Scientific Committee for NUMDIFF–15

- Martin Arnold (Halle)
- Elena Celledoni (Trondheim)
- Jason Frank (Utrecht)
- Jens Lang (Darmstadt)
- Helmut Podhaisky (Halle)
- Rüdiger Weiner (Halle)

in memoriam

- Willem Hundsdorfer (Amsterdam, 1954–2017)

Conference office

Karin Helbich, `numdiff@mathematik.uni-halle.de`

Acknowledgements

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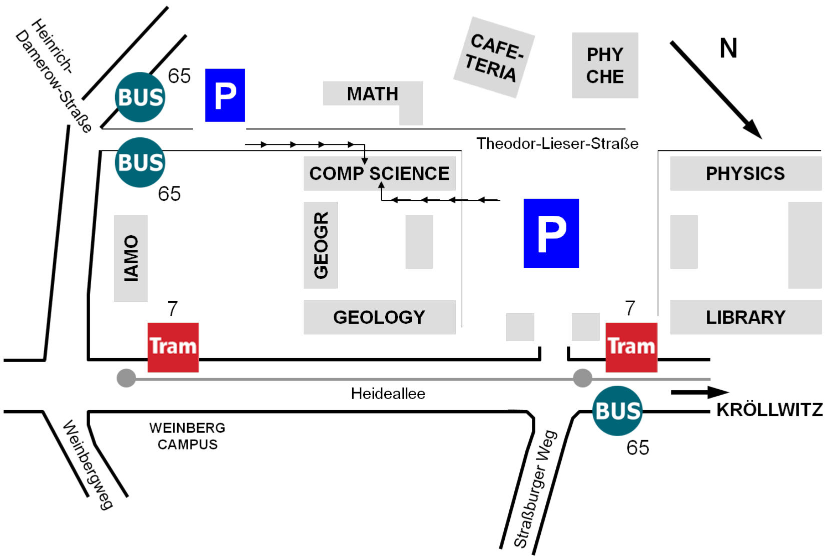
We are indebted to the *Martin Luther University Halle–Wittenberg* for making available various university facilities throughout the conference week.

last change: 22th August 2018

Contents

1. **Conference Site**
   The conference will take place in the Computer Science building situated within the Heide Campus at Von-Seckendorff-Platz 1. To get there from the "TRYP by Wyndham Halle" you can use any tram leaving eastwards from the stop "Zentrum Neustadt", then get off at stop "Rennbahnkreuz" and change to bus 65 and finally get off at stop "Heinrich-Damerow-Str./Weinberg Campus". You can also take tram No. 7 from 'Halle Hauptbahnhof' via "Marktplatz" to "Weinberg Campus" and get off at stop "Straßburger Weg".



2. **Conference Office and Registration**
   The conference office will be open on Sunday, 2 September 2018, from 17:00 to 20:00 in the lobby of the "TRYP by Wyndham Halle" (+49 345 69310). During the week it will be situated at the conference site in room 1.03. It will be open on Monday, Tuesday and Thursday from 8:00 to 16:00, and on Wednesday and Friday from 8:00 to 12:00. You can reach the conference office by phone +49 345 5524799 (active from Monday on). Participants who have not yet paid the conference fee can pay the conference fee in cash at the conference office. Please note that we cannot accept credit cards or cheques.

3. **Lectures**
   The lecture times as given in the programme already include five minutes for discussion. Session chairs will make sure that speakers do not exceed their allocated time. All lecture rooms will be equipped with laptop and data projector.

4. **Coffee and Tea Breaks, Lunch**
   Coffee and tea will be provided during the morning and afternoon breaks in a room close to the conference office. For lunch, the *Mensa Weinberg* is a 15 minute walk away.

5. **Computer and Internet Access**
At the conference site you can access the internet using eduroam or using wifi with SSID *event-net* user name *numdiff@uni-halle.de* password *FSifxre6*. Note that you may need to add a security exception in order to connect to this network. We have reserved room 1.30 for discussions.

6. **Conference Dinner**
The conference dinner will be held in the "TRYP by Wyndham Halle" on Thursday, at 19:00. The dinner ticket is included in the conference fee.

7. **Tour to Bauhaus Dessau, UNESCO World Heritage, on Wednesday afternoon**
If you are interested then please register for the excursion by Monday at the conference office. Busses will leave from the conference site at 12:30 and will return to Halle at around 19:30. After the guided tours through the main building and the "Meisterhäuser", we will have coffee and cake in the souterrain café-bistro.

The Bauhaus building **(left)** was designed by Walter Gropius in 1925. A glass facade on the load-bearing framework allows a view of the interior workings. In the workshop wing in Dessau this provides clear view of the constructive elements. The design does not visually amplify the corners of the building, which creates an impression of transparency. Gropius designed the various sections of the building differently, separating them consistently according to function.

The master's houses **(right)** were planned by Walter Gropius using industrially prefabricated components. He wished to realise the principles of rational construction, both in the architecture and in the process of building per se. In view of the technical resources available at the time, his plan was only partially realised. The buildings take the form of interlocking cubic structures of various heights. Towards the street the semi-detached houses are distinguished by generously glazed studios; vertical strip windows on the sides sheds light into the staircases. The light-coloured houses have generously-sized terraces and balconies and feature colourful accents on the window reveals, the undersides of the balconies and the drainpipes. See `https://www.bauhaus-dessau.de` for more details.

8. **Conference Proceedings**
The proceedings of NUMDIFF-15 will be published as a special issue of the Journal of Computational and Applied Mathematics. Guest editors are the members of the scientific committee and the managing guest editor is Jens Lang. Every speaker of NUMDIFF-15 can submit a manuscript for consideration of publication in this special issue. The deadline for manuscript submission is 10 January 2019. See `https://sim.mathematik.uni-halle.de/numdiff/Numdiff15/proceedings`.

1 Programme Overview

	R 3.28	R 1.26	R 1.23	R 1.27	R 1.29
Monday					
09:00	–Opening–				
09:20	Schönlieb				
10:10	–Break–				
10:40	Gunzburger				
11:30	Hansen				
12:20	–Lunch–				
14:00	März	Debrabant	Garrappa	Steinebach	Pfurtscheller
14:25	Hanke	D'Ambrosio	Abuaisha	Eisenmann	Piazzola
14:50	Arnold	Almuslimani	Jiang		Stillfjord
15:15	Mohammadi	Arara	Zhao		Kheiri Estiar
15:40	–Break–	–Break–	–Break–	–Break–	–Break–
16:10	Geiser	Snoeijer	Sandu	Hojjati	Hadjimichael
16:35	Klinge	Kulikova	Hachtel	Abdi Kalasour	Leibold
17:00	Residori	Ngnotchouye	Bauer	Paternoster	Maier
17:25	Pereira	de la Cruz	Erbay, H. A.		Krämer
18:30	Welcome reception				
Tuesday					
08:30	Constantinescu				
09:20	Scheichl				
10:10	–Break–				
10:40	Eremin	Celledoni	Kulikov	Hosseini	Cortes Garcia
11:05	Farzi	Gerisch	Meisrimel	Ávila Barrera	Fang
11:30	Rihan	Knoth	Rosemeier	Al-Hdaibat	Vulkov
11:55	Kumar	Dörich	Singh	Pandit	Koleva
12:20	–Lunch–	–Lunch–			
	Minisymposium	Minisymposium			
14:00	Jimenez	Charrier			
14:30	Wenger	Bréhier			
15:00	Couéraud	Campbell			
15:30	Martiradonna	Lang, A.			
16:00		–Break–			
16:30		Legoll			
17:00		Trstanova			
17:30		Laurent			

	R 3.28	R 1.26	R 1.23	R 1.27	R 1.29
Wednesday					
	Special session				
08:30	–Opening–				
08:40	Ruuth				
09:10	–Break–				
09:40	Lang, J.	Jax	Steinhoff	Li	
10:05	Horváth	Estévez Schwarz	Roldan	Wang	
10:30	Teunissen	Hante	Faleichyk	Egger	
10:55	Higueras	Meyer	Fekete	Liu	
11:20	–Lunch–				
12:30	Buses depart for Dessau.				
Thursday					
08:30	Cohen				
09:20	Meister				
10:10	–Break–				
10:40	in 't Hout	Hinze	Izzo	Owren	Zegeling
11:05	Sanderse	Pulch	Weiner	Wieloch	Zerulla
11:30	Vandecasteele	Paschkowski	Schneider	Wandelt	Freese
11:55	Zielinski	Tietz	Kopecz	Tapley	
12:20	–Lunch–	–Lunch–			
	Minisymposium	Minisymposium			
14:00	Benner	Jeffrey			
14:30	Himpe	Hairer			
15:00	Buhr	Mehrmann			
15:30	Peitz	Guglielmi			
16:00	–Break–	–Break–			
16:30	Banholzer	Elia			
17:00	Gräßle	Streubel			
17:30	Ullmann	Dieci			
19:00	Conference dinner				
Friday					
08:30	Van Vleck				
09:20	González Pinto				
10:10	Ketcheson				
11:00	–Break–				
11:20	Gander				
12:10	Massot				
13:00	–Closing–				

2 Scientific Programme

Monday

Room 3.28

09:00 Opening

09:20 **Schönlieb, Carola-Bibiane**
Variational models and partial differential equations for mathematical imaging

10:10 Break

10:40 **Gunzburger, Max**
A Localized Reduced-Order Modeling Approach for PDEs with Bifurcating Solutions

11:30 **Hansen, Eskil**
Domain decomposition and parabolic problems – a time integrator approach

12:20 Lunch

14:00 **März, Roswitha**
Questions concerning differential-algebraic operators

14:25 **Hanke, Michael**
A least-squares collocation method for non-linear higher index differential-algebraic equations

14:50 **Arnold, Martin**
Improving the initialization of some integrators for index-3 DAEs and related stiff ODEs

15:15 **Mohammadi, Fatemeh**
Adaptive β-blocked multistep methods for index 2 Euler-Lagrange differential algebraic equations

15:40 Break

16:10 **Geiser, Jürgen**
Serial and Parallel Iterative Splitting Methods: Algorithms and Applications

16:35 **Klinge, Marcel**
Numerical tests with AMF methods

17:00 **Residori, Mirko**
A splitting approach for the KdV equation with transparent boundary conditions

17:25 **Pereira, Matheus Fernando**
Parametric dependence of the advection-diffusion equation in two dimensions

Room 1.26

14:00 **Debrabant, Kristian**
Analysis of multilevel Monte Carlo using the Milstein discretisation

14:25 **D'Ambrosio, Raffaele**
Stability issues in the discretization of stochastic differential equations

14:50 **Almuslimani, Ibrahim**
Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations

15:15 **Arara, Alemayehu Adugna**
Stochastic B–series and order conditions for exponential integrators

15:40 Break

16:10 **Snoeijer, Jacob**
Numerical valuation of Bermudan basket options via partial differential equations

16:35 **Kulikova, Maria**
Numerical solution of the neural field equation in the presence of random disturbance

17:00 **Ngnotchouye, Jean Medard**
Weak convergence for a stochastic exponential integrator and finite element discretization of stochastic partial differential equation with additive noise

17:25 **de la Cruz, Hugo**
Numerical integration of a class of multiplicative-noise Stochastic Differential Equations via a RDE approach

Room 1.23

14:00 **Garrappa, Roberto**
Numerical simulation of Maxwell's systems in media with anomalous dielectric properties

14:25 **Abuaisha, Tareq**
On the simulation in time and frequency domain of a fractional-order model of an electrical coil within resonance frequency

14:50 **Jiang, Xingzhou**
Generalized Adams methods to solve fractional differential equations with delay

15:15 **Zhao, Wenjiao**
Lagrange hybridized discontinuous Galerkin method for fractional Navier-Stokes equations

15:40 Break

16:10 **Sandu, Adrian**
MRI-GARK: A Class of Multirate Infinitesimal GARK Methods

16:35 **Hachtel, Christoph**
A multirate implicit Euler scheme for semi-explicit DAEs of index-1: consistency and convergence analysis

17:00 **Bauer, Tobias**
Order conditions for multirate infinitesimal step methods

17:25 **Erbay, Husnu Ata**
A Semi-Discrete Numerical Method for Convolution-Type Unidirectional Wave Equations

Room 1.27

14:00 **Steinebach, Gerd**
Modelling and numerical simulation of hydrogen flow in networks

14:25 **Eisenmann, Monika**
Domain decomposition for nonlinear parabolic problems in a variational framework

15:40 Break

16:10 **Hojjati, Gholam Reza**
Multivalue–multistage methods for the numerical solution of the nonlinear Volterra integro-differential equations

16:35 **Abdi Kalasour, Ali**
A class of multivalue-multistage schemes for the numerical solution of Volterra integral equations

17:00 **Paternoster, Beatrice**
Adapted discretization of evolutionary problems by non-polynomially fitted numerical methods

Room 1.29

14:00 **Pfurtscheller, Lena-Maria**
Polynomial chaos expansion for solving stochastic control problems

14:25 **Piazzola, Chiara**
A low-rank splitting integrator for matrix differential equations

14:50 **Stillfjord, Tony**
Singular value decay of solutions to operator-valued differential Lyapunov and Riccati equations

15:15 **Kheiri Estiar, Hossein**
Numerical method for solving a fractional order HIV model arising from optimal control

15:40 Break

16:10 **Hadjimichael, Yiannis**
Accurate and stable boundary conditions for high-order discretizations of hyperbolic PDEs

16:35 **Leibold, Jan**
Linearly implicit time integration of semilinear wave equations with dynamic boundary conditions

17:00 **Maier, Bernhard**
Numerical simulation of rf-SQUIDs

17:25 **Krämer, Patrick**
Efficient Numerical Schemes for Highly Oscillatory Klein-Gordon and Dirac type Equations

Tuesday

Room 3.28

08:30 **Constantinescu, Emil**
Time Stepping Methods with Forward a Posteriori Error Estimation

09:20 **Scheichl, Robert**
Multilevel Uncertainty Quantification with Sample-Adaptive Model Hierarchies

10:10 Break

10:40 **Eremin, Alexey**
Delay dependent stability analysis of S-ROCK method

11:05 **Farzi, Javad**
Flux limiters on clustered points for solving hyperbolic conservation laws

11:30 **Rihan, Fathalla**
Parameter Identification for Delay Differential Equations

11:55 **Kumar, Vikas**
Haar wavelet quasilinearization approach for numerical solution of Burger type equation via Lie group method

12:20 Lunch

Minisymposium *Computational mechanics and geometric numerical integration*, organised by Sigrid Leyendecker (Erlangen) and Klas Modin (Chalmers)

14:00 **Jimenez, Fernando**
A discrete fractional approach for modelling dissipative mechanical systems

14:30 **Wenger, Theresa**
Numerical properties of mixed order variational integrators applied to dynamical multirate systems

15:00 **Couéraud, Benjamin**
Variational discretization of the Navier-Stokes-Fourier system

15:30 **Martiradonna, Angela**
Positive and mass-conservative integrators for biochemical systems

Room 1.26

10:40 **Celledoni, Elena**
Deep learning as optimal control problems

11:05 **Gerisch, Alf**
FFT-based evaluation of nonlocal terms in PDE systems

11:30 **Knoth, Oswald**
Split-explicit time integration methods for finite element discretizations

11:55 **Dörich, Benjamin**
Splitting methods for highly oscillatory differential equations

12:20 Lunch

Minisymposium *Numerical methods for stochastic (partial) differential equations*, organised by Gilles Vilmart (Geneva)

14:00 **Charrier, Julia**
Existence, uniqueness of the solution and convergence of finite volume approximations for hyperbolic scalar conservation laws with multiplicative noise

14:30 **Bréhier, Charles-Edouard**
Analysis of splitting schemes for the stochastic Allen-Cahn equation

15:00 **Campbell, Stuart**
Adaptive time-stepping for Stochastic Partial Differential Equations with non-Lipschitz drift

15:30 **Lang, Annika**
SPDE simulation on spheres

16:00 Break

16:30 **Legoll, Frederic**
Effective dynamics for non-reversible stochastic differential equations

17:00 **Trstanova, Zofia**
Sampling strategies and diffusion maps

17:30 **Laurent, Adrien**
Exotic aromatic B-series for the order conditions of the long time numerical integration of ergodic stochastic differential equations.

Room 1.23

10:40 **Kulikov, Gennady**
Doubly quasi-consistent fixed-stepsize implicit two-step peer methods for stiff ordinary differential equations

11:05 **Meisrimel, Peter**
Goal oriented time adaptivity using local error estimates

11:30 **Rosemeier, Juliane**
Combining a stroboscopic method with the spectral deferred correction method

11:55 **Singh, Sukhveer**
Numerical simulation to capture the pattern formation

Room 1.27

10:40 **Hosseini, Seyyed Ahmad**
Rational finite differences method based on the barycentric interpolants for ODEs

11:05 **Ávila Barrera, Andrés**
hp-FEM solutions for option price Bates' model

11:30 **Al-Hdaibat, Bashir**
Homoclinic solutions in Bazykin's predator-prey model

11:55 **Pandit, Sapna**
Haar Wavelets based Algorithms for Simulation of Hyperbolic Type Wave Equations

Room 1.29

10:40 **Cortes Garcia, Idoia**
Parallelised Waveform Relaxation for Field/Circuit Coupled Systems

11:05 **Fang, Yonglei**
Symmetric collocation ERKN methods for general second order oscillatory differential equations

11:30 **Vulkov, Lubin**
Two-grid Algorithms for Solution of Difference Equations of Compressible Fluid Flow

11:55 **Koleva, Miglena**
Fitted Finite Volume Method for Optimal Portfolio in a Exponential Utility Regime-Switching Model

Wednesday

Room 3.28

Special session in memory of Willem Hundsdorfer (1954-2017),
chaired by Karel in 't Hout (Antwerp)

08:30 Opening

08:40 **Ruuth, Steven**
Linearly Stabilized Schemes for the Time Integration of Stiff Nonlinear PDEs

09:10 Break

09:40 **Lang, Jens**
IMEX-Peer Methods Based on Extrapolation

10:05 **Horváth, Zoltán**
Positivity and SSP by implicit numerical methods for ODEs and DAEs

10:30 **Teunissen, Jannis**
Willem Hundsdorfer's role and research in the Multiscale Dynamics group at CWI

10:55 **Higueras, Inmaculada**
On Strong Stability Preserving time stepping methods

11:20 Lunch

Room 1.26

09:40 **Jax, Tim**
Linearly Implicit Rosenbrock-Wanner-Type Methods with Non-Exact Jacobian for the Numerical Solution of Differential-Algebraic Equations

10:05 **Estévez Schwarz, Diana**
InitDAE: A new approach for the computation of consistent values, the index determination and the diagnosis of singularities of DAEs

10:30 **Hante, Stefan**
Three Lie group DAE time integration methods tested on a Cosserat rod model

10:55 **Meyer, Tobias**
BDF and Newmark-Type Index-2 and Index-1 Integration Schemes for Constrained Mechanical Systems

Room 1.23

09:40 **Steinhoff, Tim**
On Singly Implicit Runge-Kutta Methods of High Stage Order that Utilize Effective Order

10:05 **Roldan, Teo**
New low-storage SSP Runge-Kutta methods

10:30 **Faleichyk, Barys**
Minimal residual linear multistep methods

10:55 **Fekete, Imre**
On the zero-stability of multistep methods on smooth nonuniform grids

Room 1.27

09:40 **Li, Lu**
Volume preserving diffeomorphisms and the Kahan method

10:05 **Wang, Bin**
Volume-preserving exponential integrators

10:30 **Egger, Herbert**
Structure preserving discretization of evolution problems with dissipation

10:55 **Liu, Changying**
Superconvergence of the structure-preserving trigonometric collocation methods for solving the nonlinear Hamiltonian wave equations

Thursday

Room 3.28

08:30 **Cohen, David**
Exponential integrators for stochastic partial differential equations

09:20 **Meister, Andreas**
Modified Patankar-Runge-Kutta Schemes for Conservative Production-Destruction Equations

10:10 Break

10:40 **in 't Hout, Karel**
On Multistep Stabilizing Correction Splitting Methods with Applications to the Heston Model

11:05 **Sanderse, Benjamin**
Runge-Kutta methods for index-2 and index-3 differential-algebraic equations arising from incompressible flow problems

11:30 **Vandecasteele, Hannes**
Efficiency of micro-macro acceleration for scale-separated stochastic differential equations

11:55 **Zielinski, Przemyslaw**
Convergence and stability of micro-macro acceleration method for scale-separated SDEs

12:20 Lunch

Minisymposium *Model order reduction for dynamical systems*,
organised by Michael Hinze (Hamburg)

14:00 **Benner, Peter**
Gramian-based Model Reduction for Classes of Nonlinear Systems

14:30 **Himpe, Christian**
From Low-Rank to Data-Driven Gramian-Based Model Reduction

15:00 **Buhr, Andreas**
Randomization in Localized Model Order Reduction

15:30 **Peitz, Sebastian**
Data driven feedback control of nonlinear PDEs using the Koopman operator

16:00 Break

16:30 **Banholzer, Stefan**
Multiobjective Optimal Control using Reduced-Order Modeling

17:00 **Gräßle, Carmen**
Adaptive trust-region POD for optimal control of the Cahn-Hilliard equation

17:30 **Ullmann, Sebastian**
Model order reduction for space-adaptive simulations of unsteady incompressible flows

Room 1.26

10:40 **Hinze, Michael**
Adaptivity in model order reduction with proper orthogonal decomposition

11:05 **Pulch, Roland**
Model order reduction for linear dynamical systems with quadratic outputs

11:30 **Paschkowski, Manuela**
Orbital convergence of timestepping schemes for non-smooth mechanics

11:55 **Tietz, Daniel Paul**
Convergence of regularised solutions of piecewise smooth differential equations

12:20 Lunch

Minisymposium *Piecewise Smooth Differential Equations*,
organised by Luca Dieci (Atlanta) and Nicola Guglielmi (L'Aquila)

14:00 **Jeffrey, Michael**
Hidden Dynamics

14:30 **Hairer, Ernst**
On the limit of regularized piecewise-smooth dynamical systems

15:00 **Mehrmann, Volker**
Regularization and numerical solution of hybrid differential-algebraic equations

15:30 **Guglielmi, Nicola**
Discontinuous ODEs and graph optimization

16:00 Break

16:30 **Elia, Cinzia**
Qualitative behavior of numerical solutions of planar discontinuous dynamical systems

17:00 **Streubel, Tom**
Piecewise smooth dynamic simulations via algorithmic piecewise differentation

17:30 **Dieci, Luca**
Is integrating a non-smooth system harder than integrating a smooth one?

<u>Room 1.23</u>

10:40 **Izzo, Giuseppe**
Construction of Strong Stability Preserving Implicit-Explicit General Linear Methods

11:05 **Weiner, Rüdiger**
Optimally zero-stable superconvergent IMEX Peer methods

11:30 **Schneider, Moritz**
Superconvergent IMEX Peer methods with A-stable implicit part

11:55 **Kopecz, Stefan**
Modified Patankar-Runge-Kutta schemes for Advection-Diffusion-Production-Destruction Systems

<u>Room 1.27</u>

10:40 **Owren, Brynjulf**
Adaptive time-stepping in Lie group integrators

11:05 **Wieloch, Victoria**
BDF integrators for mechanical systems on Lie groups

11:30 **Wandelt, Michele**
Geometric integration on Lie groups using the Cayley transformation

11:55 **Tapley, Benjamin**
Collective integration of Hamilton PDEs

Room 1.29

10:40 **Zegeling, Paul Andries**
Boundary value methods for semi-stable differential equations

11:05 **Zerulla, Konstantin**
A uniformly exponentially stable ADI scheme for Maxwell equations

11:30 **Freese, Jan Philip**
Numerical homogenization of the Maxwell-Debye system: Semidiscrete error analysis

Friday

Room 3.28

08:30	**Van Vleck, Erik** Time Dependent Stability: Computation and Applications
09:20	**González Pinto, Severiano** Some aspects of the time integration of multidimensional parabolic problems with mixed derivatives
10:10	**Ketcheson, David** The method of (uncountably many) characteristics
11:00	Break
11:20	**Gander, Martin J.** Is Optimal Really Good in Domain Decomposition ? (or why multigrid coarse spaces might not be suitable)
12:10	**Massot, Marc** Adaptive time-space algorithms for the simulation of multi-scale reaction waves with error control
13:00	Closing

3 Abstracts

A class of multivalue-multistage schemes for the numerical solution of Volterra integral equations

Ali Abdi Kalasour, Seyyed Ahmad Hosseini, Gholam Reza Hojjati, *Mon 16:35 R 1.27*

We are going to investigate a class of general linear methods combined with a quadrature rule for the numerical solution of Volterra integral equations (VIEs) of the second kind. We construct such methods up to order four in which the methods of orders one and two are A– and $V_0(\alpha)$–stable, with maximum value for α, and methods of orders three and four are stable with a large region of absolute stability. The efficiency and capability of the introduced schemes are verified by solving some stiff and nonstiff VIEs.

Keywords: Volterra integral equations, General linear methods, Order conditions, Stability analysis.

On the simulation in time and frequency domain of a fractional-order model of an electrical coil within resonance frequency

Tareq Abuaisha, Jana Kertzscher and Roberto Garrappa, *Mon 14:25 R 1.23*

As windings of an electrical coil are only separated by a thin insulating layer, there are inherent tiny capacitors formed between those windings. These tiny capacitors are added up to form together the parasitic capacitance of the coil. Thus as number of windings for a specific coil increases, the inductance and in a less manner the parasitic capacitance of the coil will also proportionally increase.

At frequencies which lie within almost a decade from the self-resonant frequency, this parasitic „stray“ capacitance will also affect the total impedance of the coil [1]. In this talk we will analyze the fractional-order model of a laboratory coil within resonance frequency. The corresponding multi-order fractional differential equation (MoFDE) will be solved numerically in time domain. In order to investigate the accuracy of the proposed solution, the results in time domain shall be compared with the exact solution in frequency domain.

Simulation results of the fractional-order model will be compared with experimental results whereas unknown parameters of the model are to be identified through an optimization process that is based on the method of least squares.

[1] T. Abuaisha, J. Kertzscher, *Fractional-order Impedance Modeling and Parameter Identification of an Electrical Coil with Interchangeable Core*, Fractional Differentiation and Its Applications (ICFDA), International Conference on, TU Bergakademie Freiberg, 2018 (in press)

Homoclinic solutions in Bazykin's predator-prey model

Bashir Al-Hdaibat, *Tue 11:30 R 1.27*

In this paper we study the homoclinic bifurcations rooted at a (nondegenerate) Bogdanov-Takens (BT) point in the Bazykin's predator-prey model. Namely, we derive an explicit approximation to the homoclinic solutions rooted there. The paper describes the use of the symbolic manipulation language MAPLE for the analysis of the homoclinic bifurcations phenomena in smooth systems of ODEs. It shows how symbolic manipulation language can effectively used to derive explicit expressions for the homoclinic solutions rooted at a (nondegenerate) BT bifurcation.

Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations

Ibrahim Almuslimani, Assyr Abdulle, Gilles Vilmart*, Mon 14:50 R 1.26*

Explicit stabilized Runge-Kutta methods are efficient for solving stiff (deterministic or stochastic) differential equations in large dimensions. In this 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.

Stochastic B–series and order conditions for exponential integrators

Alemayehu Adugna Arara, Kristian Debrabant, Anne Kværnø*, Mon 15:15 R 1.26*

We will discuss B–series for the solution of a stochastic differential equation of the form

$$\mathrm{d}X(t) = \Big(AX(t) + g_0\big(X(t)\big)\Big)\mathrm{d}t + \sum_{m=1}^{M} g_l(X(t)) \star \mathrm{d}W_m(t), \quad X(0) = x_0,$$

for which the exact solution can be written as

$$X(t) = e^{tA}x_0 + \int_0^t e^{(t-s)A} g_0(X(s))\mathrm{d}s + \sum_{m=1}^{M} \int_0^t e^{(t-s)A} g_m(X(s)) \star \mathrm{d}W_m(s).$$

Based on this, we will derive an order theory for exponential integrators for such problems. The integral w. r. t. the Wiener process has to be interpreted e. g. as an Itô or a Stratonovich integral.

References

[1] `https://arxiv.org/pdf/1801.02051.pdf`

Improving the initialization of some integrators for index-3 DAEs and related stiff ODEs

Martin Arnold*, Mon 14:50 R 3.28*

The direct application of ODE time integration methods to higher index DAEs results in numerical solutions that satisfy constraint equations with high accuracy but show a systematic deviation from the manifold that is defined by hidden constraints being obtained by differentiation of the original constraints with respect to time.

Consistent initial values of the analytical solution comply with all the original and hidden constraints in the DAE and do not share the systematic deviation of the numerical solution from hidden constraint manifolds. Therefore, some correction terms need to be added if these (analytically) consistent intial values are used for the initialization of the numerical solution since otherwise large transient error terms and order reduction may be observed in some of the solution components.

In the talk, we will discuss such improved initialization schemes for BDF and for generalized-α methods being applied to a class of semi-explicit index-3 DAEs on linear spaces or on Lie groups. Guided by this analysis for constrained systems, we extend the error analysis to second order ODEs with very stiff potential forces and discuss an improved initialization scheme for Newmark type integrators like the generalized-α method.

(The talk is based on previous joint work with O. Brüls (Liège, Belgium) and A. Cardona (Santa Fe, Argentina) on generalized-α methods and with V. Wieloch (Halle (Saale), Germany) on Lie group BDF time integration.)

hp-FEM solutions for option price Bates' model

Andrés Ávila Barrera, Cecilia Rapimán, *Tue 11:05 R 1.27*

For valuating options, several stochastic models have been developed, where several assumptions on the market are imposed. For example, Black-Scholes' model considers constant volatility and local small changes. To overcome these simplifications, Bates' model [4] includes stochastic volatility and jumps, which corresponds to the following system of stochastic differential equations

$$\begin{cases} dS_t = (\alpha - \frac{1}{2}Y_t)dt + \sqrt{Y_t}dW_1 + dq, \\ dY_t = \xi(\eta - Y_t)dt` + \theta\sqrt{Y_t}dW_2 \end{cases} \tag{1}$$

which can be reduced to a partial integro-differential equation on $\Omega \times (0,T) = (0, S_0) \times (0,1) \times (0,T)$

$$\frac{\partial C}{\partial t} + (r - q - \kappa(1)) S \frac{\partial C}{\partial S} + \frac{1}{2} y S^2 \frac{\partial^2 C}{\partial S^2} + \left[\xi(\eta - y) - \frac{1}{2}\left(\theta^2 - \rho\theta y\right) \right] \frac{\partial C}{\partial y}$$
$$\frac{1}{2}\theta^2 y \frac{\partial^2 F}{\partial y^2} + \rho\theta y S \frac{\partial^2 C}{\partial y \partial S} + \lambda \int_{-\infty}^{\infty} C(S\exp(x), y, t) W(dx) = (r + \lambda) C.$$

with boundary conditions $C(0,y,t) = 0$, $C(S_0,y,t) = S_0 - K$ and final condition $C(S,y,T) = (S-K)^+$. The conditions on y are undefined.

Based on Achdou & Tchou [1], Hilber et al. [5], [6] and Reich et al. [9], we show the variational formulation and prove a Gårding type inequality. Also localization error is obtained. We base our numerical studies on Almendral & OOsterlee [2], Ballestra & Sgarra [3] and Miglio & Sgarra [8]. We propose that *hp*-FEM methods [7], as special method of singularly elliptic problems, can be used to improve unstabilities of the FEM methods detected in the simplification of the splitting. Some studies on the parameters on the effect of convective part over the diffusion part are also considered.

Keywords: Stochastic option pricing models, *hp*-finite element method, degenerate partial integro-differential equations

Mathematics Subject Classifications (2000):35K65, 65M15, 65M60, 65N30.

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Multiobjective Optimal Control using Reduced-Order Modeling

Stefan Banholzer, Stefan Volkwein, Eugen Makarov*, Thu 16:30 R 3.28*

Many optimization problems in applications can be formulated using several objective functions, which are conflicting with each other. This leads to the notion of multiobjective or multicriterial optimization problems.
This talk discusses the application of the reference point method in combination with model-order reduction to multiobjective optimal control problems of elliptic and parabolic PDEs with up to four cost functions. Since the reference point method transforms the multiobjective optimal control problem into a series of scalar optimization problems, model-order reduction is used to lower the computational cost. Due to the lack of a-priori analysis for the model-order reduction, a-posteriori estimates are important to be able to ensure a good approximation quality. To this end, an a-posteriori estimate for the problem at hand is introduced and used for developing new strategies for efficiently updating the reduced-order model in the optimization process.

Order conditions for multirate infinitesimal step methods

Tobias Bauer, Oswald Knoth*, Mon 17:00 R 1.23*

Multirate infinitesimal step methods (MIS) are generalised split-explicit Runge-Kutta methods (RK) especially designed for problems in different temporal scales. They have been developed and investigated for up to order three. It can be shown that they are somehow related to multirate generalized additive RK methods (MGARK). Following the ideas of MGARK methods, the MIS methods can also be reformulated to partitioned RK methods.
In this presentation, applying the strategy of the reformulation, it will be shown how high-order conditions can be derived. Furthermore, a method of 4th-order is developed and presented as well as illustrated with numerical examples.

Gramian-based Model Reduction for Classes of Nonlinear Systems

Peter Benner, Pawan Kumar Goyal, *Thu 14:00 R 3.28*

For linear input-output systems, system Gramian matrices are a long established tool to quantify the properties controllability and observability. A range of associated Gramian-based model reduction methods has been developed over the last decades utilizing those attributes, starting with the landmark paper by Moore (1981) introducing balanced truncation in the form it has been used since then. During the last two decades, the method has also become computationally feasible for truly large-scale systems arising from discretizing systems with dynamics defined by unsteady PDEs. This is mainly due to low-rank techniques, allowing to compute the information necessary for implementing balanced truncation at almost linear complexity w.r.t. the order of the system (in contrast to the cubic complexity of traditional implementations).
We show that these techniques can also be used to define approximate balanced truncation methods for some classes of nonlinear systems. This is based on combing low-rank techniques for Gramian computation with the concept of truncated Gramians derived from the Volterra series representation of the system response. We introduce these techniques for bilinear, quadratic-bilinear, and polynomial systems. The performance of the new methods is illustrated by several numerical examples.

Analysis of splitting schemes for the stochastic Allen-Cahn equation

Charles-Edouard Bréhier, Jianbao Cui, Ludovic Goudenège, Jialin Hong, *Tue 14:30 R 1.26*

The stochastic Allen-Cahn equation, with additive space-time white noise perturbation, in dimension 1, is given by the following semilinear SPDE

$$dX(t) = AX(t)dt + \big(X(t) - X(t)^3\big)dt + dW(t).$$

Since the nonlinearity $x \mapsto x - x^3$ is not globally Lipschitz continuous, the design of suitable temporal discretization scheme is delicate. We propose to use a splitting strategy, taking into account that the flow $\big(\Phi_t(z)\big)_{t\geq 0}$ of the ODE $\dot{z} = z - z^3$ is exactly known.
We study numerical schemes defined as

$$X_{n+1} = e^{\Delta t A}\Phi_{\Delta t}(X_n) + \int_{n\Delta t}^{(n+1)\Delta t} e^{(n\Delta t - t)A} dW(t),$$

(exact sampling of the stochastic convolution), or as

$$X_{n+1} = S_{\Delta t}\Phi_{\Delta t}(X_n) + S_{\Delta t}\big(W((n+1)\Delta t) - W(n\Delta t)\big)$$

with $S_{\Delta t} = (I - \Delta t A)^{-1}$ (semi-implicit discretization of the stochastic convolution).
Moment estimates, as well as strong and weak convergence rates, will be presented.
I will also present numerical simulations supporting the theoretical results.

Randomization in Localized Model Order Reduction

Andreas Buhr, *Thu 15:00 R 3.28*

Localized (in space) model order reduction is a promising approach for many simulation tasks in engineering because of its good parallelization behavior and and the potential reuse of local models. Especially for highly complex structures with large geometric detail, large simulation speedups can be achieved. We focus on signal integrity simulations in printed circuit boards,

which can be performed by approximating the solution of the time harmonic Maxwell's equation. Such simulations often take several hours or days with classical methods, because even a coarse mesh easily leads to $\mathcal{O}(10^8)$ or more unknowns.
To generate local approximation spaces for localized model order reduction, we recently proposed to employ methods from randomized numerical linear algebra (RandNLA) [A. Buhr and K. Smetana, *SIAM J. Sci. Comput.*, 40(4), A2120-A2151]. We define local transfer operators which have quickly decaying singular values and approximate their left singular vectors to obtain good local approximation spaces. RandNLA provides fast algorithms having good parallelization behavior and provable convergence rates for this task.
We will showcase the application of randomized local model order reduction on the signal integrity simulation for an Olimex OLinuXino A64 mini PC (Raspberry Pi like).

Adaptive time-stepping for Stochastic Partial Differential Equations with non-Lipschitz drift

Stuart Campbell, Conall Kelly, Gabriel Lord, *Tue 15:00 R 1.26*

Traditional explicit numerical methods to simulate stochastic differential equations (SDEs) or stochastic partial differential equations (SPDEs) rely on globally Lipschitz drift and diffusion coefficients to ensure convergence. Many applications of interest include non Lipschitz drift functions. Implicit methods (when they exist) can often be too computationally expensive for practical uses. Therefore construction of explicit methods to simulate SDEs or SPDEs with non-Lipschitz drift is of interest.
Tamed methods are a class of numerical methods that perturb the drift coefficient to ensure strong convergence in the presence of non-Lipschitz drift. In this talk we present an explicit method for simulation of SPDEs which guarantees strong convergence via adaptive time-step size selection instead of drift taming. We will outline the theory behind the method and illustrate the efficiency through some numerical simulations.

Deep learning as optimal control problems

Elena Celledoni, *Tue 10:40 R 1.26*

The motivation of this talk comes from recent work of Haber and Ruthotto, where deep learning neural networks have been interpreted as discretisations of an optimal control problem. We review the first order conditions for optimality, and the conditions ensuring optimality after discretization. This leads to a class of algorithms for solving the discrete optimal control problem which guarantee that the corresponding discrete necessary conditions for optimality are fulfilled. We discuss two different deep learning algorithms and make a preliminary analysis of the ability of the algorithms to generalize.

Existence, uniqueness of the solution and convergence of finite volume approximations for hyperbolic scalar conservation laws with multiplicative noise

Julia Charrier, Caroline Bauzet, Vincent Castel, Thierry Gallouët, *Tue 14:00 R 1.26*

We are interested here in multi-dimensional nonlinear scalar conservation laws forced by a multiplicative noise with a general time and space dependent flux-function. We address simultaneously theoretical and numerical issues. More precisely we establish existence, uniqueness and some properties of the stochastic entropy solution together with the convergence of a finite volume scheme. The results proposed in this work suppose more general fluxes than the ones considered in the literature and the main novelty here is the use of the numerical approximation to get both the existence and the uniqueness of the solution. We also provide a L^∞ stability result as well as a time continuity property on the stochastic entropy solution to complete this study.

Exponential integrators for stochastic partial differential equations
David Cohen, R. Anton, G. Dujardin, S. Larsson, L. Quer-Sardanyons, M. Sigg, X. Wang, *Thu 08:30 R 3.28*

The aim of the presentation is to give a brief, and hopefully not too technical, overview on the numerical discretisation of various stochastic partial differential equations (SPDEs) by exponential-type integrators. We begin by introducing SPDEs and the main ideas behind exponential integrators. We next present recent results on the use of such numerical schemes for the time integration of stochastic wave equations, stochastic Schrödinger equations, and stochastic heat equations.

Time Stepping Methods with Forward a Posteriori Error Estimation
Emil Constantinescu, *Tue 08:30 R 3.28*

Global or *a posteriori* error represents the actual discretization error resulting after solving a system of differential equations. Calculating and controlling the *a posteriori* error is considered an expensive process, and therefore in practice only the local error (from one step to the next) is used as a proxy for the solver accuracy. However, local error estimation is not always sufficient or suitable. This talk will be focused on new time-stepping methods with built-in *a posteriori* error estimates. These methods can be cast as general linear schemes that provide pointwise global errors. Sufficient convergence conditions and order barriers are established. A few other strategies for *a posteriori* error estimation will be reviewed and shown that they can be reduced to the proposed strategy as particular cases. The theoretical findings will be illustrated on examples based on ordinary and partial differential and algebraic equations. Global error control and adaptivity will be addressed. The implementation of these methods in PETSc, a portable high-performance scientific computing library will also be discussed.

Parallelised Waveform Relaxation for Field/Circuit Coupled Systems
Idoia Cortes Garcia, Iryna Kulchytska-Ruchka, Sebastian Schöps, *Tue 10:40 R 1.29*

When coupling systems, for example describing different multiphysical problems, often each subsystem can already be solved with dedicated software. This, as well as a multirate behaviour can be exploited by using waveform relaxation. Waveform relaxation with windowing divides the simulation time interval $\mathcal{I} = [T_0, T_{\mathrm{end}}]$ into several smaller sub-intervals $\mathcal{I}_j = [T_j, T_{j+1}]$, solves there the different systems separately and exchanges information iteratively between them in order to converge to the solution of the coupled system.
On the other hand, Parareal is an algorithm that allows to parallelise time-domain simulations. The goal of this talk is to combine both methods in a multiphysics framework in order to parallelise the waveform relaxation iterations on the different sub-intervals $\mathcal{I}_j$ and eventually speed-up the time to solution. In particular, this method is used in order to simulate the coupling of the electromagnetic field inside a device with an electric circuit surrounding it. This leads to the coupling of Maxwell's equations with the system of differential algebraic equations obtained from modified nodal analysis.

Variational discretization of the Navier-Stokes-Fourier system

Benjamin Couéraud, François Gay-Balmaz*, Tue 15:00 R 3.28*

In this talk I will present an ongoing work with François Gay-Balmaz on the variational discretization of the compressible Navier-Stokes-Fourier system, in which the viscosity term and the heat conduction term are handled within the variational approach to nonequilibrium thermodynamics developed by Gay-Balmaz and Yoshimura. In order to spatially discretize the system we extend the geometric approach developped by Pavlov and al., which is particularly well-adapted for the discretization of Euler-Poincaré systems whose configuration space is the infinite-dimensional Lie group of diffeomorphisms. A careful treatment of the phenomenological constraint is necessary. After this spatial discretization, we obtain a nonholonomic, variational principle on a finite-dimensional Lie group. Finally we discretize in time the resulting system using a nonholonomic variational integrator whose associated discrete evolution equations are proved to respect the balance of energy of the system.

Stability issues in the discretization of stochastic differential equations

Raffaele D'Ambrosio*, Mon 14:25 R 1.26*

The aim of this talk is the analysis of various stability issues for numerical methods designed to solve stochastic differential equations. We first aim to consider nonlinear Itô stochastic differential equations (SDE): under suitable regularity conditions, exponential mean-square stability holds, i.e. any two solutions $X(t)$ and $Y(t)$ of a SDE with $\mathbb{E}|X_0|^2 < \infty$ and $\mathbb{E}|Y_0|^2 < \infty$ satisfy

$$\mathbb{E}|X(t) - Y(t)|^2 \leq \mathbb{E}|X_0 - Y_0|^2 e^{\alpha t}, \tag{1}$$

with $\alpha < 0$. We aim to investigate the numerical counterpart of (1) when trajectories are generated by stochastic linear multistep methods, in order to provide stepsize restrictions ensuring analogous exponential mean-square stability properties also numerically [1, 4]. This is a joint research with Evelyn Buckwar (Johannes Kepler University of Linz).

We next consider second order stochastic differential equations describing the position of a particle subject to the deterministic forcing $f(x)$ and a random forcing $\xi(t)$ of amplitude ε. The dynamics exhibits damped oscillations, with damping parameter η. We aim to analyze long-term properties for indirect stochastic two-step methods, with special emphasis to understanding the ability of such methods in retaining long-term invariance laws [2, 3]. This is a joint research with Martina Moccaldi and Beatrice Paternoster (University of Salerno).

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Analysis of multilevel Monte Carlo using the Milstein discretisation

Kristian Debrabant, Michael B. Giles, Andreas Roessler, *Mon 14:00 R 1.26*

Using a simple Monte Carlo method with a numerical discretisation with first order weak convergence, to achieve a root-mean-square error of $\mathcal{O}(\epsilon)$ would require $\mathcal{O}(\epsilon^{-2})$ independent paths, each with $\mathcal{O}(\epsilon^{-1})$ timesteps, giving a computational complexity which is $\mathcal{O}(\epsilon^{-3})$. However, Giles' multilevel Monte Carlo (MLMC) approach ([1]), which combines the results of simulations with different numbers of timesteps, reduces the cost to $\mathcal{O}(\epsilon^{-2})$ under certain circumstances.
In this presentation we analyse the efficiency of the MLMC approach for different options and scalar SDEs using the Milstein discretisation, determining or bounding the order of convergence of the variance of the multilevel estimator, and hence the computational complexity of the method.

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Numerical integration of a class of multiplicative-noise Stochastic Differential Equations via a RDE approach

Hugo de la Cruz, *Mon 17:25 R 1.26*

Many important Stochastic Differential Equations (SDEs) used to model noisy dynamical systems are driven by linear multiplicative noise diffusion-coefficients. In this work we consider an approach, based on the conjugacy between this type of SDEs and an appropriate Random Differential Equation, for constructing new integrators for the underlying system. In addition, we discuss the possibility of devising numerical methods without assuming restrictive assumptions that typically are not satisfied by many SDEs in significant applications. Details on the efficient implementation of the proposed methods are discussed and their performance is illustrated through computer simulations.

Is integrating a non-smooth system harder than integrating a smooth one?

Luca Dieci, Cinzia Elia, *Thu 17:30 R 1.26*

In this talk we first consider ways to integrate a differential system with discontinuous right-hand-side (DRHS). Then, by considering a smooth planar system having slow-fast motion, where the slow motion takes place near a curve, we explore the idea of replacing the original smooth system with a DRHS system, whereby the DRHS system coincides with the smooth one away from a neighborhood of the curve. After this reformulation, we will obtain sliding motion on the curve, and numerical methods apt at integrating for sliding motion can be applied. We further consider bypassing the sliding motion altogether, and monitor entries (transversal) and exits (tangential) on the curve. Numerical examples illustrate potential and challenges of this approach.
This talk is based on the paper "Smooth to discontinuous systems: a geometric and numerical method for slow-fast dynamics", by L. Dieci, C. Elia. In DCDS-B, 2018.

Splitting methods for highly oscillatory differential equations

Benjamin Dörich, Marlis Hochbruck, *Tue 11:55 R 1.26*

In this talk we consider the time integration of highly oscillatory differential equations of the form

$$y''(t) = -\Omega^2 y(t) + g(y(t))$$

which typically arise in the space discretizaion of semi linear wave equations. In contrast to the classical analysis we do not assume high regularity of the solution but only a so called finite energy condition. For "nice" functions g one can use trigonometric integrators with filter functions to obtain second order error estimates, cf. [1, Chapter 13] and references given there. However, for g representing a first order differential operator these integrators fail. For example in the linear case numerical experiments indicate very large error constants.

We show that much better results can be achieved by constructing new filter functions and adapting the techniques from the analysis in [2]. Numerical examples confirming the theoretical results are also presented.

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Structure preserving discretization of evolution problems with dissipation

Herbert Egger, *Wed 10:30 R 1.27*

We present a general framework for the systematic numerical approximation of dissipative evolution problems. The approach is based on rewriting the evolution problem in a particular form that complies with an underlying energy or entropy structure. Based on the variational characterization of smooth solutions, we are then able to show that the approximation by Galerkin methods in space and discontinuous Galerkin methods in time automatically leads to numerical schemes that inherit the underlying dissipative structure of the evolution problem. The proposed framework is rather general and can be applied to a wide range of applications. This is demonstrated by a detailed discussion of a variety of test problems.

Domain decomposition for nonlinear parabolic problems in a variational framework

Monika Eisenmann, Eskil Hansen, *Mon 14:25 R 1.27*

Nonlinear parabolic equations are frequently encountered in applications, but in practice constructing an approximation for these problems yields a large scale computational system. In order to obtain an efficient algorithm for the numerical approximation, it can be useful to apply a scheme that consists of a number of independently solvable subproblems to make use of a parallel computing hardware.

In our work, we introduce a general framework of non-autonomous, inhomogeneous evolution equations in a variational setting and show convergence of an operator splitting scheme via a time discretization. This approach covers a fairly general class of parabolic differential equations. We exemplify the usage to a p-Laplacian type problem with a possibly time depending domain decomposition.

Qualitative behavior of numerical solutions of planar discontinuous dynamical systems

Cinzia Elia, Luca Dieci, Timo Eirola, *Thu 16:30 R 1.26*

We consider a planar linear discontinuous system with an asymptotically stable periodic orbit and we study the qualitative behavior of the numerical approximation obtained with forward Euler with and without event location. Differences and similarities with the theory for smooth systems will be highlighted and justified both numerically and theoretically.

A Semi-Discrete Numerical Method for Convolution-Type Unidirectional Wave Equations

Husnu Ata Erbay, Saadet Erbay, Albert Erkip, *Mon 17:25 R 1.23*

In this study we prove the convergence of a semi-discrete numerical method applied to the initial value problem for a general class of nonlocal nonlinear unidirectional wave equations $u_t+(\beta * f(u))_x = 0$. Here the symbol * denotes the convolution operation in space, $(\beta * v)(x) = \int_{\mathbb{R}} \beta(x-y)v(y)dy$, and the kernel β is even function with $\int_{\mathbb{R}} \beta(x)dx = 1$. Members of the class arise as mathematical models for the propagation of dispersive waves in a variety of situations. For instance, the Benjamin-Bona-Mahony equation and the Rosenau equation are members of the class. Our calculations closely follow the approach in [1] where error analysis of a similar semi-discrete method was conducted for the nonlocal bidirectional wave equations. As in [1], the numerical method is built on the discrete convolution operator based on a uniform spatial discretization. The semi-discretization in space and a truncation of the infinite spatial domain to a finite one give rise to a finite system of ordinary differential equations in time. We prove that solutions of the truncated problem converge uniformly to those of the continuous one with the second-order accuracy in space when the truncated domain is sufficiently large. Finally, for some particular choices of the convolution kernel, we provide numerical experiments that corroborate the theoretical results.

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Delay dependent stability analysis of S-ROCK method

Alexey Eremin, *Tue 10:40 R 3.28*

The talk is concerned with the numerical solution of stochastic delay differential equations. Stochastic Runge–Kutta–Chebyshev methods (S-ROCKs) are considered. Their delay-dependent stability for a linear scalar test equation with real coefficients is studied. With help of the so-called root locus technique, the full asymptotic stability region in mean square is obtained, which is characterized by a sufficient and necessary condition in terms of the drift and diffusion coefficients as well as time stepsize and the damping parameter eta. The derived condition is compared with the analytical stability condition.

InitDAE: A new approach for the computation of consistent values, the index determination and the diagnosis of singularities of DAEs

Diana Estévez Schwarz, René Lamour, *Wed 10:05 R 1.26*

InitDAE is a prototype written in Python that computes consistent initial values of differential-algebraic equations (DAE), determines their index with a projector based decoupling and a related condition number that permits the diagnosis of singularities. The consistent initialization is determined using a projector based constrained optimization approach and the inherent differentiations required in the higher index case are provided by automatic differentiation (AD), using AlgoPy. Consequently, a detailed description of the local structural properties of the DAE becomes possible using the SVD. InitDAE has been conceived for academic purposes and is well-suited for examples of moderate size.

In this talk we give an overview of the used algorithms, demonstrate available features and discuss future possibilities, in particular the integration with Taylor series methods.

Minimal residual linear multistep methods

Barys Faleichyk, *Wed 10:30 R 1.23*

Consider an initial value problem for the system of ODEs $y' = f(t, y)$ and suppose that we have k starting values $y_0, \ldots, y_{k-1}$ at points $\{t_j\}$ which are not necessarily equidistant. To compute $y_k \approx y(t_{k-1} + \tau)$ take an explicit linear multistep method with unknown coefficients:

$$y_k = \sum_{j=0}^{k-1} (\tau \beta_j f_j - \alpha_j y_j). \tag{1}$$

On the other hand consider the corresponding classic p-step implicit BDF formula

$$c_{k-p} y_{k-p} + \ldots + c_k y_k = \tau f_k, \quad p \le k. \tag{2}$$

In the talk we discuss what happens if on each step of numerical integration the coefficients $\{\alpha_j, \beta_j\}$ of (1) are chosen to minimize the norm of the residual of method (2). The main focus will lie on the most tractable case of linear problems with $f(t, y) = A(t)y + b(t)$.

Symmetric collocation ERKN methods for general second order oscillatory differential equations

Yonglei Fang, *Tue 11:05 R 1.29*

This talk focus on the constuction of new symmetric collocation ERKN methods for second order oscillatory problems by Lagrange interpolation. Linear stability of the new ERKN methods is analyzed. Numerical experiments show the high effectiveness of the new ERKN methods compared to their RKN counterparts.

Flux limiters on clustered points for solving hyperbolic conservation laws

Javad Farzi, *Tue 11:05 R 3.28*

It is well known that the solutions of hyperbolic conservation laws have, in general, discontinuities and shocks in the domain of solution. To obtain non-oscillatory, entropy satisfying accurate solutions there are different approaches, which have been extensively studied in the literature. A well-known approach is to use the flux limiters to control the spurious oscillations and kill out the overshoots and undershoots in the vicinity of discontinuity or shock. In this paper we mainly study the effect of grid clustering to reduce the mentioned oscillations and provide sharp solutions.

On the zero-stability of multistep methods on smooth nonuniform grids

Imre Fekete, Gustaf Söderlind, István Faragó, *Wed 10:55 R 1.23*

In this talk we investigate zero stability on compact intervals and smooth nonuniform grids. The grid points $\{t_n\}_{n=0}^{N}$ are constructed as the image of an equidistant grid under a smooth deformation map, i.e., $t_n = \Phi(\tau_n)$, where $\tau_n = n/N$ and the map Φ is monotonically increasing with $\Phi(0) = 0$ and $\Phi(1) = 1$. We show that for all strongly stable linear multistep methods, there is an N^* such that a condition of zero stability is always fulfilled for $N > N^*$, provided that $\Phi \in C^2[0,1]$. Thus zero stability is maintained whenever adjacent step sizes satisfy $h_n/h_{n-1} = 1 + \mathrm{O}(N^{-1})$. This suggests that variable step size should always be implemented using smooth step size changes.

The talk is based on the paper

G. Söderlind, I. Fekete, I. Faragó: On the zero-stability of multistep methods on smooth nonuniform grids, BIT Numer. Math., `https://doi.org/10.1007/s10543-018-0716-y`, 2018.

Numerical homogenization of the Maxwell-Debye system: Semidiscrete error analysis

Jan Philip Freese, Dietmar Gallistl, Christian Wieners, *Thu 11:30 R 1.29*

In this talk we investigate time-dependent Maxwell's equations coupled with the Debye model for orientation polarization in a medium with highly oscillatory parameters. The goal is to characterize the macroscopic behavior of the solution to the resulting integro-differential system. We use analytical homogenization results to derive the effective Maxwell system with the corresponding cell problems. The Finite Element Heterogeneous Multiscale Method (FE-HMM) is applied to solve the homogenized Maxwell system and we give first insights into the semidiscrete error analysis.

Is Optimal Really Good in Domain Decomposition ? (or why multigrid coarse spaces might not be suitable)

Martin J. Gander, *Fri 11:20 R 3.28*

Domain Decomposition methods need in general a coarse correction to be scalable, and it seems natural to use for this purpose a coarse grid like in multigrid methods. I will show in this talk that while this indeed suffices to make the methods scalable, and thus "optimal" in traditional domain decomposition terminology, there are coarse corrections that lead to much faster two level domain decomposition methods. To explain this, I will introduce the notion of an optimal coarse space, and optimized approximations thereof. I will finally show that such coarse spaces can do much more than just make the domain decomposition method scalable: they can fix problems the underlying domain decomposition iteration has, like convergence problems for high contrast media, divergence of the iterative Additive Schwarz method, and even lead to a well posed Neumann-Neumann and associated FETI domain decomposition method in function space.

Numerical simulation of Maxwell's systems in media with anomalous dielectric properties

Roberto Garrappa, *Mon 14:00 R 1.23*

In materials showing anomalous dielectric properties, the polarization processes are described in the frequency domain by constitutive laws based on nonlinear models with one or more fractional powers.
As a consequence, the simulation in the time domain of Maxwell's systems for such kind of materials involves non-standard differential or pseudo-differential operators of fractional order [1] whose numerical approximation requires new and specifically devised methods.
In this talk we consider the Havriliak-Negami model which applies to a large extent of materials with anomalous dielectric relaxation properties. After discussing the mean features and properties of this model, we analyze the fractional derivative of Prabhakar type [2] involved for its description in the time domain and we propose some approaches for the numerical simulation of Maxwell's systems.
The extension to other dielectric models, such as the Excess Wing model, is also addressed.

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Serial and Parallel Iterative Splitting Methods: Algorithms and Applications

Jürgen Geiser, J.L.Hueso, E.Martinez,, *Mon 16:10 R 3.28*

In the lecture, we discuss the ideas of serial and parallel iterative splitting methods. The ideas and properties of iterative splittig methods with serial versions have been studied since recent years. We extend the itertative splitting methods to a class of parallel versions, which allow to reduce the computational time and keep the benefit of the higher accuracy with each iterative step.
We present the novel parallel splitting methods, which are nowadays important to solve large problems. While decomposing into simpler subproblems, such subproblems can be computed independently with the different processors.
We discuss the numerical convergence of the serial and parallel iterative splitting methods. Then, we present different numerical applications based on convection-diffusion problems to validate the benefit of the parallel versions.

FFT-based evaluation of nonlocal terms in PDE systems

Alf Gerisch, *Tue 11:05 R 1.26*

Cellular adhesion or repulsion is an important aspect in many biological systems and has been implicated in processes related the pigmentation pattern in fish, the sorting of cells in embryonal tissue, the invasion of healthy tissue by cancer cells and also tissue growth in bioreactors. In PDE-type modelling of these processes this aspect is often successfully accounted for by a solution-dependent spatially nonlocal term. The nonlocality here represents the observation that the state of the sourrounding tissue of a cell influences its adhesive or repulsive behaviour. The evaluation of the nonlocal term in such models often amounts to the computational bottleneck in numerical schemes.

In this presentation we outline an efficient FFT-based technique for the evaluation of this nonlocal term on one- and higher dimensional uniform grids and for spatially periodic boundary conditions. We also show how more general boundary condition can be accomodated for by slightly increasing the problem dimension and at a moderate increase in computational cost. The methodology is also applicable in the case of certain iterated integrals. We finally also discuss an application of the method on unstructured grids and/or non-box shaped spatial domains.

Some aspects of the time integration of multidimensional parabolic problems with mixed derivatives

Severiano González Pinto, *Fri 09:20 R 3.28*

We start by reviewing a few schemes based on directional splitting for the time integration of multidimensional parabolic problems in case that mixed derivatives are present and where it is assumed a spatial semi-discretization based on central differences. Then, we focus on unconditional stability aspects, particularly on W-methods based on the Approximated Matrix Factorization (AMF) to perform the directional splitting. The linear constant coefficient problem with Homogeneous Boundary Conditions of Dirichlet type will be analyzed and a relevant scalar test problem stemming from it, will play a relevant role in the stability analysis. The empirical order of convergence in PDE sense of some relevant schemes will be illustrated with a few linear test PDE problems, one of them meeting applications in Finance. It will be seen that often the convergence order presents a stronger reduction when the boundary conditions are time-dependent. A way to circumvent this drawback will be shown.

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Adaptive trust-region POD for optimal control of the Cahn-Hilliard equation

Carmen Gräßle, Michael Hinze, Jan Oke Alff, Nicolas Scharmacher, *Thu 17:00 R 3.28*

We consider the optimal control of a Cahn-Hilliard system in a trust-region framework. For an efficient numerical solution, the expensive high dimensional PDE systems are replaced by reduced order models utilizing proper orthogonal decomposition (POD-ROM). Within the trust-region POD (TR-POD), the accuracy of the surrogate models is controlled in the course of the optimization. The POD modes are computed corresponding to snapshots of the governing equations which are discretized utilizing adaptive finite elements. Different types of snapshots and POD basis generations for the different system variables are analyzed. In the numerical examples, the smooth as well as the double-obstacle free energy potential are considered.

Discontinuous ODEs and graph optimization

Nicola Guglielmi, Eleonora Andreotti (L'Aquila and Torino), Dominik Edelmann and Christian Lubich (Tuebingen), *Thu 15:30 R 1.26*

In this talk I will discuss some optimization methods in spectral graph theory aimed to cluster a weighted undirected graph under certain constraints. The use of a gradient system is the main tool in the methodology. Due to the non-negativity constraint on the weights of the graph, it is possible that a discontinuous ODE is encountered which leads to the possibility that only a generalized solution of the gradient system exists. This situation has to be handled accurately in a numerical integration of the system. This is a joint work with Eleonora Andreotti (L'Aquila and Torino), Dominik Edelmann and Christian Lubich (Tuebingen).

A Localized Reduced-Order Modeling Approach for PDEs with Bifurcating Solutions

Max Gunzburger, Alessandro Alla, Martin Hess, Gianluigi Rozza, Annalisa Quaini, *Mon 10:40 R 3.28*

Reduced-order modeling (ROM) commonly refers to the construction, based on a few solutions (referred to as snapshots) of an expensive discretized partial differential equation (PDE), and the subsequent application of low-dimensional discretizations of partial differential equations (PDEs) that can be used to more efficiently treat problems in control and optimization, uncertainty quantification, and other settings that require multiple approximate PDE solutions. In this work, a ROM is developed and tested for the treatment of nonlinear PDEs whose solutions bifurcate as input parameter values change. In such cases, the parameter domain can be subdivided into subregions, each of which corresponds to a different branch of solutions. Popular ROM approaches, such as proper orthogonal decomposition (POD), results in a global low-dimensional basis that does not respect nor take advantage of the often large differences in the PDE solutions corresponding to different subregions. Instead, in the new method, the k-means algorithm is used to cluster snapshots so that within cluster snapshots are similar to each other and are dissimilar to those in other clusters. This is followed by the construction of local POD bases, one for each cluster. The method also can detect which cluster a new parameter point belongs to, after which the local basis corresponding to that cluster is used to determine a ROM approximation. Numerical experiments show the effectiveness of the method both for problems for which bifurcation cause continuous and discontinuous changes in the solution of the PDE.

A multirate implicit Euler scheme for semi-explicit DAEs of index-1: consistency and convergence analysis

Christoph Hachtel, Andreas Bartel, Michael Günther, *Mon 16:35 R 1.23*

The mathematical modelling of electrical circuits often leads to large scale systems of differential equation with components which provide a very different dynamical behaviour. These systems can be integrated efficiently by multirate time integration schemes. Such multirate schemes employ inherent step sizes according to the dynamical properties of the components of the system.

In general, electrical circuits are described by differential algebraic equations. In this talk, we will apply multirate time integration schemes to semi-explicit differential-algebraic equations of index 1. We focus on systems where the algebraic constraints only occur in the slow changing components. On the basis of the implicit Euler-scheme, we will point out the details of the multirate time integration for DAEs. We will discuss different coupling approaches between the subsystems consisting of components with similar dynamic behaviour. For the analysis of the integration scheme, we follow the indirect approach and write the algebraic variables as a function of the differential variables. We will show that the order of consistency of the classical ODE multirate scheme can be maintained under suitable assumptions. We will complete our talk by an adaption of the proof of [1] that shows that by using a constant macro step-size the multirate implicit Euler scheme also converges for semi-explicit DAEs of index-1.

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Accurate and stable boundary conditions for high-order discretizations of hyperbolic PDEs

Yiannis Hadjimichael, *Mon 16:10 R 1.29*

In this talk, we provide a rigorous analysis of various boundary conditions applicable to Runge–Kutta methods for hyperbolic conservation laws. In particular, we focus on perturbed Runge–Kutta methods that use both upwind- and downwind-biased discretizations; such methods have been used until now only with periodic boundary conditions. Moreover, we examine the boundary conditions under which a perturbed Runge–Kutta method coupled with a TVD spatial discretization maintains the TVD property. Several examples in one- and two-dimensional hyperbolic problems exhibit the robustness of the boundary condition treatment and the high order of accuracy at the boundaries.

On the limit of regularized piecewise-smooth dynamical systems

Ernst Hairer, Nicola Guglielmi, *Thu 14:30 R 1.26*

This work deals with piecewise-smooth dynamical systems and with regularizations, where the jump discontinuities of the vector field are smoothed out in an ε-neighbourhood by using a continuous transition function. It addresses the following questions:

- does the solution of the regularization, for $\varepsilon \to 0$, converge to a Filippov solution of the discontinuous problem ?
- under which condition is the limit for $\varepsilon \to 0$ of the regularized solution independent of the transition function ?

Emphasis is put on the situation, where there is non-uniqueness of solutions for the discontinuous problem. The results are complemented by numerical simulations.

This work is a continuation of the results in the publications

N. Guglielmi and E. Hairer, *Classification of hidden dynamics in discontinuous dynamical systems.* SIAM J. Appl. Dyn. Syst. 14(3) (2015) 1454–1477.

N. Guglielmi and E. Hairer, *Solutions leaving a codimension-2 sliding.* Nonlinear Dynamics 88(2) (2017) 1427-1439

which can be downloaded from

`http://www.unige.ch/~hairer/preprints.html`

A least-squares collocation method for non-linear higher index differential-algebraic equations

Michael Hanke, Roswitha März, *Mon 14:25 R 3.28*

Differential-algebraic equations (DAEs) with higher index give rise to essentially ill-posed problems. We regularize the DAEs by a least-squares collocation method. Its realization is not much more computationally expensive than standard collocation methods used in the numerical solution of ordinary differential equations and index-1 DAEs. Thus, it is much cheaper than methods based on index reductions. In numerical experiments, this approach has displayed excellent convergence properties both for linear and non-linear DAEs. A strict convergence proof has been given earlier for the general class of linear index-μ tractable DAEs.
The present paper is devoted to present new results about the convergence of this least-squares collocation method and a Gauss-Newton scheme for non-linear DAEs under rather general conditions

Domain decomposition and parabolic problems – a time integrator approach

Eskil Hansen, Monika Eisenmann, *Mon 11:30 R 3.28*

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 [2]. We will outline a convergence analysis [1] 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.

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Three Lie group DAE time integration methods tested on a Cosserat rod model

Stefan Hante, Martin Arnold, *Wed 10:30 R 1.26*

We will consider three Lie group DAE time integration methods: Firstly, the generalized-α Lie group method, which slowly gains popularity in multi-body simulation, secondly the BLieDF Lie group method, which is a recently developed multistep method based on the popular BDF methods and lastly a variational integrator which is a Lie group analogon to the well-known SHAKE and RATTLE integration schemes.
All three Lie group DAE time integrators are implemented in Fortran and are applied to a nontrivial constrained Cosserat rod model in order to compare performance, accuracy and energy behaviour.

On Strong Stability Preserving time stepping methods
Inmaculada Higueras, *Wed 10:55 R 3.28*

During the last decades, the study of Strong Stability Preserving (SSP) properties for different kinds of time-stepping schemes has been an active research area. SSP methods aim at preserving qualitative properties of the exact solution (e.g., monotonicity, contractivity, positivity, discrete maximum principles, etc.), in general, under step size restrictions. The basic assumption is the numerical preservation of these properties by the explicit Euler method.
However, for some problems, the performance of SSP and non-SSP schemes is quite similar. On the other hand, for some other problems, SSP methods preserve qualitative properties even though the explicit Euler does not preserve them.
In this talk we give an overview on SSP methods trying to clarify some issues on this topic.

The use of time series filters in numerical instability control
Adrian Hill,

The use of the standard time series filters of signal processing to control numerical instability is investigated. Two main categories of filter are considered: (i) finite impulse response (FIR or non-recursive) filters, e.g. the Gragg filter in the Gragg-Bulirsch-Stoer Method, and (ii) infinite impulse response (IIR or recursive) filters, e.g. the discrete Butterworth filter. The known properties of such filters are numerically reinterpreted as order preservation, approximate energy preservation, and the filtering out of oscillatory unstable components. The design and construction of filters is considered. Computations are presented for both stiff and energy conserving problems. Two main types of filtering strategy are considered: (a) filtering after the main computation is complete (passive filtering) and (b) intermittent filtering, with filtered solutions fed back into the main computation (active filtering).

From Low-Rank to Data-Driven Gramian-Based Model Reduction
Christian Himpe, Peter Benner, *Thu 14:30 R 3.28*

For input-output systems, system Gramian matrices are a long established tool to quantify the properties controllability and observability. A range of associated Gramian-based model reduction methods has been developed over the last decades utilizing those attributes, starting with the classic balanced truncation for linear systems. Typically, these methods are targeted towards systems with a certain structure, such as bilinear, quadratic-bilinear or polynomial, which is exploited to efficiently obtain reduced order models using low-rank truncated Gramians. Yet, some classes of systems have complex structures that (currently) cannot be reduced by such an ansatz, for example general nonlinear control-affine systems.
For nonlinear input-output systems, system Gramian matrices can also be defined based on controllability and observability, yet their numerical computation is usually infeasible. A compromise between computability and Gramian-based model reduction for nonlinear systems is a data-driven computation, that incorporates nonlinear behavior inside an attractor and reproduces algebraic results for linear systems. These so-called empirical Gramians extend Gramian-based model reduction methods to otherwise intangible input-output systems. Their computation is based on simulated trajectories for systematic perturbations of the steady-state configuration. More recently, the empirical cross Gramian was enhanced to low-rank computation; we will demonstrate low-rank computation of the empirical controllability and observability Gramians.

Adaptivity in model order reduction with proper orthogonal decomposition
Michael Hinze, Carmen Gräßle, *Thu 10:40 R 1.26*

A crucial challenge within snapshot-based POD model order reduction for time-dependent systems lies in the input dependency. In the 'offline phase', the POD basis is computed from snapshot data obtained by solving the high-fidelity model at several time instances. If a dynamical structure is not captured by the snapshots, this feature will be missing in the ROM solution. Thus, the quality of the POD approximation can only ever be as good as the input material. In this sense, the accuracy of the POD surrogate solution is restricted by how well the snapshots represent the underlying dynamical system. If one restricts the snapshot sampling process to uniform and static discretizations, this may lead to very fine resolutions and thus large-scale systems which are expensive to solve or even can not be realized numerically. Therefore, offline adaptation strategies are introduced which aim to filter out the key dynamics. On the one hand, snapshot location strategies detect suitable time instances at which the snapshots shall be generated. On the other hand, adaptivity with respect to space enables us to resolve important structures within the spatial domain. Motivated from an infinite-dimensional perspective, we explain how POD in Hilbert spaces can be implemented. The advantage of this approach is that it only requires the snapshots to lie in a common Hilbert space. This results in a great flexibility concerning the actual discretization technique, such that we even can consider r-adaptive snapshots or a blend of snapshots stemming from different discretization methods. Moreover, in the context of optimal control problems adaptive strategies are crucial in order to adjust the POD model according to the current optimization iterate. In this talk, recent results in this direction are discussed and illustrated by numerical experiments.

Multivalue–multistage methods for the numerical solution of the nonlinear Volterra integro-differential equations
Gholam Reza Hojjati, Ali Abdi, Hassan Mahdi, *Mon 16:10 R 1.27*

We are going to design a numerical scheme based on the general linear methods (GLMs) for the numerical solution of a class of Volterra integro-differential equations (VIDEs). In this scheme, we construct a special class of GLMs for ODEs and combine them with Gregory quadrature rule to approximate the integral term of the underlying VIDE. The convergence and linear stability properties are analyzed. Implementation of the constructed methods on the well-known VIDEs confirms their efficiency.
Keywords: Volterra integro-differential equations, General linear methods, Gregory quadrature rule, Convergence and stability analysis.

Positivity and SSP by implicit numerical methods for ODEs and DAEs
Zoltán Horváth, Volker Mehrmann, *Wed 10:05 R 3.28*

Theoretical settings and implementations of time stepping methods for ODEs that guarantee the positivity and/or SSP property have required the same property for the Explicit Euler method. In this talk we shall present theoretical and experimental results on cases when, instead of that for the Explicit Euler method, condition on the Implicit Euler method is applied for implicit numerical methods. Also, we shall show how the presented results apply for DAEs.

Rational finite differences method based on the barycentric interpolants for ODEs

Seyyed Ahmad Hosseini, Ali Abdi, Helmut Podhaisky, *Tue 10:40 R 1.27*

Stiff systems of ODEs arise widely in the mathematical modeling of physical and biological phenomena. In this study, we first employ the linear barycentric rational finite differences method for the numerical solution of stiff systems of ODEs which is derived by exactly differentiating the linear barycentric rational interpolant. The linear stability behavior of the proposed method with respect to the standard test problem of Dahlquist is also investigated. In addition, for obtaining the methods with more desirable stability properties in this class, the adaptive version of such methods is introduced. The efficiency and capability of the introduced methods are verified by solving some well-known stiff problems.

On Multistep Stabilizing Correction Splitting Methods with Applications to the Heston Model

Karel in 't Hout, Willem Hundsdorfer, *Thu 10:40 R 3.28*

In this talk we consider splitting methods based on linear multistep methods and stabilizing corrections. To enhance the stability of the methods, we employ an idea of Bruno & Cubillos (2016) who combine a high-order extrapolation formula for the explicit term with a formula of one order lower for the implicit terms. Several examples of the obtained multistep stabilizing correction methods are presented, and results on linear stability and convergence are derived. The methods are tested in the application to the well-known Heston model arising in financial mathematics and are found to be competitive with well-established one-step splitting methods from the literature.

Construction of Strong Stability Preserving Implicit-Explicit General Linear Methods

Giuseppe Izzo, Zdzislaw Jackiewicz, *Thu 10:40 R 1.23*

Many practical problems in science and engineering are modeled by large systems of ordinary differential equations (ODEs) which arise from space discretization of partial differential equations (PDEs). For such differential systems there are often natural splittings of the right hand sides into two parts, so they can 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, for example advection, and $g(y)$ represents stiff processes, for example diffusion or chemical reaction, in semidiscretization of advection-diffusion-reaction equations. For efficient integration of such kind of systems we consider the class of 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], we consider IMEX General Linear Methods (GLMs) to obtain methods where the explicit part has the so-called strong stability preserving (SSP) property [2, 3, 4], and the implicit part of the method is A-, or L-stable. Since the good properties of the explicit and implicit part do not ensure good performances when the two schemes interact with each other, we also analyze the absolute stability of the overall IMEX method to obtain large regions of *combined stability*. We provide examples of IMEX GLMs with order $p \leq 4$ and high stage order, $q = p$, and report the results of numerical experiments based on the solution of several large stiff problems, that confirm that the proposed methods have good performances.

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Linearly Implicit Rosenbrock-Wanner-Type Methods with Non-Exact Jacobian for the Numerical Solution of Differential-Algebraic Equations

Tim Jax, *Wed 09:40 R 1.26*

Solving differential-algebraic equations (DAEs) effectively is an ongoing topic in applied mathematics. In this context, especially regarding the computation of large networks in different fields of practical interest leads to extensive systems that must be evaluated efficiently. Due to given stiffness properties of DAEs, time-integration of such problems by linearly implicit Runge-Kutta methods in the form of Rosenbrock-Wanner (ROW) schemes is generally convenient. Compared to fully implicit schemes, they are easy to implement and avoid having to solve non-linear equations by including Jacobian information within their formulation. However, particularly when having to deal with large coupled systems, computing the exact Jacobian is costly and, therefore, proves to be a considerable drawback.

In this talk, concepts of Rosenbrock-Wanner-Type methods will be shown that allow for non-exact Jacobian entries with respect to differential and algebraic parts given when computing semi-explicit DAEs of index-1, thus enabling to apply versatile strategies that reduce computational efforts. Order conditions for realizing these methods will be presented, introducing an approach inspired by the works of Steihaug and Wolfbrandt [3] as well as Roche [2] that allows for their general derivation using an algebraic theory based on rooted trees. In this context, strategies described in [1] will be enhanced.

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Hidden Dynamics

Michael Jeffrey, *Thu 14:00 R 1.26*

In the last few years we have discovered a number of "illusions of noise" induced by the presence of discontinuities (e.g. switches, decisions, jumps in physical constants) in dynamical systems. When a system switches abruptly between two or more modes of behaviour, it can begin evolving along the discontinuity threshold between modes — so-called sliding dynamics. Such behaviour is usually highly robust, but it turns out that the tight constraint of the variables involved in sliding motion can unleash a frustration on other variables that makes them wild

and unpredictable. Their erratic variation and sensitivity to modelling assumptions creates the illusion of underlying noise when in fact none is present.
These kinds of behaviour are changing the way we understand the dynamics that occurs at the thresholds between different regimes of behaviour. Most importantly they have implications for our very notion of determinism in systems that can switch between different modes. Hidden dynamics provides a way to open up the sites of discontinuity, and explore how far we can extend determinism. There are limits to predictability of systems as they transition between regimes, and these can manifest as arbitrary pauses in motion, or spurious illusions of noise.
The most simple and striking illusion of noise is called "jitter". If two investors trading stocks in a company seem to reach a steady trading level, jitter can send the company value into unexpected erratic fluctuations. If the supply and demand of a commodity, such as oil, are regulated to a steady level, jitter can cause the commodity price to become volatile and unstable. The basic idea can be applied to mechanical, fluid flow, electronic, or other physical systems.
In this phenomenon the devil really is in the details. A sliding mode is a dynamical solution that evolves perfectly along the threshold where a discontinuity occurs in a set of differential equations. The notion of stability of a system to perturbations at a discontinuity is not a standard one in dynamical systems, so the study of real world non-ideal switching has been a long running challenge. We now understand how the tiniest non-idealities in the description of a discontinuity can manifest themselves as enormous large scale sensitivity. Depending on the application the true system might glide smoothly along the threshold (e.g. in mechanical sticking), or it might chatter along the threshold (e.g. in electronic variable structure control or thermostatic switching). There may be factors of time delay, hysteresis, or stochasticity in the switching process. Any of these can have a huge affect on variable not constrained by the sliding mode, but a combination of Filippov's inclusions, recent piecewise smooth dynamical theory, and singular perturbations, reveal that certain geometry constraints the erratic outcomes.
A single switch or discontinuity is very robust to non-idealities, which is part of the reason why sliding modes have been so successfully applied in electronic and mechanical control, but also in ecology, physiology, and a growing range of life science modelling. Two or more switches or discontinuities, however, become highly unstable to such perturbations, allowing them to vastly affect the outcome. Their effects can be understood within a range of behaviours known as "hidden dynamics" associated with switching. A coincidence of switches creates a sensitivity responsible for erratic or 'jittery' dynamics, which creates the illusion of underlying noise.

Generalized Adams methods to solve fractional differential equations with delay

Xingzhou Jiang, Jingjun Zhao, Yang Xu, *Mon 14:50 R 1.23*

In this talk, we use the fractional convolution quadrature based on generalized Adams methods to get a numerical solvers for fractional differential equations with delay. The convergence of the method is proved by the inverse of matrix. We also get the numerical stability region based on generalized Adams methods and Adams methods. The linear stability properties of generalized Adams methods when applied to linear fractional delay differential equation is studied. The numerical experiments confirm the valuable properties of this approach.

A discrete fractional approach for modelling dissipative mechanical systems

Fernando Jimenez, Sina Ober-Blöbaum, *Tue 14:00 R 3.28*

This talk is about the modelling of dissipative systems using fractional derivatives and also about some particular integrators obtained from their discretisation. We put our emphasis in obtaining numerical integrators via the discretisation of a restricted variational principle that provides the dynamical equations of dissipative mechanical systems with linear damping. We shall display their numerical behaviour and show their superior performance when approximating the dynamics and the energy decreasing of these systems.

A Numerical Algorithm for Approximation and Analysis of Burgers'-Fisher Equation

Ram Jiwari,

In this talk article, the authors proposed a numerical algorithm for approximation and analysis of Burgers'-Fisher equation $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + au\frac{\partial u}{\partial x} + bu(1-u) = 0$. Existence and uniqueness of weak solution, a priori error estimates of semi-discrete solution in $L^\infty(0,T;L^2(\Omega))$ norm are proved. Nonlinearity of the problem is handled by lagging it to previous known level. The scheme is found to be convergent. Finally, numerical experiments are performed on some examples to demonstrate the effectiveness of the scheme. The proposed scheme found to be fast, easy and accurate.

The method of (uncountably many) characteristics

David Ketcheson, Randall J. LeVeque, Jithin George, *Fri 10:10 R 3.28*

The method of characteristics is a standard technique for solving hyperbolic PDEs with constant or piecewise-constant coefficients. In the presence of more complicated spatial variation of coefficients, the method appears impractical since the number of characteristics arriving at any given point is uncountable. Problems of this kind arise naturally for wave propagation in the atmosphere and the ocean, for example. We present a numerical method for dealing with this infinity of characteristics and demonstrate an application to shoaling of ocean waves. Some interesting connections to other areas of mathematics will also be presented.

Numerical method for solving a fractional order HIV model arising from optimal control

Hossein Kheiri Estiar, Mohsen Jafari, *Mon 15:15 R 1.29*

In this paper, A fractional order HIV model with both virus-to-cell and cell-to-cell transmissions is considered. We incorporate into the model a combined antiretroviral (cARV) drug , as time dependent control, aimed at controlling the spread of HIV infection, and formulate an optimal control problem with free terminal time. Necessary conditions for a state/control/terminal time triplet to be optimal are obtained. We present a general formulation for a FOCP, in which the state and co-state equations are given in terms of the left fractional derivatives. We develop the Forward-Backward sweep method (FBSM) and the Adapted Forward-Backward Sweep method (AFBSM) using the Adams-type predictor-corrector method to solve the FOCP with fixed and free terminal time, respectively. Numerical examples show the efficiency of the proposed method.

Numerical tests with AMF methods

Marcel Klinge, Domingo Hernández-Abreu, Rüdiger Weiner*, Mon 16:35 R 3.28*

In this talk, we consider numerical methods for the solution of stiff initial value problems

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e]\,. \tag{1}$$

Implicit integration methods require the solution of linear systems, which can be very expensive for high dimensional problems (1). One possibility is to apply an Approximate Matrix Factorization (AMF) technique. The AMF approach uses some splitting of the right-hand side of (1) and exploits special structures of the corresponding Jacobians. We consider linearly-implicit one-step W-methods and two-step W-methods with AMF. Furthermore, we discuss AMF peer methods, which require the application of Newton iteration. We compare these schemes in numerical experiments on a linear model.

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Split-explicit time integration methods for finite element discretizations

Oswald Knoth, Katrin Lubashevksy*, Tue 11:30 R 1.26*

There is a new interest in finite element methods for solving the equations in numerical weather forecasting. In contrast to finite difference and finite volume methods explicit time integration methods are hampered by non-diagonal mass matrices in front of the time derivatives. We will compare different mixed finite and discontinuous Galerkin methods for the two-dimensional linear Boussinesq approximation in the context of split-explicit time integration schemes. Especially different lumping procedures are investigated which replaces non-diagonal mass matrices by simple diagonal block-diagonal matrices.

Fitted Finite Volume Method for Optimal Portfolio in a Exponential Utility Regime-Switching Model

Miglena Koleva, Tihomir Gyulov, Lubin Vulkov*, Tue 11:55 R 1.29*

The focus of the present work is a system of weakly coupled degenerate semi-linear parabolic equations of optimal portfolio in a regime-switching with exponential utility function. We extend this model, developing additional problems - IBPM and IWPM for solving indifference buyer's and writer's prices, respectively. Further, we establish comparison principle for the first model and on this base we prove a maximum principle for IBPM and IWPM. The above models are solved numerically by fitted finite volume method. We prove the discrete maximum principle and convergence of the numerical solutions in maximal norm. Numerical results, illustrating the theoretical statements are presented and discussed.

Modified Patankar-Runge-Kutta schemes for Advection-Diffusion-Production-Destruction Systems

Stefan Kopecz, Andreas Meister*, Thu 11:55 R 1.23*

Modified Patankar-Runge-Kutta (MPRK) schemes are numerical methods for the solution of positive and conservative production-destruction systems. They adapt explicit Runge-Kutta schemes in a way to ensure positivity and conservation of the numerical approximation irrespective of the chosen time step size.
In this talk we present an investigation of MPRK schemes in the context of convection-diffusion-reaction equations with source terms of production-destruction type. The time-splitting approach is used to integrate the reaction terms with MPRK schemes. In particular, the efficiency of MPRK schemes in case of stiff reactions will be discussed.

Efficient Numerical Schemes for Highly Oscillatory Klein-Gordon and Dirac type Equations

Patrick Krämer, Katharina Schratz*, Mon 17:25 R 1.29*

Klein–Gordon and Dirac equations physically describe the motion of relativistic particles. The construction of efficient numerical time integration schemes for solving these equations in the nonrelativistic limit regime, i.e. when the speed of light c formally tends to infinity, is numerically very delicate, as the solution becomes highly-oscillatory in time. In order to resolve the oscillations, standard time integrations schemes require severe restrictions on the time step $\tau \sim c^{-2}$ depending on the small parameter c^{-2} which leads to high computational costs.
In my talk, I will present numerical techniques based on [1] for efficiently solving these highly oscillatory systems without any time step restriction by exploiting their inherent time-oscillatory structure. We carry out the construction of these schemes by filtering out the highly oscillatory phases (in time) explicitly, which allows us to break down the numerical task to solving slowly oscillatory Schrödinger-type systems.

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Doubly quasi-consistent fixed-stepsize implicit two-step peer methods for stiff ordinary differential equations

Gennady Kulikov, Rüdiger Weiner*, Tue 10:40 R 1.23*

Recently, Kulikov [1] presented the idea of double quasi-consistency, which facilitates the global error estimation and control, considerably. More precisely, a local error control implemented in such methods plays a part of global error control at the same time. Unfortunately, the property of double quasi-consistency is unavailable in the classical numerical integration formulas of Runge-Kutta or multistep type, including Nordsieck methods as well. That is why Kulikov and Weiner [2, 3, 4] extended their search for doubly quasi-consistent numerical integration tools to general linear methods and constructed the first formulas of such sort within explicit parallel peer schemes.
The focus of the present research is on accurate numerical integration formulas for treating stiff ODEs, which often arise in practice and for which explicit methods are shown to be ineffective. In this talk, we make the first step towards an accurate and efficient numerical solution of stiff ODEs and prove existence of *implicit* stepping formulas. We fulfill our investigation of double quasi-consistency within the family of fixed-stepsize implicit two-step peer schemes

and construct two methods of convergence orders 3 and 4, which possess excellent stability properties. Then, these methods are equipped with an efficient local (and, hence, global) error estimation mechanism based on the embedded method approach, whose quality is assessed in numerical experiments with both nonstiff and stiff test problems with known solutions.

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Numerical solution of the neural field equation in the presence of random disturbance

Maria Kulikova, Pedro Lima, Gennady Kulikov, *Mon 16:35 R 1.26*

This paper aims at presenting an efficient and accurate numerical method for treating both deterministic- and stochastic-type *neural field equations* (NFEs) in the presence of external stimuli input (or without it) [1]. The devised numerical integration means belongs to the class of Galerkin-type spectral approximations grounded mathematically in [2, Proposition 2.1.10]. The particular effort is focused on an efficient practical implementation of the novel technique because of the partial integro-differential fashion of the NFEs, which are to be integrated, numerically. Our method is implemented in MATLAB. Its practical performance and efficiency is investigated on three variants of a particular NFE model with external stimuli inputs. We study both the deterministic case of the mentioned model and its stochastic counterpart to observe important differences in the solution behavior. First, we observe only stable one-bump solutions in the deterministic neural field scenario, which, in general, will be preserved in our stochastic NFE scenario if the level of random disturbance is sufficiently small. Second, if the area of the external stimuli is large enough and exceeds the size of the bump, considerably, the stochastic neural field solution's behavior may change dramatically and expose also two- and three-bump patterns. In addition, we show that strong random disturbances, which may occur in neural fields, fully alter the behavior of the deterministic NFE solution and allow multi-bump (and even periodic-type) solutions to appear in all variants of the stochastic NFE model studied in this paper.

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Haar wavelet quasilinearization approach for numerical solution of Burger type equation via Lie group method
Vikas Kumar, *Tue 11:55 R 3.28*

In this talk, an initial and boundary value problem for Burgers type equation is considered. With the help of Lie group approach, initial and boundary value problem for Burgers type equation reduced to an initial value problem for nonlinear ordinary differential equations. Moreover, the ordinary differential equations are solved to obtain soliton solutions. Further, Haar wavelet quasilinearization approach is applied to systems of ordinary differential equations for constructing numerical solutions of Burgers type equation. Numerical solutions are computed, and accuracy of numerical scheme is assessed by applying the scheme half mesh principal to calculate maximum errors.

IMEX-Peer Methods Based on Extrapolation
Jens Lang, Willem Hundsdorfer, *Wed 09:40 R 3.28*

In [1], we have investigated a new class of implicit–explicit (IMEX) two-step methods of Peer type for systems of ordinary differential equations with both non-stiff and stiff parts included in the source term. An extrapolation approach based on already computed stage values is applied to construct IMEX methods with favourable stability properties. For equidistant nodes, IMEX-Peer methods are equivalent to the well known IMEX-BDF methods. New optimised IMEX-Peer methods with general nodes of order $p = 2, 3, 4$, are given as result of a search algorithm carefully designed to balance the size of the stability regions and the extrapolation errors. Numerical experiments and a comparison to other implicit–explicit methods will be presented.

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SPDE simulation on spheres
Annika Lang, Peter Creasey, *Tue 15:30 R 1.26*

The simulation of solutions to stochastic partial differential equations requires besides discretization in space and time the approximation of the driving noise. This problem can be transfered to the simulation of a sequence of random fields on the underlying domain. In this talk I will concentrate on domains that are spheres and review some recent developments.

Exotic aromatic B-series for the order conditions of the long time numerical integration of ergodic stochastic differential equations.
Adrien Laurent, Gilles Vilmart, *Tue 17:30 R 1.26*

We introduce a new algebraic framework based on aromatic trees and Butcher-series for the systematic study of the accuracy of numerical integrators for sampling the invariant measure of a class of ergodic stochastic differential equations.

Effective dynamics for non-reversible stochastic differential equations

Frederic Legoll, *Tue 16:30 R 1.26*

Coarse-graining is central to reducing dimensionality in molecular dynamics, and is typically characterized by a mapping which projects the full state of the system to a smaller class of variables. While extensive literature has been devoted to coarse-graining starting from reversible systems, not much is known in the non-reversible setting. Starting with a non-reversible dynamics, we study an effective dynamics which approximates the (non-closed) projected dynamics. Under fairly weak conditions on the system, we prove error bounds on the trajectorial error between the projected and the effective dynamics. In addition to extending existing results to the non-reversible setting, our error estimates also indicate that the notion of mean force motivated by this effective dynamics is a good one.
Joint work with T. Lelièvre and U. Sharma (ENPC).

Linearly implicit time integration of semilinear wave equations with dynamic boundary conditions

Jan Leibold, Marlis Hochbruck, *Mon 16:35 R 1.29*

In this talk we present a linearly implicit time integration scheme for semilinear wave equations with a non-stiff nonlinearity. Such methods treat the (stiff) linear part of the differential equation implicitly and the nonlinear part explicitly. Thus they require only the solution of one linear system of equations in each time step. We investigate the stability of the scheme and show a second order error bound.
As an application, we consider a finite element discretization of a semilinear acoustic wave equation with dynamic boundary conditions as in [2]. Based on the analysis in [1] we derive a full discretization error bound. Afterwards we present numerical experiments which show that the linearly implicit method is competitive to standard time integration methods like the Crank-Nicolson or the leapfrog scheme.

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Volume preserving diffeomorphisms and the Kahan method

Lu Li, Elena Celledoni, *Wed 09:40 R 1.27*

Kahan's method is a special numerical integration method that works very well for certain quadratic differential equations. A modified measure and one or several modified integrals are preserved by this method for some special classes of quadratic vector fields. In this talk, we apply Kahan's method to a general vector filed F and give a general condition on its Jacobian matrix F' guaranteeing that a modified measure is preserved. Connections to the discretization of the group of volume preserving diffeomorphisms arising in certain classes of partial differential equations will be discussed.

Superconvergence of the structure-preserving trigonometric collocation methods for solving the nonlinear Hamiltonian wave equations

Changying Liu, Kai Liu, Xinyuan Wu, *Wed 10:55 R 1.27*

This work is devoted to the error estimate of the trigonometric collocation time integrators for solving the nonlinear Hamiltonian wave equations We propose the trigonometric collocation time integrators, which could take full advantage of the oscillation introduced by the spatial discretisation. The superconvergence of the trigonometric collocation time integrators is rigorously analysed. Moreover, we also prove that the trigonometric collocation time integrators could be symmetric and symplectic with suitable collocation points. Numerical experiments verify our theoretical analysis results.

Numerical simulation of rf-SQUIDs

Bernhard Maier, Marlis Hochbruck, Marvin Müller, Carsten Rockstuhl, *Mon 17:00 R 1.29*

We study the interaction of electromagnetic waves with rf-SQUIDs aligned on a thin film [1]. This yields a system of Maxwell's equations coupled with an anharmonic oscillator via a jump condition for the normal derivative at the interface. Since our main interest is the calculation of the reflection and transmission coefficients of the film, we introduce transparent boundary conditions [2], which drastically reduce the computational effort. In fact, the spatial resolution of our numerical examples does not affect the computational cost.
In this talk, we show well-posedness using [3] for a first order reformulation of this system. We further discuss the discretization with finite elements in space and the Crank-Nicolson method in time and prove convergence results. Finally, we confirm these results presenting numerical examples.

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Positive and mass-conservative integrators for biochemical systems

Angela Martiradonna, G. Colonna (CNR-IMIP, Bari, Italy), F. Diele (CNR-IAC, Bari, Italy), *Tue 15:30 R 3.28*

The state variables involved in a biochemical process are non-negative, since they model the concentration of chemical elements and compounds. In addition, biochemical systems are mass-conservative, in the sense that the total amount of any chemical element involved in the process does not change over time. The numerical schemes for the integration of this type of equations must be unconditionally positive and mass-conservative, if they are to produce meaningful results.
In this talk I will give an overview of the existing numerical schemes for biochemical systems in the recent literature [1, 4]. Then, I will propose a novel explicit scheme based on the composition of the (non-Newtonian) geometric Euler scheme in [2] with a non-standard positive integrator [3].
This work has been supported by GNCS-INDAM.

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Questions concerning differential-algebraic operators

Roswitha März, *Mon 14:00 R 3.28*

The nature of differential-algebraic operators (DA operators) is constitutive for the direct treatment of differential-algebraic equations (DAEs) in function spaces. In particular, respective characteristics of the involved DA operators are responsible for both the effectiveness and the failure of direct discretizations of DAEs. In the first part we will concentrate on linear first-order higher-index DA operators acting in most natural Hilbert spaces. We provide their basic characteristics as well as the related background for the overdetermined least-squares polynomial collocation to work well. Respective numerical experiments are clearly promising. The inverse of an injective first-order higher-index DA operator and as the case may be the inverse of a injective composed DA operator involves again a DA-operator, but now it is a higher-order one. Higher-order DA operators arise also in different application. In our second part we will address characteristics of linear higher-order DA operators

Adaptive time-space algorithms for the simulation of multi-scale reaction waves with error control

Marc Massot, *Fri 12:10 R 3.28*

Numerical simulations of multi-scale phenomena are commonly used for modeling purposes in many applications such as combustion, chemical vapor deposition, or air pollution modeling. These models raise several difficulties created by the high number of unknowns, the wide range of temporal scales due to detailed chemical kinetic mechanisms, as well as steep spatial gradients associated with very localized fronts of high chemical activity. Furthermore, a natural stumbling block to perform 3D simulations with all scales resolution is either the unreasonably small time step due to stability requirements or the unreasonable memory requirements for implicit methods. In this work, we introduce a new resolution strategy for multi-scale reaction waves based mainly on time operator splitting and space adaptive multiresolution. It considers high order time integration methods for reaction, diffusion and convection problems, in order to build a time operator splitting scheme that exploits efficiently the special features of each problem. Based on theoretical studies of numerical analysis, such a strategy leads to a splitting time step which is not restricted neither by fast scales in the source term nor by restrictive stability limits of diffusive or convective steps, but only by the physics of the phenomenon. Moreover, this splitting time step is dynamically adapted taking into account a posteriori error estimates, carefully computed by a second embedded and economic splitting method. The main goal is then to perform computationally very efficient as well as accurate in time and space simulations of the complete dynamics of multi-scale phenomena under study, considering large simulation domains with conventional computing resources and splitting time steps purely dictated by the physics of the phenomenon and not by any stability constraints associated with mesh size or source time scales. Applications will be presented in the fields of combustion waves and plasma discharges dynamics. We will also briefly address the question of parallelism as well as the coupling with a hydrodynamics solver.

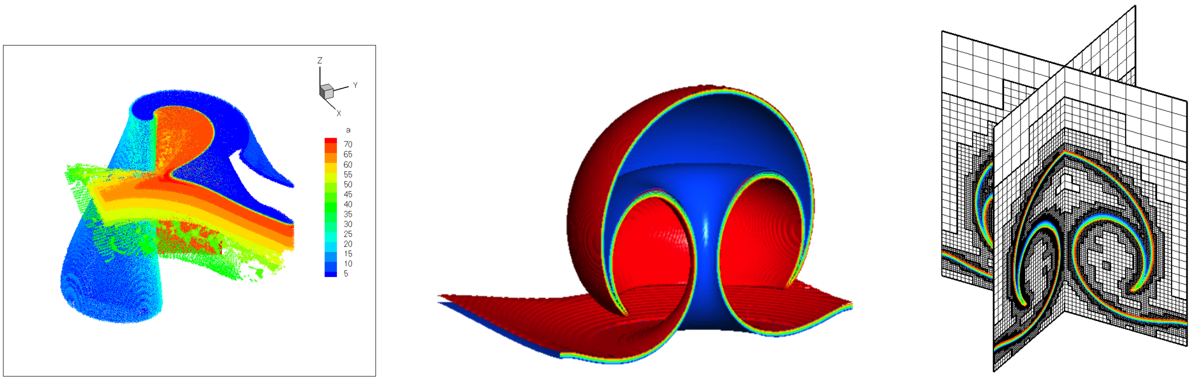

Figure 1: Left: Simulation of scroll waves using Belousov-Zhabotinsky model with detailed mechanism in 3D, Right: Simulation of the interaction of a premixed flame front with a toroidal vortex in 3D and mesh adaptation (Ph.D. M. Duarte).

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Regularization and numerical solution of hybrid differential-algebraic equations

Volker Mehrmann, Peter Kunkel, *Thu 15:00 R 1.26*

The solvability and regularity of hybrid differential-algebraic systems (DAEs) is studied, and classical stability estimates are extended to hybrid DAE systems. Different reasons for non-regularity are discussed and appropriate regularization techniques are presented. This includes a generalization of Filippov regularization in the case of so-called chattering. The results are illustrated by several numerical examples

Goal oriented time adaptivity using local error estimates

Peter Meisrimel, Philipp Birken, *Tue 11:05 R 1.23*

When solving ODEs or PDEs, one is not always interested in the solution, but rather a quantity of interest (QoI) derived from it. Starting from an IVP (semidiscretized PDE) with solution $\mathbf{u}(t)$, we consider QoIs of the form

$$J(\mathbf{u}) = \int_0^T j(t, \mathbf{u}(t))\, dt$$

with $j : [0, T] \times \mathbb{R}^n \to \mathbb{R}$. Examples for this are the average energy production of a turbine or the drag coefficient for a vehicle.
The standard approach for controlling the error in the QoI is the dual-weighted residual method [1]. To obtain an estimate the error in the QoI, this method requires solving the given ODE (PDE) forward in time and its adjoint problem backwards in time, multiple times each, to reach a desired precision.
An alternative approach is to use time-adaptive schemes based on local error estimates [2], which require only one forward solve, but give no estimate of $J(\mathbf{u})$.
We propose a new, goal oriented and adaptive method [3] based on local error estimates. Taking the local error approach, we determine timesteps using only the quantities that are relevant for $J(\mathbf{u})$. Our error estimate consists of local error estimates in $j(t, \mathbf{u})$ and estimates of a quadrature approximation $J_h \approx J$. This gives us a new easy to implement timestep controller. In the talk, we will present results on convergence, order of convergence and necessary requirements for these. We outline a performance analysis of the new method. In numerical test, we verify our results, show strengths and weaknesses of the method and compare it to the dual-weighted residual method and classical time-adaptivity based on local error estimates.

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Modified Patankar-Runge-Kutta Schemes for Conservative Production-Destruction Equations

Andreas Meister, Stefan Kopecz*, Thu 09:20 R 3.28*

Modified Patankar-Runge-Kutta (MPRK) schemes are numerical methods for the solution of positive and conservative production-destruction systems. They adapt explicit Runge-Kutta schemes in a way to ensure positivity and conservation irrespective of the time step size. With the talk we introduce a general definition of MPRK schemes and present a thorough investigation of necessary as well as sufficient conditions to derive first, second and third order accurate MPRK schemes. The theoretical results will be confirmed by numerical experiments in which MPRK schemes are applied to solve non-stiff and stiff systems of ordinary differential equations.

BDF and Newmark-Type Index-2 and Index-1 Integration Schemes for Constrained Mechanical Systems

Tobias Meyer, Pu Li, Bernhard Schweizer*, Wed 10:55 R 1.26*

Various methods for solving DAE systems, e.g. constrained mechanical systems, are known from literature. Here, an alternative approach is presented using intermediate time points. The idea of the method is inspired by a co-simulation technique recently published in [1]. The approach is very general and can basically be applied for arbitrary DAE systems (mechanical or non-mechanical DAE systems with higher-index). In this talk, implementations of this approach are presented for BDF and Newmark-type integrator schemes. We discuss index-2 formulations with one intermediate time point and index-1 implementations based on two intermediate time points. A direct application of the approach for BDF or Newmark-type integrators yields a system of discretized equations with larger dimensions. Roughly speaking, the system increases by factor 2 for the index-2 and by factor 3 in case of the index-1 formulation. It is possible to reduce the size of the discretized DAE system by using simple interpolation techniques. Examples are presented, which demonstrate the straightforward application of the approach.

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Adaptive β-blocked multistep methods for index 2 Euler-Lagrange differential algebraic equations

Fatemeh Mohammadi, Carmen Arévalo, Claus Führer, *Mon 15:15 R 3.28*

It is common to use BDF methods to solve index 2 DAE systems numerically even for non-stiff state space form of a problem. Because the solution with non-stiff integrators such as Adams-Moulton discretizations, is unstable. A technique designed to overcome this instability is β-blocking [1, 4, 2]. This stabilizing technique was developed for fixed step-size multistep methods.

In this talk we present a polynomial formulation of $\beta-$blocked multistep methods [3] that allows the use of variable step-sizes by construction. We formulate adaptive singular and regular $\beta-$blocked multistep methods and demonstrate their performance by some numerical examples.

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Weak convergence for a stochastic exponential integrator and finite element discretization of stochastic partial differential equation with additive noise

Jean Medard Ngnotchouye, Antoine Tambue, *Mon 17:00 R 1.26*

We consider a finite element approximation of a general semi-linear stochastic partial differential equation driven by space-time additive noise. We examine the full weak convergence rate for non-self-adjoint linear operator with additive noise. Key part of the proof does not rely on Malliavin calculus. For non-self-adjoint operators, we analyse the optimal strong error for spatially semi discrete approximations for additive noise with truncated and non-truncated noise. Depending on the regularity of the noise and the initial solution, we found that in some cases the rate of weak convergence is twice the rate of the strong convergence. We present some numerical results in two dimensions to support our convergence rate result.

Adaptive time-stepping in Lie group integrators

Brynjulf Owren, Charles Curry, *Thu 10:40 R 1.27*

We introduce variable stepsize commutator free Lie group integrators, where the error control is achieved using embedded Runge-Kutta pairs. For orders 3 and 4, we are able to obtain such pairs with the minimal number of flow calculations (exponentials). The methods make use of reusal of exponentials from previous stages. We present some numerical examples where we apply the schemes to some well-known problems in mechanics as well as the stiff van der Pol oscillator.

Haar Wavelets based Algorithms for Simulation of Hyperbolic Type Wave Equations

Sapna Pandit, R C Mittal*, Tue 11:55 R 1.27*

In this article, the authors developed two algorithms based on Haar wavelets operational matrix for simulation of nonlinear hyperbolic type wave equations. These types of equations describe a variety of physical model in the nonlinear optics, relativistic quantum mechanics, solitons and condensed matter physics, interaction of solitons in collisionless plasma and solid state physics etc. The algorithms reduced the equations into a system of algebraic equations and then the system is solved by Gauss-elimination procedure. Some well-known hyperbolic type wave problems are considered as numerical problems to check the accuracy and efficiency of the proposed algorithm. The numerical results are shown in figures and RMS, L2 errors form.

Orbital convergence of timestepping schemes for non-smooth mechanics

Manuela Paschkowski, Martin Arnold*, Thu 11:30 R 1.26*

When simulating mechanical systems with impacts, velocity jumps occur. Timestepping schemes are well-known possibilities to integrate such dynamical systems. Their advantage is the avoided event detection such that a large number of changes of the active set – especially accumulation points of velocity jumps – can be handled with higher computational efficiency, in particular when single events are less important than the mean. These schemes are always of integration order one with respect to discrete L^p-norms. This is a consequence of the identification of impact points only with order one independently of the approximation order in the smooth phases. In this talk, the idea of orbital convergence of timestepping schemes is presented, which is a more reasonable tool to compare the approximation accuracy of different timestepping methods [1, 2, 3]. Using the framework of measure differential inclusions, the orbital convergence order of these schemes is studied for scalar problems. An experimental convergence analysis with the bouncing ball and the impact oscillator examples will underline the benefits of this approach.

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Adapted discretization of evolutionary problems by non-polynomially fitted numerical methods

Beatrice Paternoster*, Mon 17:00 R 1.27*

The talk is devoted to the discretization of selected evolutionary problems generating periodic wavefronts [5] and aims to explain the benefits gained by adapting the numerical scheme to the problem. Such an adaptation is carried out by merging the a-priori known qualitative information on the problem, as well as the structure of the vector field itself, into the numerical scheme.

Particular emphasis will be given to advection-reaction-diffusion problems, for which the adaptation in space is developed by means of a finite difference scheme based on trigonometrical basis functions [3], rather than on algebraic polynomials which could strongly reduce the stepsize in order to accurately reproduce the prescribed oscillations of the exact solution. The adaptation in time takes into account that the spatially discretized problem is characterized by a vector field consisting in stiff and nonstiff terms, hence it makes sense to adopt an implicit-explicit (IMEX) time integration, which implicitly integrate only the stiff constituents, while the nonstiff part is computed explicitly. Clearly, the employ of non-polynomial basis functions makes the coefficients of the numerical method dependent on unknown parameters (i.e. the frequency of the oscillations), which need to be properly estimated [4]; the proposed estimation relies on a minimization procedure of the local truncation error that is carried out a-priori, without affecting the computational cost of the integration. A rigorous analysis on the stability and accuracy properties of the overall method is presented, together with some numerical tests, in order to highlight the effectiveness of the approach. The introduced technique also covers the case of periodic dynamics generated by evolutionary problems with memory [1, 2], discretized in terms of non-polynomially fitted quadrature methods able to accurately reproduce the oscillatory behavior with a reduced computational cost with respect to their analogous polynomial version, when a good estimate of the unknown frequency is provided. Stability issues for such a discretization are also addressed.

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Data driven feedback control of nonlinear PDEs using the Koopman operator

Sebastian Peitz, Stefan Klus*, Thu 15:30 R 3.28*

In this talk we present a data driven reduced order modeling approach for control of nonlinear PDEs which relies on the Koopman operator. We construct a bilinear surrogate model via linear interpolation between two Koopman operators corresponding to constant controls. Using a recent convergence result for Extended Dynamic Mode Decomposition, convergence of the reduced order model based control problem towards the true optimum can be guaranteed if the control system depends linearly on the input. The resulting feedback controller is used to control the Burgers equation as well as the flow around a cylinder governed by the Navier-Stokes equations.

Parametric dependence of the advection-diffusion equation in two dimensions
Matheus Fernando Pereira, Varese Salvador Timóteo*, Mon 17:25 R 3.28*

In this work we have solved the two-dimensional advection-diffusion equation numerically for a spatially dependent solute dispersion along non-uniform flow with a pulse type source in order to make a systematic study on the influence of medium heterogeneity, initial flow velocity and initial dispersion coefficient parameters on the solutions of the equation. The behavior of the solutions is then investigated as we change the three parameters independently. Our results show that even though the parameters represent different physical features of the system, the effect on their variation is very similar. We also observe that the effects caused by the parameters on the concentration depend on the distance from the source. Finally, our numerical results are in good agreement with the exact solutions for all values of the parameters we used in our analysis.

Polynomial chaos expansion for solving stochastic control problems
Lena-Maria Pfurtscheller, Tijana Levajkovic, Hermann Mena*, Mon 14:00 R 1.29*

We consider the infinite dimensional stochastic linear quadratic optimal control problem and provide a numerical framework for solving this problem using a polynomial chaos expansion approach. The resulting system consists of a set of deterministic partial differential equations in terms of the coefficients of the state and the control variables. For each equation, we then set up an optimal control problem. We solve the arising problems by deterministic numerical methods and thus obtain an approximation of the stochastic problem. We show some numerical examples and compare our approach to the standard one. Moreover, we discuss the difference between the finite and infinite horizon case.

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A low-rank splitting integrator for matrix differential equations
Chiara Piazzola*, Mon 14:25 R 1.29*

In this talk we present a numerical integrator for determining low-rank approximations to solutions of large-scale matrix differential equations. In particular, we consider semilinear stiff problems and propose a low-rank integrator based on splitting methods to separate the stiff linear part of the equation from the non-stiff nonlinear one. Then the solutions of the subproblems are approximated by low-rank ones. The strength of the proposed approach is that the time integration is performed only on the low-rank factors of the solution. We provide a convergence analysis and discuss some numerical results.
This is joint work with H. Mena, A. Ostermann, L.-M. Pfurtscheller and H. Walach.

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Model order reduction for linear dynamical systems with quadratic outputs

Roland Pulch, Akil Narayan, *Thu 11:05 R 1.26*

We consider initial value problems for linear time-invariant systems consisting of ordinary differential equations

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \qquad x(t_0) = x_0 \\ y(t) &= x(t)^\top M x(t) \end{aligned}$$

with state variables x and inputs u. The quadratic output y represents a quantity of interest defined by a symmetric matrix M of rank k. We investigate model order reduction (MOR) for systems of high dimension. The system can be transformed into a linear dynamical system with k linear outputs, see [1]. However, many MOR methods for linear dynamical systems become inefficient or even infeasible in the case of large numbers k. Alternatively, we transform the system into a quadratic-bilinear (QB) form with a single linear output. The properties of this QB system are analyzed. We apply the MOR technique of balanced truncation from [2] to the QB system, where a stabilization is required. The solution of quadratic Lyapunov equations is traced back to the solution of linear Lyapunov equations. We present numerical results for a relevant example including a high rank k, where the two MOR approaches are compared.

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A splitting approach for the KdV equation with transparent boundary conditions

Mirko Residori, *Mon 17:00 R 3.28*

In this talk we propose a numerical approach for the linearized 1-D Korteweg–de Vries (KdV) equation with space dependent coeffcients

$$u_t + a(x)u_x + b(x)u_{xxx} = 0,$$

where the spatial domain is unbounded ($x \in \mathbb{R}$). We cut off a finite computational domain from the unbounded one and we employ transparent boundary conditions. We follow a splitting strategy in order to divide the full equation into its dispersive part $u_t + b(x)u_{xxx} = 0$ and its transport part $u_t + a(x)u_x = 0$. The transparent boundary conditions are then derived in a full discrete setting using the Crank–Nicolson and the explicit Euler finite different schemes for the dispersive and the transport equation respectively. Numerical simulations are presented that illustrate the theoretical results.
This is a joint work with Einkemmer Lukas and Alexander Ostermann.

Parameter Identification for Delay Differential Equations
Fathalla Rihan, *Tue 11:30 R 3.28*

In this talk, we present the theoretical framework to solve inverse problems for Delay Differential Equations (DDEs). Given a parameterized DDE and experimental data, we estimate the parameters appearing in the model, using least squares approach. Some issues associated with the inverse problem, such as nonlinearity and discontinuities which make the problem more ill-posed, are studied. Sensitivity and robustness of the models to small perturbations in the parameters, using variational approach, are also investigated. The sensitivity functions may provide guidance for the modelers to determine the most informative data for a specific parameter, and select the best fit model. The consistency of delay differential equations with bacterial cell growth is shown by fitting the models to real observations.
keywords: DDEs - Nonlinearity - Parameter estimation - Sensitivity analysis - Time-lags

New low-storage SSP Runge-Kutta methods
Teo Roldan, Inmaculada Higueras, *Wed 10:05 R 1.23*

Low-storage implementations are highly recommended for the numerical resolution of differential problems where memory management considerations are as important as accuracy and stability considerations. These differential problems usually are obtained after a spatial discretization of some partial differential equations.
For Runge-Kutta schemes, most of the classic low-storage methods are based on the ideas of Williamson and van der Houwen. However, some other approaches, based on Shu-Osher representations of Runge-Kutta methods, have also been considered in the literature. In some cases, optimal Strong Stability Preserving (SSP) methods have sparse Shu Osher matrices and this sparse structure can be exploited to reduce the number of registers required for its implementation.
In this talk we show new low-storage SSP Runge-Kutta methods that can be implemented in two memory registers. Although their SSP coefficients are not optimal, they have some other additional relevant properties. Some numerical experiments show the efficiency of these new schemes.

Combining a stroboscopic method with the spectral deferred correction method
Juliane Rosemeier, *Tue 11:30 R 1.23*

In natural sciences, problems with periodic forcings are studied often; for instance for an idealized ice cloud model the impact of gravity waves can be represented by such a forcing. Therefore, we implemented a new method for stroboscopic problems. For a first test, we chose the inverted Kapitsa pendulum equation which is an appropriate test problem for this kind of methods. Our numerical scheme is a combination of two existing methods. We used a stroboscopic method proposed by Calvo et al. (2011) and the method of spectral deferred correction. The first above-mentioned method consists of a micro-solver and a macro-solver. The method of spectral deferred correction is an iterative scheme and used as a macro-solver for the first method. The iterations of the spectral deferred correction method are used to increase the accuracy of the macro-solver.

Linearly Stabilized Schemes for the Time Integration of Stiff Nonlinear PDEs

Steven Ruuth, Kevin Chow*, Wed 08:40 R 3.28*

In many applications, the governing PDE to be solved numerically contains a stiff component. When this component is linear, an implicit time stepping method that is unencumbered by stability restrictions is preferred. On the other hand, if the stiff component is nonlinear, the complexity and cost per step of using an implicit method is heightened, and explicit methods may be preferred for their simplicity and ease of implementation. In this talk, we consider new and existing linearly stabilized schemes for the purpose of integrating stiff nonlinear PDEs in time. These schemes compute the nonlinear term explicitly and, at the cost of solving a linear system with a matrix that is fixed throughout, are unconditionally stable, thus combining the advantages of explicit and implicit methods. Applications are presented to illustrate the use of these methods.

Runge-Kutta methods for index-2 and index-3 differential-algebraic equations arising from incompressible flow problems

Benjamin Sanderse, Arthur Veldman*, Thu 11:05 R 3.28*

Many computational physics problems can be modelled by partial differential equations (PDEs) with constraints. In particular, we are interested in single-phase and multi-phase incompressible fluid flow problems, in which the constraint is that the velocity field is divergence-free. After discretizing the PDEs in space, a differential-algebraic equation (DAE) system is obtained. In previous work we have analyzed the accuracy of explicit Runge-Kutta methods for the single-phase incompressible Navier-Stokes equations, which form an index-2 DAE. In the current work we consider the extension to multi-phase incompressible flow problems in pipelines and channels, where a different constraint leads to a DAE with index 3. Existing time integration methods for this system lack either conservation, accuracy, or constraint-consistency.
We propose a third order half-explicit Runge-Kutta method (Hairer et al., 1989) that is consistent with the constraints of the index-3 DAE system, and with coefficients chosen such that order reduction due to the DAE nature of the equations is prevented. The method is explicit for the mass and momentum equations and implicit for the pressure. The resulting method is (i) constraint-consistent: exact conservation of the volume constraint and the incompressibility constraint; (ii) accurate: high order temporal accuracy for differential and algebraic variables; (iii) conservative: the original mass and momentum equations are solved, so that the proper shock conditions are satisfied; (iv) efficient: the only implicit part is the pressure Poisson equation, and the time step for the explicit part is restricted by a benign CFL condition based on the convective wave speeds.
Several testcases show the effectiveness of the time-integration methods: Kelvin-Helmholtz instabilities in a pipeline, liquid sloshing in a tank, and ramp-up of gas production in a multiphase pipeline.

MRI-GARK: A Class of Multirate Infinitesimal GARK Methods

Adrian Sandu*, Mon 16:10 R 1.23*

Differential equations arising in many practical applications are characterized by multiple time scales. Multirate time integration seeks to solve efficiently multiscale systems by discretizing each component with a different, appropriate time step, while ensuring the overall accuracy and stability of the numerical solution. Multirate methods of linear multistep and Runge-Kutta type have been proposed in the literature. In a seminal paper Wensch, Knoth, and Galant (BIT Numerical Mathematics 49, 2009) developed multirate infinitesimal step (MIS) methods

that discretize the slow component with an explicit Runge-Kutta method, and advance the fast component via a modified fast ODE system. Günther and Sandu (Numerische Mathematik 133, 2016) explained MIS schemes as a particular case of multirate general-structure Runge-Kutta (GARK) methods.
This work constructs a family of multirate infinitesimal GARK schemes (MRI-GARK) that extends the hybrid dynamics idea of the MIS approach. The order conditions theory and stability analyses are developed. Particular methods of order up to four are derived. Numerical results are presented confirm the theoretical findings. We expect the new MRI-GARK family to be useful for differential equations with widely disparate time scales, where the influence of the fast component on the slow one is weak.

Multilevel Uncertainty Quantification with Sample-Adaptive Model Hierarchies

Robert Scheichl, *Tue 09:20 R 3.28*

Sample-based multilevel uncertainty quantification tools, such as multilevel Monte Carlo, multilevel quasi-Monte Carlo or multilevel stochastic collocation, have recently gained huge popularity due to their potential to efficiently compute robust estimates of quantities of interest (QoI) derived from PDE models that are subject to uncertainties in the input data (coefficients, boundary conditions, geometry, etc). Especially for problems with low regularity, they are asymptotically optimal in that they can provide statistics about such QoIs at (asymptotically) the same cost as it takes to compute one sample to the target accuracy. However, when the data uncertainty is localised at random locations, such as for manufacturing defects in composite materials, the cost per sample can be reduced significantly by adapting the spatial discretisation individually for each sample. Moreover, the adaptive process typically produces coarser approximations that can be used directly for the multilevel uncertainty quantification. In this talk, we present two novel developments that aim to exploit these ideas. In the first part we will present Continuous Level Monte Carlo (CLMC), a generalisation of multilevel Monte Carlo (MLMC) to a continuous framework where the level parameter is a continuous variable. This provides a natural framework to use sample-wise adaptive refinement strategies, with a goal-oriented error estimator as our new level parameter. We introduce a practical CLMC estimator (and algorithm) and prove a complexity theorem showing the same rate of complexity as MLMC. Also, we show that it is possible to make the CLMC estimator unbiased with respect to the true quantity of interest. Finally, we provide two numerical experiments which test the CLMC framework alongside a sample-wise adaptive refinement strategy, showing clear gains over a standard MLMC approach with uniform grid hierarchies. In the second part, we extend the sample-adaptive strategy to multilevel stochastic collocation (MLSC) methods providing a complexity estimate and numerical experiments for a MLSC method that is fully adaptive in the dimension, in the polynomial degrees and in the spatial discretisation.
This is joint work with Gianluca Detommaso (Bath), Tim Dodwell (Exeter) and Jens Lang (Darmstadt).

Superconvergent IMEX Peer methods with A-stable implicit part

Moritz Schneider, Jens Lang, Willem Hundsdorfer, Rüdiger Weiner, *Thu 11:30 R 1.23*

The spatial discretization of certain time-dependent partial differential equations (e.g. advection-diffusion-reaction systems) yields large systems of ODEs where the right-hand side can be split into a stiff and a non-stiff part. We are interested in the construction of time integrators that combine the favorable stability properties of implicit methods and the low computational cost of explicit schemes. In order to guarantee consistency and thus convergence, the implicit and explicit integrator must fit together. A natural way to construct these so called implicit-explicit (IMEX) methods is to start with an appropriate implicit scheme and extrapolate it in a suitable manner. Promising candidates are implicit Peer methods as shown by Lang and Hundsdorfer [1].

In this talk, we discuss the construction of superconvergent methods with A-stable implicit part [2]. To this end, we begin with the derivation of conditions for constant step size sequences and, later, extend this notion to the setting of variable step sizes.

We start by recalling basic properties of s-stage IMEX Peer methods, such as consistency and stability, which are analyzed in detail in [1]. The main part of the talk is devoted to the concept of superconvergence, i.e. convergence of order $s+1$, and its application to IMEX Peer methods. After a short introduction to the subject, we derive necessary and sufficient conditions on the coefficient matrices that guarantee superconvergence of the full scheme for constant step sizes. Further, we present a construction procedure for superconvergent implicit Peer methods and the subsequent extrapolation. In the second part, we discuss how the previously derived consistency conditions have to be modified such that the resulting method is superconvergent for variable step size sequences as well. In addition, we comment on the stability of these new schemes. Finally, we illustrate the advantage of the new superconvergent schemes in numerical examples and compare them with established methods, including those recently developed by Soleimani, Knoth and Weiner in [3, 4].

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Variational models and partial differential equations for mathematical imaging

Carola-Bibiane Schönlieb, *Mon 09:20 R 3.28*

Images are a rich source of beautiful mathematical formalism and analysis. Associated mathematical problems arise in functional and non-smooth analysis, the theory and numerical analysis of partial differential equations, harmonic, stochastic and statistical analysis, and optimisation. Starting with a discussion on the intrinsic structure of images and their mathematical representation, in this talk we will learn about variational models for image analysis and their connection to partial differential equations, and go all the way to the challenges of their mathematical analysis as well as the hurdles for solving these - typically non-smooth - models computationally. The talk is furnished with applications of the introduced models to image de-noising, motion estimation and segmentation, as well as their use in biomedical image reconstruction such as it appears in magnetic resonance imaging.

Numerical simulation to capture the pattern formation

Sukhveer Singh, *Tue 11:55 R 1.23*

This work deals to capture the different types of patterns of nonlinear time dependent coupled reaction diffusion models. To accomplish this work, a new differential quadrature (DQ) algorithm is developed with the help of modified trigonometric cubic B-spline functions. The stability part of the developed algorithm is studied by matrix stability analysis method. In the experimental part, different types of patterns of Gray–Scott, Schnakenberg, Isothermal Chemical and Brusselator Models are captured which are similar to the existing patterns of the models.

Numerical valuation of Bermudan basket options via partial differential equations

Jacob Snoeijer, Karel in 't Hout, *Mon 16:10 R 1.26*

This talk deals with numerical methods to approximate the fair values of European and Bermudan basket options, which constitute common products in the financial markets. If there are $d \geq 2$ assets in the basket, then the fair value of such a financial option satisfies a time-dependent d-dimensional partial differential equation. For its efficient numerical solution, we discuss in this talk a useful dimension reduction technique and numerically investigate its convergence behaviour by ample experiments.

Modelling and numerical simulation of hydrogen flow in networks

Gerd Steinebach, *Mon 14:00 R 1.27*

In this talk fluid flow problems in networks are considered. The focus is on the simulation of metal hydride storage systems integrated into a hydrogen network for energy supply. First, the general modelling approach for flow simulation in networks is introduced. Suitable semi-discretization in space by WENO methods leads to large DAE systems. Simple problems are used as examples to discuss some numerical difficulties.
The simulation of large networks requires robust and efficient integrators for DAEs. Nunmerical investigations with different methods are presented.

On Singly Implicit Runge-Kutta Methods of High Stage Order that Utilize Effective Order

Tim Steinhoff, *Wed 09:40 R 1.23*

The abscissae c_i of a classical singly implicit Runge–Kutta method (SIRK) of order p, that also has a stage order of p, are tightly bound to the roots of the p-degree Laguerre polynomial. Utilizing the concept of effective order lifts this restriction allowing for arbitrary choices of c_i in principal. To provide further flexibility in terms of error constants and stability we discuss in this talk a combination of the effective order concept with SIRK methods, that are based on perturbed collocation. Furthermore, the concept of finite iteration is taken into account to ensure that a predefined number of Newton iteration steps suffices to meet the (effective) order of the corresponding fully implicit SIRK method.

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

Tony Stillfjord, *Mon 14:50 R 1.29*

It is frequently observed in practice that the singular values of the solutions to differential Lyapunov equations or differential Riccati equations 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 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.

Piecewise smooth dynamic simulations via algorithmic piecewise differentation

Tom Streubel, Andreas Griewank, Caren Tischendorf, *Thu 17:00 R 1.26*

Given some piecewise differentiable ODE, the order of consistency of any Runge-Kutta method or any multistep method will drop to 2 while crossing a non differentiability. We will discuss changes during the derivation of the midpoint rule and the trapezoidal method such that they attain their consistency order of 3 again. These modified versions of both integrators are considered to be nonsmooth generalizations in that they are still equivalent to their classical counterparts on sufficiently smooth systems of ODEs. We will discuss energy preservation and symplectic properties of both the classical and generalized midpoint rule for piecewise smooth Hamiltonian systems. We will conclude the talk with an outlook to semi explicit DAEs and the generalization of multistep methods based on piecewise polynomial Taylor expansions.

Collective integration of Hamilton PDEs

Benjamin Tapley, Christian Offen, Robert McLachlan, Elena Celledoni, Brynjulf Owren, *Thu 11:55 R 1.27*

Many PDEs (e.g., Burgers', KdV and Camassa-Holm) can be written in the Hamiltonian formulation on a Poisson manifold; however, no general-purpose Poisson integrators are available for such systems. In [1] Poisson integrators are found for ODEs by first finding a symplectic realisation of the Poisson manifold then applying a symplectic integrator to the collective system. In this presentation we extend the work done in [1] by considering the action of the diffeomorphism group on the circle $\mathrm{Diff}(S^1)$. The realisation is obtained as the momentum map of the cotangent lift of the group action of $\mathrm{Diff}(S^1)$ on $C^\infty(S^1)$. In our examples we consider Burgers' and other Hamiltonian PDEs and show that by implementing symplectic integrators on a collective system, we obtain more long-term stable solutions and better preservation of the Casimir and Hamiltonian when compared to integrating the system on $\mathrm{diff}^*(S^1)$.

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Willem Hundsdorfer's role and research in the Multiscale Dynamics group at CWI

Jannis Teunissen, *Wed 10:30 R 3.28*

This talk gives a brief overview of Willem Hundsdorfer's role and research in the Multiscale Dynamics group at CWI (Centrum Wiskunde & Informatica), Amsterdam. Having joined CWI in 1984, he was part of the Multiscale Dynamics group since 2002. Teamed up with Ute Ebert, Willem brought in the numerical expertise to develop numerical models of electric discharges. An important contribution was for example the use of adaptive mesh refinement for solving advection-diffusion-reaction as well as elliptic equations. With his students, Willem also worked on multirate time-stepping techniques for stiff ODEs and PDEs and on monotonicity preserving schemes.

Convergence of regularised solutions of piecewise smooth differential equations

Daniel Paul Tietz, Martin Arnold, *Thu 11:55 R 1.26*

We study piecewise smooth differential equations in which the discontinuity of the vector field occurs on two smooth surfaces of the phase space and may result in codimension-2 sliding.
First we will regularise the associated differential inclusion with a small regularisation parameter ϵ. Based on the ideas presented in [1] and [2], especially some asymptotic expansion techniques, we will then discuss the linear convergence of the regularised solutions in ϵ for the most common cases.
Finally we will analyse some problems given from electrical engineering and validate the theoretical result.

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Sampling strategies and diffusion maps

Zofia Trstanova, Ben Leimkuhler, *Tue 17:00 R 1.26*

The main challenge for sampling Boltzmann-Gibbs distributions comes from the high dimensionality of the system and complicated (metastable) energies. In this talk, I will focus on Langevin dynamics, and diffusion maps. Diffusion maps are a dimension reduction technique that can provide an approximation of the generator of Langevin dynamics. This approximation can serve as an automatic tool for exploration of the local geometry of the underlying manifold. I will explain how this strategy can accelerate sampling and highlight these ideas by numerical simulations.

Model order reduction for space-adaptive simulations of unsteady incompressible flows

Sebastian Ullmann, Carmen Gräßle, Michael Hinze, Jens Lang, *Thu 17:30 R 3.28*

We consider model order reduction for unsteady incompressible Navier-Stokes problems. A reduction of computational complexity is achieved by a Galerkin projection of the solution of a high-dimensional reference problem onto a low-dimensional subspace. We focus on subspaces generated by a proper orthogonal decomposition (POD) of space-adapted finite element snapshots. In previous works, we have investigated adaptive POD-Galerkin modeling for elliptic and parabolic problems [1, 2]. Incompressible flows pose additional challenges regarding the stability of the resulting reduced-order models and regarding the implementation of inhomogeneous initial and boundary condition.

We propose two approaches to computing reduced spaces which result in stable POD-Galerkin models. The first approach employs a projection of the adapted velocity snapshots onto a space of functions which are weakly divergence-free with respect to a pressure reference space. The resulting reduced-order model is a system of ordinary differential equations for the velocity POD coefficients. The second approach is based on separate PODs of the adapted velocity and pressure snapshots. Here, the velocity POD basis is enriched by supremizer functions computed on a reference velocity space. The stability of the velocity-pressure pair of reduced spaces is linked to the inf-sup constant of the reference discretization.

We analyze the complexity of the proposed reduced-order models, present numerical results for a benchmark problem, and compare our methods in terms of accuracy per computational cost.

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[2] S. Ullmann, M. Rotkvic and J. Lang, POD-Galerkin reduced-order modeling with adaptive finite element snapshots, *J. Comput. Phys.* (2016), 325:244–258, doi: 10.1016/j.jcp.2016.08.018.

Efficiency of micro-macro acceleration for scale-separated stochastic differential equations

Hannes Vandecasteele, Przemyslaw Zielinski, Giovanni Samaey, *Thu 11:30 R 3.28*

Many stochastic systems in nature have an inherent time-scale separation, while 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 model is a stiff stochastic differential equation.

The proposed algorithm interleaves short bursts of stochastic microscopic simulation with extrapolation of the macroscopic states over a larger time interval. .Since the extrapolation step is larger than the 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.

For slow-fast SDEs, it is often also possible to derive an approximate macroscopic model for the non-stiff variable in the limit of infinite time-scale separation. This approximate model however induces a modelling error when the separation is finite. Our results show that the micro-macro acceleration method can attain a lower error than the approximate macroscopic model, while increasing efficiency with respect to the microscopic simulation.

Time Dependent Stability: Computation and Applications

Erik Van Vleck, *Fri 08:30 R 3.28*

Time dependent stability spectra such as Lyapunov exponents and Sacker-Sell spectrum provide stability information for time dependent solutions of differential equations. These stability spectra fill roles that real parts of eigenvalues play for time independent solutions. In this talk we review time dependent stability spectra and their properties, numerical techniques for extracting stability spectra and their approximation properties, and then turn our attention to applications of such stability spectra. Particular attention will be paid to time dependent stability of numerical time stepping techniques and stiffness detection and to applications to data assimilation via decomposition of the tangent space of nonlinear time evolving models into time dependent stable and unstable subspaces.

Two-grid Algorithms for Solution of Difference Equations of Compressible Fluid Flow

Lubin Vulkov, Miglena Koleva, *Tue 11:30 R 1.29*

We propose two-grid algorithms for solving 1D and 2D compressible flow systems of equations on a bounded domain. In the first step, the nonlinear boundary value problem is discretized on a coarse grid of size H. In the second step, the nonlinear problem is linearized around an interpolant of the computed solution at the first step. Then, the linear problem is solved on a fine mesh of size h, $h < H$. On this base, we develop two-grid iteration algorithms, that achieve optimal accuracy as long as the mesh size satisfies $h = (H^{2^r})$, $r = 1, 2, \ldots$, where r is the r-th Newton's iteration for the linearized differential problem. Numerical experiments are discussed

Geometric integration on Lie groups using the Cayley transformation

Michele Wandelt, M. Günther, M. Muniz, *Thu 11:30 R 1.27*

This talk deals with geometric numerical integration on a Lie group using the Cayley transformation.
We investigate a coupled system of differential equations in a Lie group setting that occurs in Lattice Quantum Chromodynamics. Here, elementary particles are simulated which means expectation values of some operators are computed using the Hybrid Monte Carlo method. In this context, Hamiltonian equations of motion are solved with a time-reversible and volume-preserving integration method. Usually, the exponential function is used in the integration method as mapping from the Lie algebra to the Lie group.

The focus is put on geometric numerical integration using the Cayley transformation instead of the exponential function. The geometric properties of the method are shown for the example of the Störmer-Verlet method, both theoretically and numerically. Moreover, its advantages and disadvantages are discussed.

Volume-preserving exponential integrators

Bin Wang, Xinyuan Wu, *Wed 10:05 R 1.27*

This talk is about the volume-preserving property of exponential integrators in different vector fields. We derive a necessary and sufficient condition of volume preservation for exponential integrators, and with this condition, volume-preserving exponential integrators are analysed in detail for four kinds of vector fields. It turns out that symplectic exponential integrators can be volume preserving for a much larger class of vector fields than Hamiltonian systems. On the basis of the analysis, novel volume-preserving exponential integrators are derived for solving highly oscillatory second-order systems and extended RKN integrators of volume preservation are presented for separable partitioned systems. Moreover, the volume preservation of RKN methods is also discussed.

Optimally zero-stable superconvergent IMEX Peer methods

Rüdiger Weiner, Behnam Soleimani, Jens Lang, Moritz Schneider, *Thu 11:05 R 1.23*

Many systems of ODEs are of the form

$$y' = f(t, y) + g(t, y)$$

with stiff part f and nonstiff part g, for instance MOL discretizations of diffusion-advection-reaction equations. This kind of problems can be treated efficiently by implicit-explicit (IMEX) methods. In IMEX methods the stiff part is solved by an implicit method, the nonstiff part is solved by an explicit method.

In this talk we consider s-stage IMEX peer methods of order $p = s$ for variable and of order $p = s + 1$ for constant step sizes. They are combinations of s-stage superconvergent implicit and explicit peer methods. Due to their high stage order no order reduction appears. This is in contrast to one-step IMEX methods. On the other hand compared with multistep methods there is no order bound for A-stability of the implicit part.

We construct methods of order $p = s + 1$ for $s = 3, 4, 5$ where we compute the free parameters numerically to give good stability with respect to a general linear test problem frequently used in the literature. Numerical tests and comparison with two-step IMEX Runge-Kutta methods confirm the high potential of the superconvergent IMEX peer methods.

Numerical properties of mixed order variational integrators applied to dynamical multirate systems

Theresa Wenger, Sina Ober-Blöbaum, Sigrid Leyendecker, *Tue 14:30 R 3.28*

Dynamical systems having components that act on different time scales are a challenge for numerical integration. Established approaches are to split the potential forces into fast and slow ones or separating the configurations into fast and slow degrees of freedom allowing for different treatment. Embedded in the framework of variationally derived integrators, the idea here is, to use polynomials of different degrees to approximate the components that act on different time scales. Together with quadrature rules of different orders to approximate the parts of the action integral, the discrete Lagrangian is defined. Numerical investigations reveal, that within this approach run-time savings can be achieved while the accuracy stays nearly the same. However, linear stability can suffer, what is shown by analysing the eigenvalues of the propagation matrices. Some of the presented integrators are reformulated as modified trigonometric integrators and the modulated Fourier expansion is used to analyse the capture of the slow energy exchange and the conservation of total energy and stiff oscillatory energy in the Fermi-Pasta-Ulam problem.

BDF integrators for mechanical systems on Lie groups

Victoria Wieloch, Martin Arnold*, Thu 11:05 R 1.27*

Multistep methods of BDF type are the methods-of-choice in many industrial multibody system simulation packages. Matrix Lie groups can be used to describe large rotations without singularities. In this framework, BLieDF is a k-step Lie group integrator for constrained second order systems. Order reduction can be avoided 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.
We compare this integrator with multistep methods on Lie groups suggested by Faltinsen et al. [1] and show the advantages of the BLieDF integrator.

References

[1] S. Faltinsen, A. Marthinsen, and H. Munthe-Kaas, "Multistep methods integrating ordinary differential equations on manifolds," *Applied Numerical Mathematics*, vol. 39, p. 349–365, 2001.

Boundary value methods for semi-stable differential equations

Paul Andries Zegeling*, Thu 10:40 R 1.29*

In this talk I present a boundary-value method (BVM) that can be used for partial (PDE) and ordinary differential equation (ODE) models with semi-stable, or even ill-posed, properties. Traditionally, step-by-step methods, such as Runge-Kutta and linear multistep methods, are being utilized for time-dependent models. However, their numerical stability regions (this holds both for explicit and implicit methods) are usually such that a significant part does not intersect with areas in the complex plane which are of importance for a successful time-integration. BVMs, that need an extra numerical condition at the final time, are global methods and are, in some sense, free of such barriers. As an example, a BVM, based on the explicit midpoint method combined with an implicit-Euler final condition, possesses the whole complex plane (excluding the imaginary axis) as stability region. On the other hand, they loose efficiency, since an extended linear or nonlinear system has to be solved for the whole time range of interest. Numerical experiments illustrating these properties are given for, among others, a dispersive wave equation and the backward heat equation.

A uniformly exponentially stable ADI scheme for Maxwell equations

Konstantin Zerulla*, Thu 11:05 R 1.29*

Alternating direction implicit (ADI) schemes are a very efficient tool for time integration of linear isotropic Maxwell equations on cuboids as they are unconditionally stable and decouple into essentially one-dimensional problems.
We study the Maxwell system with Ohm's law and a strictly positive conductivity. In this case the solutions tend to zero exponentially for large times. However, works by Nicaise, Tucsnak, Zuazua and others for the discretization of wave equations suggest, that the uniform decay properties of the continuous Maxwell system get lost when discretizing in time or space without additional damping.
We thus construct a modified ADI scheme by including artificial viscous damping. In this way we obtain uniformly exponentially stable time-discrete approximations to the Maxwell equations and an unconditionally stable scheme with similar effort as the original one. Finally, we will also give a bound on the error of the modified scheme.

Lagrange hybridized discontinuous Galerkin method for fractional Navier-Stokes equations

Wenjiao Zhao, Jingjun Zhao, Yang Xu, *Mon 15:15 R 1.23*

In this talk, a particular Lagrange hybridized discontinuous Galerkin method is applied to time-dependent incompressible fractional Navier-Stokes equations. The stability of the fully scheme is proved, and error estimates for the L^2-norm both in velocity and pressure are analysed in detail. In addition, existence and uniqueness of weak solution are also considered. Finally, the effectiveness of the proposed method is shown by some numerical examples.

Convergence and stability of micro-macro acceleration method for scale-separated SDEs

Przemyslaw Zielinski, Kristian Debrabant, Tony Lelievre, Giovanni Samaey, *Thu 11:55 R 3.28*

Many dynamical systems of current interest exhibit behavior on a wide range of time scales and cannot be simulated directly on long (macroscopic) time intervals. I present and discuss a multi-scale method to efficiently simulate the macroscopic observables of SDEs having strong separation between time-scales.

The method couples short bursts of stochastic path simulation with extrapolation of spatial averages forward in time. After each extrapolation, a new microscopic state is obtained by matching the last available microscopic distribution with the extrapolated macroscopic state. The matching is an inference procedure that renders a minimal perturbation of a prior microscopic state (available just before the extrapolation) consistent with the extrapolated macroscopic state.

I introduce the matching operator based on minimization of Kullback-Leibler divergence and indicate why it provides a convenient numerical approach. Then, I discuss the relation of the method to coarse graining, establish the convergence in the numerically weak sense, and inquire about the stability for appropriately chosen test models.

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List of Speakers