistical sampling is perfect. It has been the purpose of many works in the past twenty years to quantify precisely the bias in the time step for ergodic properties of stochastic processes, but this had not been done yet for these Feynman-Kac dynamics, which are of interest in many situations. I will present a recent work with G. Stoltz that provides precise error estimates in this case, depending on the numerical scheme at hand. We will see that the difficulty relies on the non-linear feature of the dynamics, for which we designed new technical tools. Numerical simulations in various situations will be presented in order to illustrate the theoretical results.

Room: SR 17 | Wednesday 11:00am - 11:30am

A convergent discretisation scheme for diffusion process transition path theory

Nada Cvetkovic[1], **Tim Conrad**[1] **and Han Cheng Lie**[2]

[1] *Freie Universität, Berlin, Germany*
[2] *Universität Potsdam, Germany*

Many applications involve analysing dynamical systems that undergo rare transitions between two metastable subsets A and B of state space. E and Vanden-Eijnden (J. Stat. Phys., 2006) formulated transition path theory (TPT) for ergodic diffusion processes, by constructing objects that describe the statistics of 'reactive trajectories', i.e. trajectory segments that leave A and enter B before re-entering A. These objects include the committor function, which assigns to each state the probability that a trajectory starting at that state enters B before A, and a vector field called the 'probability current', the integral curves of which describe the average behaviour of reactive trajectories. To compute these objects, one often needs to solve the backward Kolmogorov equation, which is a second order partial differential equation and is hence difficult to solve in high dimensions using standard methods.
We use Voronoi tessellations to discretise state space, and model the underlying diffusion process by a jump process on the associated Delaunay graph. For this process, we construct the analogues of the committor and probability current that can be approximated using sampled trajectory data. Our Monte Carlo approach thus avoids direct solution of the Kolmogorov equation. Our approach differs from the TPT developed by Metzner et al. (Multiscale Model. Simul., 2009), because we do not require our jump process to be Markovian. Furthermore, we derive rigorous estimates of the approximation errors of our discrete TPT objects with respect to their continuous counterparts in TPT for diffusion processes, and use these estimates to prove convergence in the limit of fine discretisation.

Room: SR 17 | Wednesday 11:30am - 12:00pm

Time-discretization of stochastic 2-D Navier–Stokes equations with a penalty-projection method

Tsiry Avisoa Randrianasolo[1] **and Erika Hausenblas**[2]

[1] *Bielefeld university, Germany*
[2] *Montanuniversitaet Leoben, Austria*

In this talk, a time-discretization of the stochastic incompressible Navier–Stokes problem by penalty method is analyzed. Some error estimates are derived, combined, and eventually arrive at a speed of convergence in probability of order 1/4 of the main algorithm for the pair of variables velocity and pressure. Also, using the law of total probability, we obtain the strong convergence of the scheme for both variables.

Room: SR 17 | Wednesday 12:00pm - 12:30pm

The truncated method for highly nonlinear stochastic differential equations

Qian Guo[1], **Wei Liu**[1], **Xuerong Mao**[2] **and Rongxian Yue**[1]

[1] *Department of Mathematics, Shanghai Normal University, Shanghai, China*
[2] *Department of Mathematics and Statistics, University of Strathclyde, Glasgow G1 1XH, UK*

When the global Lipschitz condition is disturbed, the classical Euler–Maruyama method has been proved divergent for solving stochastic differential equations(SDEs) with highly nonlinear coefficients. The tamed method is one of the most popular explicit methods that were developed particularly for the highly nonlinear SDEs. In this talk, we introduce another efficient approach, named the truncated method. The finite-time strong L^r-convergence theory for the truncated methods are established. We also demonstrate the real benefit of the method by showing that the method can preserve the asymptotic stability and boundedness of the underlying SDEs.

CS 06
Highly oscillatory problems, symplecticity

Room: SR 17

Friday 10:30am - 11:00am
Winfried Auzinger
Precise local error control for symmetric one-step schemes applied to nonlinear evolution equations

Friday 11:00am - 11:30am
Jitse Niesen
Convergent modified Hamiltonians for integrable discretization schemes

Friday 11:30am - 12:00pm
Hongjiong Tian
Asymptotic-numerical solvers for highly oscillatory Hamiltonian systems

Friday 12:00pm - 12:30pm
Philip William Sharp
The Crossover Point for Symplectic Methods Applied to N-Body Simulations of the Solar System

Room: SR 17

Friday 10:30am - 11:00am

Precise local error control for symmetric one-step schemes applied to nonlinear evolution equations

Winfried Auzinger[1], **Harald Hofstätter**[2] **and Othmar Koch**[2]

[1] *Technische Universität Wien, Austria*
[2] *Universität Wien, Austria*

Controlling the local error in time (and adapting the stepsize) of one-step methods for evolution equations can be performed in different ways. For a number problem classes (e.g., equations of Schrödinger type) defect-based techniques are useful because the defect (residual) of the numerical solution can be evaluated efficiently, resulting in an asymptotically correct local error estimator.
We recall the idea of this technique, and concentrate on the case of symmetric schemes. Here the asymptotic quality of the estimator can be further be increased by computing a 'symmetrized' version of the defect. This can also be used as a corrector resulting in a higher-order scheme. We demonstrate that this inherits symmetry, and also symplecticity, of the underlying lower-order scheme asymptotically in a very precise way. Numerical examples are presented.

Room: SR 17 | Friday 11:00am - 11:30am

Convergent modified Hamiltonians for integrable discretization schemes

Shami Alsallami[1], **Jitse Niesen**[2] **and Frank Nijhoff**[2]

[1] *Umm Al-Qura University, Saudi Arabia*
[2] *University of Leeds, United Kingdom*

Backward error analysis shows that when a Hamiltonian system is solved by a symplectic integrator, the numerical result is (almost) the exact solution of a modified Hamiltonian system. However, for most nonlinear systems the modified Hamiltonian does not really exist because the series defining it diverges. Here we describe an example of a nonlinear system where the modified Hamiltonian has a closed-form expression and hence converges. This discretization arises as an integrable lattice equation discretizing the potential KdV equation on a periodic domain; we will mention a similar construction for the Boussinesq equation. Numerical results indicate how useful these discretizations may be in practice.

Room: SR 17 | Friday 11:30am - 12:00pm

Asymptotic-numerical solvers for highly oscillatory Hamiltonian systems

Hongjiong Tian and **Zhongli Liu**

Shanghai Normal University, China, People's Republic of

We are concerned with asymptotic-numerical solvers for highly oscillatory ordinary differential equations and Hamiltonian systems. First, we derive an asymptotic expansion of the exact solution in inverse powers of the oscillatory parameter, featuring only a finite number of non-zero expansion coefficients in each term. We then use the truncation with the first few terms of the asymptotic expansion as an effective means to approximate the highly oscillatory problems. The error estimation of the asymptotic-numerical solver is analyzed and nearly conservation of the energy in the Hamiltonian case is proved. The numerical experiments on the Fermi-Pasta-Ulam problem are implemented to show the efficiency of our proposed methods.

Room: SR 17 | Friday 12:00pm - 12:30pm

The Crossover Point for Symplectic Methods Applied to N-Body Simulations of the Solar System

Philip William Sharp

University of Auckland, New Zealand

It is well known that the error in the position when symplectic methods are applied to N-body simulations varies as t as against t^2 for non-synplectic methods. Hence for sufficiently large t symplectic methods should be more efficient than non-symplectic methods. We investigate numerically for representative explicit Runge Kutta Nystrom methods just how large t must be for simulations of the Solar System and how this value of t compares with the time scales in the Solar System.

CS 07
Time integration

Room: SR 17

Monday 02:00pm - 02:30pm
Saghir Ahmad
Stiffness switching in general linear methods

Monday 02:30pm - 03:00pm
Zdzislaw Jackiewicz
Local error estimation for implicit-explicit general linear methods

Monday 03:00pm - 03:30pm
Laurent O. Jay
A starting approximation algorithm of arbitrarily high order for implicit methods

Monday 03:30pm - 04:00pm
Chengming Huang
Stability analysis of VDRK methods for the second kind Volterra integro-differential equations

Room: SR 17 | Monday 02:00pm - 02:30pm

Stiffness switching in general linear methods

Saghir Ahmad[1], **John Charles Butcher**[2] **and Winston Sweatman**[3]

[1] *Auckland Institute for Studies, New Zealand*
[2] *University of Auckland New Zealand*
[3] *Massey University New Zealand*

General linear methods (GLMs) have been recently implemented using both variable order and variable stepsize. The selection of order and stepsize is based on minimizing error and work combined using a Lagrange multiplier.
Using the Lagrange approach for the GLMs in [1, 2], some heuristics can be avoided, along with optimal selection of stepsize, and order during the integration. These heuristics include the safety factor used in classical controllers, to avoid un-necessary rejection of steps. This idea has been tested numerically to solve stiff problems [2] as well as non-stiff problems [1] on separate occasions.
Existing ODE solvers treat stiff and non–stiff problems separately. However, our aim is to construct a solver which automatically detects stiffness and switches between stiff and non-stiff modes using the variant of the Lagrange multiplier techniques. Numerical tests can be based on stiff, non-stiff, and mildly stiff problems, to further optimize cost and accuracy in a numerical integrator.

References

[1] S. Ahmad, J. C. Butcher, W. Sweatman, *Variable order and stepsize in general linear methods*, Numerical Algorithms 80, 2019

[2] J. C. Butcher, H. Podhaisky, *On error estimation in general linear methods for stiff ODEs*, Appl. Numer. Math. 56, 345-357, 2006.

Room: SR 17 | Monday 02:30pm - 03:00pm

Local error estimation for implicit-explicit general linear methods

Zdzislaw Jackiewicz[1], **Angelamaria Cardone**[2] **and Giuseppe Izzo**[3]

[1] *Arizona State University, United States of America*
[2] *University of Salerno, Italy*
[3] *University of Naples, Italy*

We investigate implicit-explicit methods for differential systems with stiff and non-stiff parts. Stage order and order conditions are formulated and estimation of local discretization errors in fixed and variable stepsize environments is discussed. We also describe the construction of such methods with desirable accuracy and stability properties.

Room: SR 17 | Monday 03:00pm - 03:30pm

A starting approximation algorithm of arbitrarily high order for implicit methods

Laurent O. Jay

The University of Iowa, United States of America

We consider the application of any type of implicit methods to initial value problems. We illustrate the results in particular for implicit Runge-Kutta (IRK) methods. We propose a new starting approximation algorithm for the internal stages of IRK methods based on the iterated correction of any starting approximation such as one based on continuous output, on additional function evaluations, on equistage approximation, or even on the new starting approximation algorithm itself. Arbitrarily high order approximations for the internal stages can be obtained. This general acceleration technique is flexible, embarrassingly parallel, and it does not require any additional function evaluations. The numerical solution of Hamiltonian and Lagrangian systems by symplectic IRK methods, such as Gauss methods will greatly benefit from this algorithm which can drastically reduce the number of function evaluations needed in the modified Newton/fixed point iterations process, making thus implicit methods extremely efficient even for separable problems.

Room: SR 17 | Monday 03:30pm - 04:00pm

Stability analysis of VDRK methods for the second kind Volterra integro-differential equations

Jiao Wen, Chengming Huang and Min Li

Huazhong University of Science and Technoloy, China, People's Republic of

In this talk, we are concerned with the stability of Runge-Kutta methods for the second kind Volterra integro-differential equations. Both the basic test equation and a convolution test equation are considered. Some fixed order recurrence relations and the corresponding stability matrices are derived. The concept of V_0-stability is introduced, and some A_0-stable and V_0-stable methods are obtained. Also, the stability regions of some one-stage and two-stage fully implicit discretized collocation methods are given and compared.

CS 08
Exponential integrators

Room: SR 16

Tuesday 02:00pm - 02:30pm
Tobias Jawecki
Computable upper error bounds for Krylov subspace approximations to matrix exponentials

Tuesday 02:30pm - 03:00pm
Othmar Koch
Adaptive exponential methods

Tuesday 03:00pm - 03:30pm
Christoph Zimmer
Exponential Integrators for Semi-linear Parabolic Problems with Linear Constraints

Tuesday 03:30pm - 04:00pm
Ai Ishikawa
Equivalence of two energy-preserving numerical methods that are based on time translation symmetry

Room: SR 16 | Tuesday 02:00pm - 02:30pm

Computable upper error bounds for Krylov subspace approximations to matrix exponentials

Tobias Jawecki[1], Winfried Auzinger[1] and Othmar Koch[2]

[1] *TU Wien, Austria*
[2] *Universität Wien, Austria*

The reliability of well-known a posteriori error estimates for Krylov approximations to the matrix exponential is discussed. In many cases error estimates constitute upper error bounds and even can be tightened. Additionally, a new defect-based a posteriori error estimate is introduced. This error estimate constitutes an upper norm bound on the error without further assumptions and can be computed during the construction of the Krylov subspace with nearly no computational effort.
The matrix exponential function itself can be understood as a time propagation with restarts. In practice, we are interested in finding time steps for which the error of the Krylov subspace approximation is smaller than a given tolerance. Apart from step size control, the new upper error bound can be used on the fly to test if the dimension of the Krylov subspace is already sufficiently large to solve the problem in a single time step with the required accuracy.

Room: SR 16 | Tuesday 02:30pm - 03:00pm

Adaptive exponential methods

Othmar Koch[1], **Winfried Auzinger**[2], **Harald Hofstätter**[1], **Tobias Jawecki**[2], **Karolina Kropielnicka**[3] **and Pranav Singh**[4]

[1] *Universität Wien, Austria*
[2] *Technische Universität Wien, Austria*
[3] *University of Gdansk*
[4] *University of Oxford*

We investigate exponential-based adaptive numerical time integrators for time-dependent systems of linear ordinary differential equations of Schrödinger type. Applications in the study of the design of novel solar cells motivate the interest in finding efficient adaptive time integration methods for this task. We consider commutator-free Magnus-type methods, classical Magnus integrators and novel integrators based on a splitting approach. In all the methods, efficient time-stepping is realized based on defect-based estimators for the local error constructed especially for the task. We show the asymptotical correctness of the error estimators and demonstrate the advantages of adaptive time-stepping.

Room: SR 16 | Tuesday 03:00pm - 03:30pm

Exponential Integrators for Semi-linear Parabolic Problems with Linear Constraints

Christoph Zimmer[1] **and Robert Altmann**[2]

[1] *TU Berlin, Germany*
[2] *University of Augsburg, Germany*

Exponential integrators provide a powerful tool for the time integration of parabolic partial differential equations (PDE), by allowing large time steps even for very restrictiv CFL conditions. On the other hand, PDEs with an additional underling constraint (PDAE) include applications such as PDEs with dynamical boundary conditions or the transient Stokes problem.
In this talk, we construct and analyze exponential integrators for semi-linear parabolic PDAEs. The resulting schemes only require the solution of linear stationary as well as transient but homogeneous saddle point problems in each time step. Further, no linearization steps or regularizations of the transient system are needed. The talk concludes with some numerical examples.

Room: SR 16 | Tuesday 03:30pm - 04:00pm

Equivalence of two energy-preserving numerical methods that are based on time translation symmetry

Ai Ishikawa and Takaharu Yaguchi

Kobe University, Japan

In this talk we investigate a relation between the two approaches to deriving energy-preserving numerical methods proposed by Yaguchi(2013) and Ishikawa–Yaguchi(2016). In both approaches energy-preserving numerical schemes are derived by using time translation symmetry and the discrete gradient, but the former is based on the Lagrangian formalism and the latter on the Hamiltonian. Hence it is expected that there exists a natural correspondence between the two approaches similar to the Legendre transformation; however, such a correspondence has not been revealed yet. In fact, because the numerical schemes derived by the two approaches have a degree of freedom of choice of the discrete gradient, it is not straightforward to introduce a well-defined correspondence between them. In this contribution, we show that the two approaches are certainly equivalent under a certain condition on the choice of the discrete gradient. Besides, the relation of the condition to the Legendre transformation is also discussed.

CS 09
Schrödinger Equations

Room: SR 16

Monday 10:30am - 11:00am
Robert Altmann
Computation of localized Schrödinger eigenstates under random potentials

Monday 11:00am - 11:30am
Marnix Van Daele
The efficient and accurate solution of the 2D Schrödinger eigenvalue problem

Monday 11:30am - 12:00pm
Toon Baeyens
PySlise: a Python Package for solving Schrödinger Equations

Room: SR 16 | Monday 10:30am - 11:00am

Computation of localized Schrödinger eigenstates under random potentials

Robert Altmann and **Daniel Peterseim**

Augsburg University, Germany

We consider the linear Schrödinger operator with oscillatory high-amplitude random potentials on bounded domains. In this case, the lowermost eigenstates localize in the sense that these eigenstates decay exponentially. This can be proven using iterative solvers in combination with an optimal local preconditioning. In this talk we apply these techniques also numerically in order to actually compute the first eigenstates of the random Schrödinger operator.

Room: SR 16 | Monday 11:00am - 11:30am

The efficient and accurate solution of the 2D Schrödinger eigenvalue problem

Marnix Van Daele and **Toon Baeyens**

Ghent University, Belgium

The constant perturbation (CP) methods were originally devised for the solution of the time-independent one-dimensional Schrödinger equation. Yet they have proven to be very efficient for different classes of Sturm-Liouville problems and they now form the basis of the very succesful Matlab package Matslise [1].
Also for coupled channel Schrödinger equations CP-based codes have been developed, such as the Matlab-package Matscs [2] and the Fortran program LILIX [3].
The CP methods can also be successfully applied to other types of problems. In this talk we present an improved version of the algorithm first formulated by Ixaru in [4] for the efficient and accurate solution of the eigenvalue problem of the 2D Schrodinger equation.
To build this improved algorithm some of the above mentioned Matslise and Matscs algorithms had to be redesigned. This will be the topic of the talk of Toon Baeyens.
References:
[1] Ledoux V. and Van Daele M., Matlise 2.0: A Matlab Toolbox for Sturm-Liouville Computations, ACM Trans. Math. Softw. 42, 4, Article 29 (June 2016).
[2] Ledoux V., Van Daele M. and Vanden Berghe G., A numerical procedure to solve the multichannel Schrodinger eigenvalue problem, Comp. Phys. Comm. 176 (2007) 191-199.
[3] Ixaru L. Gr., LILIX—A package for the solution of the coupled channel Schrödinger equation, Comp. Phys. Comm. 147 (2002) 834-852.
[4] Ixaru L. Gr., New numerical method for the eigenvalue problem of the 2D Schrödinger equation, Comput. Phys. Commun. 181 (2010) 1738-1742.

Room: SR 16 | Monday 11:30am - 12:00pm

PySlise: a Python Package for solving Schrödinger Equations

Toon Baeyens and **Marnix Van Daele**

UGent, Belgium

This is an introduction to a new Python package that is able to solve numerically the one and two-dimensional time independent Schrödinger equation. Accompanying this package there is a web based gui. The main motivator of this research is modernizing and bringing together existing techniques and proven methods.

Matslise is a very effective implementation of CP-methods for the one-dimensional Sturm-Liouville equation. But due to the numerous features, this implementation isn't highly optimised for efficiency. For this reason we have reimplemented and optimised the algorithms of Matslise and Matscs in C++. This reimplementation became the computation engine for the Python package and the web based GUI (WebAssembly).

The Python package is less feature-rich than the original Matslise and Matscs (only Schrödinger equation, no degenerate case detection...), but a lot more optimised. These optimisations include: very efficient eigenfunction calculations, smarter backward propagation, higher order method for Matscs, on request error calculation, using C++ with Eigen. On top of that there is a unified interface to communicate with Matslise, Matscs and the new code for the two-dimensional case.

CS 10
Dynamical Systems

Room: SR 17

Monday 10:30am - 11:00am
Sandip Saha
Reduction of Kinetic Equations to Liénard–Levinson–Smith Form: Counting Limit Cycles

Monday 11:00am - 11:30am
Mohammad Sajid
On Dynamical Properties including Chaotic Behaviour of Two-parameter Family of Functions associated with Exponential Map

Monday 11:30am - 12:00pm
Asma Farooq
How perturbations propagate along solutions of linear ordinary differential equations: a relative error analysis.

Monday 12:00pm - 12:30pm
Sigurdur Freyr Hafstein
Numerical methods for computing Lyapunov functions for nonlinear systems

Room: SR 17 | Monday 10:30am - 11:00am

Reduction of Kinetic Equations to Liénard–Levinson–Smith Form: Counting Limit Cycles

Sandip Saha[1], **Gautam Gangopadhyay**[1] **and Deb Shankar Ray**[2]

[1] *S N Bose National Centre for Basic Sciences, India*
[2] *Indian Association For The Cultivation Of Science, Kolkata, India*

We have presented an unified scheme to express a class of system of equations in two variables into a Liénard–Levinson–Smith (LLS) oscillator form. We have derived the condition for limit cycle with special reference to Rayleigh and Liénard systems for arbitrary polynomial functions of damping and restoring force. Krylov–Boguliubov (K–B) method is implemented to determine the maximum number of limit cycles admissible for a LLS oscillator atleast in the weak damping limit. Scheme is illustrated by a number of model systems with single cycle as well as the multiple cycle cases.

Room: SR 17 | Monday 11:00am - 11:30am

On Dynamical Properties including Chaotic Behaviour of Two-parameter Family of Functions associated with Exponential Map

Mohammad Sajid

Qassim University, Saudi Arabia

The main goal of the present paper is to study the dynamical properties of two-parameter family of functions associated with exponential map as well as chaos in the dynamics of this family on the real line. In many cases, dynamical systems are concerned with mathematical modeling of engineering and scientific systems. To study the dynamical properties, the real fixed points of the family of functions are to be determined theoretically while the real periodic points are to be computed numerically. We plot the bifurcation diagrams for the real dynamics, by changing parameter values. The graphs of numerical data are plotted to see the behavior of orbits. From the bifurcation diagrams, the existence of chaos in the dynamics of our family explores for looking period-doubling. In spite of this, chaos in the real dynamics is identified by calculating positive Lyapunov exponents.

Room: SR 17

Monday 11:30am - 12:00pm

How perturbations propagate along solutions of linear ordinary differential equations: a relative error analysis.

Asma Farooq[1] **and Stefano Maset**[2]

[1] *University of Trieste, Trieste Italy*
[2] *University of Trieste, Trieste Italy*

In this talk we study how perturbations in initial value y_0 or in the matrix A propagate along the solutions of linear ordinary differential equations

$$\begin{cases} y'(t) = Ay(t),\ t \geq 0, \\ y(0) = y_0. \end{cases}$$

In other words we are considering the conditioning of the problem

$$(y_0, A) \mapsto e^{tA} y_0$$

and an asymptotic analysis of condition numbers, as $t \to +\infty$, will be given. The analysis is accomplished for the case where A is normal matrix.

We remark that our study is different from known conditioning studies for the matrix exponential: we look attentively at the relative errors

$$\frac{\|e^{tA}\widetilde{y}_0 - e^{tA}y_0\|}{\|e^{tA}y_0\|} \text{or } \frac{\|e^{t\widetilde{A}}y_0 - e^{tA}y_0\|}{\|e^{tA}y_0\|}$$

relevant to a perturbation $\widetilde{y}_0$ of the initial value y_0 or to a perturbation $\widetilde{A}$ of the matrix A rather than the relative error

$$\frac{\|e^{\widetilde{A}} - e^{A}\|}{\|e^{A}\|}$$

considered in many papers in literature.

Room: SR 17 | Monday 12:00pm - 12:30pm

Numerical methods for computing Lyapunov functions for nonlinear systems

Sigurdur Freyr Hafstein

University of Iceland, Iceland

Lyapunov functions are the generalisation of energy for dissipative physical systems to general dynamical systems. A Lyapunov function for an attractor of a dynamical system delivers lower bounds on its basin of attraction, a complete Lyapunov function delivers information on the qualitative behaviour of the system flow.
Several methods have been suggested to generate Lyapunov functions for nonlinear systems. We give a short overview and discuss in more detail combined approaches, where a Lyapunov function candidate is first generated by either solving a series of initial-values problems or by solving numerically a first order PDE using radial basis functions. Subsequently, the quality of the Lyapunov function candidate is validated using a linear programming problem and interpolation over a simplicial complex.

CS 11
Boundaries and boundary layers

Room: SR 16

Tuesday 10:30am - 11:00am
Manfred Trummer
Resolving boundary layers with coordinate transformations

Tuesday 11:00am - 11:30am
Paul Muir
Recent Advances in Error Control Gaussian Collocation Software for Boundary Value ODEs and 1D PDEs

Tuesday 11:30am - 12:00pm
Marc Josien
Some quantitative homogenization results for an interface

Room: SR 16 | Tuesday 10:30am - 11:00am

Resolving boundary layers with coordinate transformations

Manfred Trummer[1] **and Conor McCoid**[2]

[1] *Simon Fraser University, Canada*
[2] *University of Geneva*

We are solving singularly perturbed two-point boundary value problems; the linear equation is

$$\epsilon u''(x) + p(x)u'(x) + q(x)u(x) = f(x), \qquad x \in [-1, +1].$$

We are most interested in the case of very small $\epsilon > 0$, and propose a new algorithm to improve the accuracy of spectral collocation methods for such problems.
When discretizing this equation via spectral collocation (for example, using Chebyshev points), one typically replaces the first and last of the collocation equation with the boundary conditions. Driscoll and Hale suggest resampling as an alternative to row replacement when including boundary conditions. Testing this with an iterated sine–transformation designed for resolving boundary layers reveals artificial boundary conditions imposed by the transformation. The transformation is regularized to prevent this. The new regularized sine–transformation is employed to solve boundary value problems with and without resampling. It shows superior accuracy provided the regularization parameter is chosen from an optimal range.

Room: SR 16 | Tuesday 11:00am - 11:30am

Recent Advances in Error Control Gaussian Collocation Software for Boundary Value ODEs and 1D PDEs

Paul Muir

Saint Mary's University, Canada

This talk will describe two numerical software projects that employ Gaussian collocation for the error controlled numerical solution of boundary value ordinary differential equations (BVODEs) and time-dependent partial differential equations with one spatial dimension (1D PDEs).
The Fortran 77 Gaussian collocation BVODE solver, COLNEW, which first appeared several decades ago, continues to be widely used; COLNEW interfaces in Python, Scilab, and R have recently been developed. Our BVODE software project involves a major update of COLNEW; the new version, implemented in Fortran 95, greatly enhances the ease-of-use of the solver and features the implementation of a superconvergent interpolant to augment the collocation solution that is coupled with a new error estimation scheme, leading to significant improvements in the efficiency of the computation. We are also developing a Python interface for the new solver.
The 1D PDE project involves the development of a new Fortran 95 solver, BACOLRI, that implements our recent algorithms for interpolation-based spatial error estimation to yield an update of the Fortran 77 1D PDE solver, BACOLR. The new solver is based on a Gaussian collocation spatial discretization scheme and a new spatial error estimation/control scheme, coupled with a Runge-Kutta solver for the error controlled treatment of the time dimension. BACOLRI features a much simplified calling sequence and we have also developed a Python interface for the solver.

Room: SR 16

Tuesday 11:30am - 12:00pm

Some quantitative homogenization results for an interface

Marc Josien

Max Planck Institut, Germany

We consider a linear elliptic equation in divergence form with a small scale $\epsilon \ll 1$

$$-\mathrm{div}\,(a(x/\epsilon) \cdot \nabla u^{\epsilon}(x)) = f(x),$$

where the matrix a represents a flat interface between two heterogeneous media. Remarkably enough, the homogenized matrix $\bar{a}$ is not constant, but only piecewise constant and discontinuous through the interface. We propose a generalization of the two-scale expansion to obtain a precise approximation of the oscillating gradient ∇u^{ϵ}. Then, by combining Avellaneda and Lin's work in homogenization and Li and Vogelius' work concerning regularity of elliptic equation with discontinuous coefficients, we recover Lipschitz estimates and a (near-optimal and uniform in space) convergence rate up to the interface. This result paves the way for studying complex structures of non-stationary heterogeneous materials, such as inclusions.

CS 12
Model order reduction

Room: SR 17

Thursday 02:00pm - 02:30pm
Gianluca Ceruti
Dynamical low-rank approximation of (skew-)symmetric matrices.

Thursday 02:30pm - 03:00pm
Marcus W.F.M. Bannenberg
Coupling of Model Order Reduction and Multirate Techniques

Room: SR 17 | Thursday 02:00pm - 02:30pm

Dynamical low-rank approximation of (skew-)symmetric matrices.

Gianluca Ceruti and **Christian Lubich**

University of Tübingen, Germany

Dynamical low-rank approximation is introduced and a numerical integrator that computes a symmetric or skew-symmetric low-rank approximation to large symmetric or skew-symmetric time-dependent matrices that are either given explicitly or are the unknown solution to a matrix differential equation is presented. We show that low-rank time-dependent matrices are reproduced exactly, and the error behavior is robust to the presence of small singular values of the solution or the approximate solution.

Room: SR 17

Thursday 02:30pm - 03:00pm

Coupling of Model Order Reduction and Multirate Techniques

Marcus W.F.M. Bannenberg[1], **Michael Günther**[1] **and Angelo Ciccazzo**[2]

[1] *Bergische Universitat Wuppertal, Germany*
[2] *ST Microelectronics, Italy*

In industrial circuit and device simulation, e.g. for estimating failure probabilities due to aging, simulation problems have to be run many times in the loop of an optimization flow. This can only be done by drastically reducing simulation costs via model order reduction (MOR). This is particularly challenging for coupled systems of various simulation packages for the different subcomponents and physical domains. For efficiency, MOR and multirate error estimates have to be linked to define overall error estimates, balanced to the accuracy requirements of the iteration level of the optimization flow.

CS 13
Runge-Kutta methods

Room: SR 17

Tuesday 02:00pm - 02:30pm
Inmaculada Higueras
Strong Stability Preserving properties of composition Runge-Kutta schemes

Tuesday 02:30pm - 03:00pm
Sebastiano Boscarino
A Unified IMEX Runge–Kutta Approach for Hyperbolic Systems with Multiscale Relaxation

Tuesday 03:00pm - 03:30pm
Zoltán Horváth
SSP and Positivity for Implicit Methods

Tuesday 03:30pm - 04:00pm
Ines Ahrens
The Pantelides Algorithm for DAEs with delay

Room: SR 17 | Tuesday 02:00pm - 02:30pm

Strong Stability Preserving properties of composition Runge-Kutta schemes

Inmaculada Higueras and **Teo Roldan**

Public University of Navarre, Spain

During the last decades, the study of Strong Stability Preserving (SSP) properties (e.g., monotonicity, contractivity, positivity, discrete maximum principles, etc.) for Runge-Kutta methods has been an active research topic.
In this talk we analyze strong stability preserving (SSP) properties of Runge-Kutta (RK) methods obtained by composing k different schemes with different step sizes. We will show how the SSP coefficient of a composition method can be obtained and an upper bound on this coefficient will be given. Some examples will illustrate these results. Other issues related to SSP composition methods, like low-storage SSP RK methods, will also be considered [1].
[1] I. Higueras, T. Roldan, Strong Stability Preserving Properties of Composition Runge–Kutta Schemes, J. Sci. Comput. (2019), DOI 10.1007/s10915-019-00956-9.
Supported by Ministerio de Economía y Competividad (Spain), Project MTM2016-77735-C3-2-P.

Room: SR 17 | Tuesday 02:30pm - 03:00pm

A Unified IMEX Runge–Kutta Approach for Hyperbolic Systems with Multiscale Relaxation

Sebastiano Boscarino, Lorenzo Pareschi and Giovanni Russo

Università di Catania, Italy

In this paper we consider the development of Implicit-Explicit (IMEX) Runge-Kutta schemes for hyperbolic systems with multiscale relaxation. In such systems the scaling depends on an additional parameter which modifies the nature of the asymptotic behavior which can be either hyperbolic or parabolic. Because of the multiple scalings, standard IMEX Runge-Kutta methods for hyperbolic systems with relaxation loose their efficiency and a different approach should be adopted to guarantee asymptotic preservation in stiff regimes. We show that the proposed approach is capable to capture the correct asymptotic limit of the system independently of the scaling used. Several numerical examples confirm our theoretical analysis.

Room: SR 17 | Tuesday 03:00pm - 03:30pm

SSP and Positivity for Implicit Methods

Zoltán Horváth and **Tihamér A. Kocsis**

Széchenyi István University, Győr, Hungary

The state-of-the-art theory for strong stability preservation (SSP) and that for forward invariance of sets (positivity preservation, PP), rely on the SSP/PP of the Explicit Euler (EE) method with a positive step size. However, this theory does not apply in many cases of practical importance when FE is not of SSP/PP for any positive step size (e.g. FEM without lumping, higher order DG, spectral methods).
In this talk we shall present our results for diagonally implicit methods (e.g. diagonally implicit Runge-Kutta methods, DIMSIMMs) that use assumptions only on the property of the Implicit Euler (IE) method, instead of the condition on EE method. We quantify the SSP/PP step sizes in terms of a measure of the IE-step on the given problem and a new parameter of the scheme. We remark that the applied IE condition can be considered as a new family of circle conditions. Further, the introduced scheme parameter of the analysis shows similar properties to the classical absolute monotonicity radius of the scheme used in the theory with the EE condition. We shall investigate optimal scheme parameters up to order 4.
In addition, the new theory proposes an efficient implementation procedure as well of the diagonally implicit methods. We shall present this implementation, too.
To illustrate the new theoretical findings, we shall present results of computational experiments for FEM with FEniCS.

Room: SR 17 | Tuesday 03:30pm - 04:00pm

The Pantelides Algorithm for DAEs with delay

Ines Ahrens and **Benjamin Unger**

TU Berlin, Germany

Differential algebraic equations (DAEs), consisting of both differential and algebraic equations, are used to model the dynamical behavior of physical systems. A well-known strategy to solve DAEs is to differentiate certain equations in time. In a large-scale setting, this might become computationally infeasible. However, if it is known a priori which equations of the original system need to be differentiated the computational cost can be reduced. One way to determine these equations is the Pantelides algorithm.

If the DAE features in addition a delay term, taking derivatives might not be sufficient, and instead, the derivative array must be shifted in time, thus increasing the computational complexity even further. In this talk, I will explain how one can modify the Pantelides algorithm such that it determines the equations which need to be shifted and/or differentiated. This is joint work with Benjamin Unger (TU Berlin).

CS 14
Space discretization

Room: SR 16

Thursday 02:00pm - 02:30pm
Bernd Feist
Fractional Laplacian - Approximation of the dense FEM stiffness matrix by $\mathcal{H}$-matrices

Thursday 02:30pm - 03:00pm
Daisuke Furihata
Structure-preserving method using discrete Gauss, Green and Stokes laws on Voronoi meshes

Thursday 03:00pm - 03:30pm
Maximilian Bauer
The Coupling of low-rank Approximations with the Solution Process for discretised Boundary Integral Equations

Thursday 03:30pm - 04:00pm
Massimo Frittelli
Virtual Element Method for bulk-surface reaction-diffusion systems with electrochemical applications

Room: SR 16 | Thursday 02:00pm - 02:30pm

Fractional Laplacian - Approximation of the dense FEM stiffness matrix by $\mathcal{H}$-matrices

Bernd Feist and **Mario Bebendorf**

Universität Bayreuth, Germany

$\mathcal{H}$-matrices are a well suited method to approximate discrete elliptic operators. Here, we want to show that the fractional Laplacian $L^s = (-\Delta)^s$, $0 < s < 1$, can also be approximated by $\mathcal{H}$-matrices. Although, the fractional Laplacian is an elliptic operator, there a some special features, which we have to consider, before we can start the approximation. In particular, the operator is non-local and its integral form is used for the FEM approach. Therefore, we have to handle a dense stiffness matrix. Additionally, each entry consists of combinations of volume and surface integrals, which make the computation quite costly. Thus, an efficient treatment of these entries is needed. We will use the similarity between the integral form of the fractional Laplacian and boundary integral equations to develop an efficient computation method. For this, existing techniques for the treatment of boundary integral equations are adapted to the fractional Laplacian. Finally, the Adaptive Cross Approximation (ACA) is used to get an $\mathscr{H}$-matrix approximation of the dense stiffness matrix. Some numerical examples will be shown to prove the efficiency of the approach.

Room: SR 16 | Thursday 02:30pm - 03:00pm

Structure-preserving method using discrete Gauss, Green and Stokes laws on Voronoi meshes

Daisuke Furihata

Osaka University, Japan

We have developed a few numerical methods to inherit essential and mathematical properties from the target differential equations. We commonly call them structure-preserving methods, and we indicated they are efficient, reliable and durable via some numerical computations on one-dimensional problems. However, if we would like to introduce reference/mesh points located arbitrarily in two- or three-dimensional regions, it is hard to design some structure-preserving methods. The reason is that we should define some finite difference/volume operators to discretize differential operators, however, in general, it is also severe problems to find/design some discrete Gauss, Green and Stokes formulae based on them. This difficulty often prevents to design structure-preserving methods since such formulae are an essential key for variational calculation included in the process of the design.
In these years, we have found that there exist some rigorous discrete Gauss, Green and Stokes formulae among finite difference/volume operators based on the Voronoi decompositions. Furthermore, we can apply them to design some structure-preserving numerical methods for some PDE problems and run numerical computations.
In this talk, we would like to indicate those finite difference/volume operators, Green, Gauss and Stokes formulae and the obtained discrete variational derivative methods, which is one of the structure-preserving methods for PDEs, based on Voronoi cells.

Room: SR 16 | Thursday 03:00pm - 03:30pm

The Coupling of low-rank Approximations with the Solution Process for discretised Boundary Integral Equations

Maximilian Bauer and Mario Bebendorf

University of Bayreuth, Germany

The Adaptive Cross Approximation (ACA) is known for the efficient approximation of discretizations of integral operators via the generation of low-rank approximations on suitable matrix blocks. This talk aims to the extension of ACA to a block adaptive version. Since the usual way of constructing hierarchical matrix approximations with ACA, i.e. having the same prescribed accuracy on each block of the partition, is not the most efficient for the solution of linear systems, we adapt the accuracy on each block to the actual error of the solution. This means that some blocks may be more important for the solution error than others. In order to detect those blocks and to automatically improve the block-wise matrix approximation error, error estimation techniques known from adaptive mesh refinement are applied to ACA. With these extensions we are able to couple the assembling of the coefficient matrix with the iterative solution process. The performance of the investigated algorithm will be shown with some numerical examples at the end of the talk.

Room: SR 16 | Thursday 03:30pm - 04:00pm

Virtual Element Method for bulk-surface reaction-diffusion systems with electrochemical applications

Massimo Frittelli[1], Anotida Madzvamuse[2] and Ivonne Sgura[1]

[1] *University of Salento, Italy*
[2] *University of Sussex, UK*

We present a Bulk-Surface Virtual Element Method (BSVEM) for the spatial discretisation of bulk-surface reaction-diffusion systems (BSRDSs) in two dimensions. To the best of the authors' knowledge, the proposed method is the first application of the Virtual Element Method [Beirao da Veiga et al, "Basic principles of Virtual Element Methods", 2013] to bulk-surface PDEs. The method is based on the discretisation of the bulk into polygonal elements with arbitrarily many edges, instead of triangles. The bulk-surface finite element method (BSFEM) on triangular meshes [Elliott and Ranner, "Finite element analysis for a coupled bulk-surface partial differential equation", 2013] is a special case of the BSVEM. From the numerical point of view, the contribution is twofold. First, we show that the usage of arbitrary polygons can be exploited to reduce the computational complexity of matrix assembly. Second, we introduce an optimised matrix implementation of the method that can be also exploited in the special case of BSFEM. We consider a fully discrete scheme by applying the Implicit-Explicit (IMEX) Euler method to the BSVEM spatially discrete problem. We present a novel bulk-surface model for electrodeposition based on the reaction-diffusion model considered in [Lacitignola et al, "Spatio-temporal organization in a morphochemical electrodeposition model", 2015]. The proposed model couples a linear diffusion system in the bulk with a RDS on the boundary through nonlinear boundary conditions. Numerical examples illustrate (i) pattern formation in the proposed BSRDS for electrodeposition, (ii) the computational advantages of BSVEM and (iii) the optimal convergence rate in space and time of IMEX Euler-BSVEM.

CS 15
Partial differential equations

Room: SR 17

Tuesday 10:30am - 11:00am
Yuto Miyatake
On the equivalence between SOR-type methods for linear systems and Itoh–Abe-type discrete gradient methods for gradient systems

Tuesday 11:00am - 11:30am
Peter Meisrimel
Waveform Relaxation using asynchronous time-integration

Tuesday 11:30am - 12:00pm
Dohyun Kim
Emergent behaviors of the Schrödinger-Lohe model on cooperative-competitive networks

Tuesday 12:00pm - 12:30pm
Ruili Zhang
Classical Instabilities of Conservative Systems are the Results of Parity-Time Symmetry Breaking

Room: SR 17 | Tuesday 10:30am - 11:00am

On the equivalence between SOR-type methods for linear systems and Itoh–Abe-type discrete gradient methods for gradient systems

Yuto Miyatake[1], **Tomohiro Sogabe**[2] **and Shao-Liang Zhang**[2]

[1] *Osaka University, Japan*
[2] *Nagoya University, Japan*

The successive overrelaxation (SOR) method and its variants are typical stationary iterative methods for solving linear systems. In this talk, we show that when the coefficient matrix is symmetric positive definite, these methods are equivalent to Itoh–Abe-type discrete gradient methods for certain gradient systems. This discussion leads to new interpretations of SOR-type methods. For example, a new derivation of SOR-type methods is found, these methods monotonically decrease a certain quadratic function, and the relaxation parameter is interpreted as the stepsize following a certain change of variables. Based on the new interpretation of the relaxation parameter, we also present new adaptive SOR-type methods.

Room: SR 17

Tuesday 11:00am - 11:30am

Waveform Relaxation using asynchronous time-integration

Peter Meisrimel and **Philipp Birken**

Lund University, Sweden

We consider the coupling of two multi-physics systems of time-dependent ODEs. We solve the coupling using Waveform Relaxation (WR) methods. WR methods solve a given system using a function approximation of the solution to the other system to get an improved solution and then iterates. The two main variants of this are Jacobi and Gauss-Seidel WR. For Jacobi one runs both systems in parallel, for which convergence is slow, whereas Gauss-Seidel converges faster, but is sequential.
We propose a new WR type method which uses asynchronous communication. Instead of exchanging whole discrete functions in the update process, we asynchronously exchange results of all time-integration steps which make up the discrete functions. The proposed method is always parallel and gets speed-up from increased data exchange. We show convergence in the discrete setting and numerical results showing good performance for two coupled heat equations.

Room: SR 17

Tuesday 11:30am - 12:00pm

Emergent behaviors of the Schrödinger-Lohe model on cooperative-competitive networks

Hyungjin Huh[1], **Seung-Yeal Ha**[2] and **Dohyun Kim**[3]

[1] *Chung Ang University, Korea, Repbulic of*
[2] *Seoul National University, Korea, Republic of*
[3] *National Institute for Mathematical Sciences, Korea, Republic of*

We present several sufficient frameworks leading to the emergent behaviors of the coupled Schrödinger-Lohe (S-L) model under the same one-body external potential on cooperative-competitive networks. The S-L model was first introduced as a possible phenomenological model exhibiting quantum synchronization and its emergent dynamics on all-to-all cooperative networks has been treated via two distinct approaches: Lyapunov functional approach and finite-dimensional reduction based on pairwise correlations. In this talk, we further generalize the finite-dimensional dynamical systems approach for pairwise correlation functions on cooperative-competitive networks and provide several sufficient frameworks leading to the collective exponential synchronization. For small systems consisting of three and four quantum subsystem, we also show that the system for pairwise correlations can be reduced to the Lotka-Volterra model with cooperative and competitive interactions, in which lots of interesting dynamical patterns appear, e.g., existence of closed orbits and limit-cycles.

Room: SR 17 | Tuesday 12:00pm - 12:30pm

Classical Instabilities of Conservative Systems are the Results of Parity-Time Symmetry Breaking

Ruili Zhang

Beijing Jiaotong University, China, People's Republic of

We show that the governing equations of the classical two-fluid interaction and the incompressible fluid system are PT-symmetric, and the well-known Kelvin-Helmholtz instability and the two-stream instability are the results of spontaneous PT-symmetry breaking. By proving the theorem that all PT-symmetric Hamiltonians are pseudo-Hermitian (G-Hamiltonian), we show that PT-symmetry breaking is actually the onset of instability of pseudo-Hermitian Hamiltonian, which has been well studied Krein et al. Specifically, it is shown that the boundaries between the stable and unstable regions are locations for Krein collisions between eigenmodes with different Krein signatures. It is anticipated that this mechanism of destabilization is valid for other collective instabilities in conservative systems in plasma physics, accelerator physics, and fluid dynamics systems.

Poster Session

Poster Session

Room: Foyer

Tuesday 18:45 - 20:00

Guillaume Bertoli
A correction in the Strang splitting method for semilinear parabolic problems with inhomogeneous boundary conditions based on the nonlinearity flow only.

Georg Maierhofer
Filon-type methods for highly oscillatory integrals with singularities

Jian Liu
Lorentz covariance of Geometric Algorithms

Stefano Di Giovacchino
Mean-square contractivity of stochastic θ-methods

Teng Zhang
Numerical simulations of vortex interactions in the nonlinear Schrödinger equation with periodic boundary conditions

Mary Durojaye
Valuation of Option Pricing with Meshless Radial Basis Functions Aproximation

Shuenn-Yih Chang
Weak instability in time integration methods

Christian Offen
Boundary Value Problems and Symplectic Integration

Room: Foyer | Tuesday 06:45pm - 08:00pm

A correction in the Strang splitting method for semilinear parabolic problems with inhomogeneous boundary conditions based on the nonlinearity flow only.

Guillaume Bertoli and **Gilles Vilmart**

University of Geneva, Switzerland

The Strang splitting method, formally of order two, can suffer from order reduction when applied to semilinear parabolic problems with inhomogeneous boundary conditions. The recent work [L .Einkemmer and A. Ostermann. Overcoming order reduction in diffusion-reaction splitting. Part 1. Dirichlet boundary conditions. SIAM J. Sci. Comput., 37, 2015. Part 2: Oblique boundary conditions, SIAM J. Sci. Comput., 38, 2016] introduces a modification of the method to avoid the reduction of order based on the nonlinearity. In this work, we introduce a new correction constructed directly from the flow of the nonlinearity and which requires no evaluation of the source term or its derivatives. The goal is twofold. One, it reduces the computational effort to construct the correction, especially if the nonlinearity is numerically heavy to compute. Second, numerical experiments suggest it is well suited in the case where the nonlinearity is stiff. We provide a convergence analysis of the method for a smooth nonlinearity and perform numerical experiments to illustrate the performances of the new approach.

Room: Foyer

Tuesday 06:45pm - 08:00pm

Filon-type methods for highly oscillatory integrals with singularities

Georg Maierhofer, **Arieh Iserles and Nigel Peake**

University of Cambridge, United Kingdom

Motivated by boundary integral methods for acoustic scattering problems in 2D we consider the extended Filon method for the efficient numerical approximation of highly oscillatory integrals in the presence of integrable singularities. A fundamental part for the construction of these methods is the Filon paradigm and we present an extension of the former to the singular setting, where we treat a general class of frequency independent singularities and the specific case of a Hankel kernel with a non-linear oscillator for the frequency dependent case. These results show that from an asymptotic point of view it is desirable to interpolate the regular part of the integrand and to separate singular and oscillatory behaviour.

For the frequency independent case we describe a natural interpolation basis whose moments are known exactly. We provide a new error bound on the quality of polynomial interpolation at endpoint derivatives and interior Clenshaw–Curtis points which forms the basis for an error bound on these singular oscillatory methods that is explicit in both the number of interpolation points and the frequency of oscillations. For the frequency dependent case we present a stable algorithm for computing the standard moments for a Hankel kernel with a linear oscillator and show that, together with the Filon paradigm, this yields quadrature methods which can attain an arbitrary high asymptotic order as the frequency increases.

Room: Foyer

Tuesday 06:45pm - 08:00pm

Lorentz covariance of Geometric Algorithms

Jian Liu and **Yulei Wang**

University of Science and Technology of China, China, People's Republic of

In this post, the Lorentz covariance of algorithms is introduced. Under Lorentz transformation, both the form and performance of a Lorentz covariant algorithm are invariant. To acquire the advantages of symplectic algorithms and Lorentz covariance, a general procedure for constructing Lorentz covariant canonical symplectic algorithms (LCCSA) is provided, based on which an explicit LCCSA for dynamics of relativistic charged particles is built. LCCSA possesses Lorentz invariance as well as long-term numerial accuracy and stability, due to the preservation of discrete symplectic structure and Lorentz symmetry of the system. For situations with time-dependent electromagnetic fields, which is difficult to handle in traditional construction procedures of symplectic algorithms, LCCSA provides a perfect explicit canonical symplectic solution by implementing the discretization in 4-spacetime. We also show that LCCSA has built-in energy-based adaptive time steps, which can optimize the compuation performance when the Lorentz factor varies.

Room: Foyer

Tuesday 06:45pm - 08:00pm

Mean-square contractivity of stochastic θ-methods

Raffaele D'Ambrosio and Stefano Di Giovacchino

University of L'Aquila, Italy

We focus our attention on the numerical discretization of nonlinear stochastic differential equations by means of stochastic θ-methods. In particular, we investigate their nonlinear stability properties with respect to nonlinear test problems such that the mean-square deviation between two solutions exponentially decays, i.e., a mean-square contractive behaviour is visible along the stochastic dynamics. We aim to make the same property visible also along the numerical discretization via stochastic θ-methods: this issue is translated into sharp stepsize restrictions depending on parameters of the problem, here accurately estimated. A selection of numerical tests confirming the effectiveness of the analysis and its sharpness is also provided for both scalar and vector valued problems.

Room: Foyer | Tuesday 06:45pm - 08:00pm

Numerical simulations of vortex interactions in the nonlinear Schrödinger equation with periodic boundary conditions

Teng Zhang

National University of Singapore, Singapore

The nonlinear Schrödinger equation (NLSE) is a fundamental equation to model quantum vortices in superfluids and superconductors. In this poster, we present the numerical simulations on quantized vortex interactions in the 2D NLSE with periodic boundary conditions. The numerical vortex trajectory results are compared with the reduced dynamical laws, and some interesting moving patterns are also shown.

Room: Foyer

Tuesday 06:45pm - 08:00pm

Valuation of Option Pricing with Meshless Radial Basis Functions Aproximation

Mary Durojaye and **Kayode Odeyemi**

UNIVERSITY OF ABUJA, Nigeria

This work focuses on valuation scheme of European option of single asset with meshless radial basis approximations. The prices are governed by Black – Scholes equations. The option price is approximated with four infinitely smooth positive definite radial basis functions (RBFs), namely, Gaussian (GA), Multiquadrics (MQ), Inverse Multiquadrics (IMQ) and Inverse Quadratic (IQ). The RBFs were used for discretizating the space variables while Runge-Kutta method was used as a time-stepping marching method to integrate the resulting systems of differential equations. The accuracy of the RBF-FD discretization can be increased by considering not only the data sites but also the derivative values on the nodes present in the supporting region. Numerical examples are shown to illustrate the strength of the method developed.

Room: Foyer

Tuesday 06:45pm - 08:00pm

Weak instability in time integration methods

Shuenn-Yih Chang[1] and **Chiu-Li Huang**[2]

[1] *National Taipei University of Technology, Taiwan*
[2] *Fu Jen Catholic University, Taiwan*

Three integration methods have been successfully developed for solving equations of motion, which are second-order ordinary differential equations, for earthquake engineering applications and structural dynamics. Although they generally have the same numerical properties, such as explicit formulation, unconditional stability and second-order accuracy, a drastically different performance is found in solving the free vibration response to either linear elastic or nonlinear systems with high frequency modes. The cause of this different performance in free vibration responses is analytically explored herein. As a result, it is verified that a weak instability is responsible for the significantly different performance of the integration methods. In general, a weak instability will result in an inaccurate solution or even numerical instability in the free vibration responses of high frequency modes. Hence, a weak instability must be prohibited for time integration methods.

Room: Foyer

Tuesday 06:45pm - 08:00pm

Boundary Value Problems and Symplectic Integration

Christian Offen

Massey University, New Zealand

Catastrophe theory has been attracting researcher for more than half a century. Nowadays a highly-developed framework is available to describe singularities and bifurcations. My research shows how bifurcations of solutions to Hamiltonian boundary value problems fit into this setting and that symplectic structure needs to be preserved to resolve bifurcations correctly in numerical computations.

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