The seminar NUMDIFF–14 is jointly organised by the *Institute of Mathematics, Martin Luther University Halle–Wittenberg*, the *Center for Mathematics and Computer Science* (CWI) in Amsterdam and *the Mathematical Institute of the University of Utrecht*.

Scientific Committee

- Martin Arnold (Halle)
- Jason Frank (Utrecht)
- Willem Hundsdorfer (Amsterdam)
- Helmut Podhaisky (Halle)
- Rüdiger Weiner (Halle)

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Acknowledgements

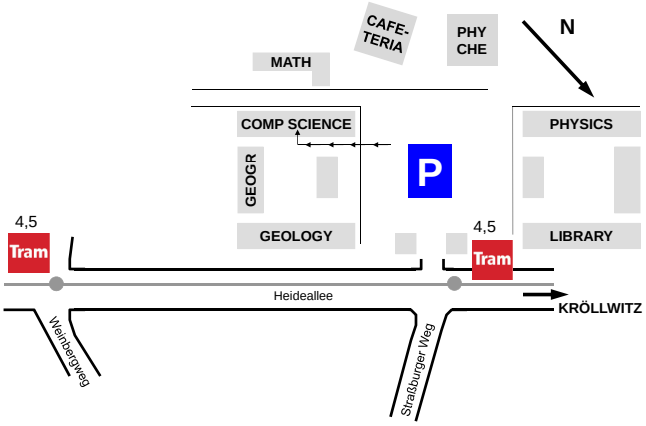
We acknowledge the generous support of:

- Martin Luther University Halle–Wittenberg
- Deutsche Forschungsgemeinschaft
- Stadt Halle, Dienstleistungszentrum Wirtschaft und Wissenschaft
- SIMPACK AG, Gilching

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

Contents

1. **Conference Site and Duration**
   The conference will take place in the lecture rooms of the Computer Science building situated within the Heide Campus at Von-Seckendorff-Platz 1. Parking spaces are available.



   The conference will begin at 9:00 on Monday, 7 September 2015, and will finish around 13:15 on Friday, 11 September 2015. From Tuesday to Friday, the lectures will start at 8:30. To reach the conference site from the "Tryp by Wyndham" Hotel you can use the tram lines 2,9,10 and 11 first, leaving in front of the hotel from stop "Zentrum Neustadt" towards "Beesen" or "Hauptbahnhof", then get off at the third stop "Rennbahnkreuz" and change to tram line 4 or 5, direction "Kröllwitz", leaving from the track perpendicular to the arriving track (100 meter walk), and finally get off at the third stop "Straßburger Weg".

2. **Conference Office and Registration**
   The conference office will be open on Sunday, 6 September 2015, from 17:00 to 20:00 in the lobby of the "Tryp by Wyndham Hotel" Halle-Neustadt (+49 345 69310). On the other days the conference office 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 and by fax +49 345 5527004. These lines will be active from Monday, 7 September 2015.

   Please register at the conference office after your arrival. Participants who have not paid the conference fee in advance can pay the conference fee in cash at the conference office. Please note that we cannot accept credit cards or cheques.

3. **Lecture Rooms and Audio-Visual Requirements**
   The opening of the seminar as well as all plenary lectures will take place in lecture room 3.07.

   All lecture rooms will be equipped with laptop and data projector.

4. **Time of Lectures and Discussion**
   Please note that 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.

5. **Coffee and Tea Breaks, Lunch**
   Coffee and tea will be provided during the morning and afternoon breaks in room 1.02 next to the conference office.

   For lunch, the *Mensa Weinberg* is a 15 minute walk away. Please ask local participants or the staff in the conference office for further information. A small cafeteria is located west of conference site, see map on page 2.

6. **Computer and Internet Access**
   At the conference site you can access the internet using eduroam or using WLAN SSID *event-net* with network key *Un!@HALWB*, user name *numdiff14* and password *l3iR4Kbx*. For the computer terminals in room 3.02, use domain *UNIPOOL*, the password *numdiff* and the login *poolxxx* where *xxx* is the three digit number contained in the name tag of the pc. For example, the login for the PC named *poolpc204* will be *pool204*. We have reserved room 1.30 for discussions and there you can also use your own computer.

7. **Conference Dinner**
   The conference dinner will be held in the Tryp by Wyndham Hotel Halle–Neustadt on Thursday, 10 September at 19:00. One dinner ticket is included in the conference fee.

8. **Tour to BMW plant Leipzig on Wednesday afternoon**
   If you are interested then please register on Monday for the excursion at the conference office. Busses will leave from the conference site at 12:30 and will return to Halle at around 19:30.

9. **Conference Proceedings**
   The proceedings of NUMDIFF-14 will be published as a special issue of the *Journal of Computational and Applied Mathematics*. Guest editors are M. Arnold, J. Frank, W. Hundsdorfer, H. Podhaisky and R. Weiner.

   Every speaker of NUMDIFF-14 can submit a manuscript for consideration of publication in this special issue. Submitted manuscripts must deal with original work not published elsewhere and will be refereed according to the standard journal procedure.

   For a statement of the journal's objectives and the instructions for authors, see:

   `http://www.journals.elsevier.com/journal-of-computational-and-applied-mathematics`

   Authors are encouraged to use the journal style files. The paper length is restricted to 20 style file pages. The deadline for manuscript submission is 15 December 2015.

   The manuscripts should be submitted through `http://ees.elsevier.com/cam/`. Please indicate that your article is for this special issue by selecting article type *"NUMDIFF14"*. Please also send a copy directly to willem.hundsdorfer@cwi.nl.

1 Programme Overview

Monday, September 7, 2015

	R 3.07	*R 1.04*	*R 1.26*	*R 1.27*
9:00	–Opening–			
9:20	Botchev			
10:10	–Break–			
10:40	Celledoni			
11:30	Hesthaven			
12:20	–Lunch–			
14:00	Kumar	Schmitt	Anwar	Soll
14:25	Wieloch	Podhaisky	Ha	Feng
14:50	Hante	Schröder	Rihan	Ahmad
15:15	Kolpakov	Soleimani	Unger	Hachtel
15:40	–Break–			
16:10	Baum	Gonzalez-Pinto	Göckler	D'Ambrosio
16:35	Köbis	Rang	Kandolf	Reguera
17:00	Niroomand Rad	Klinge	de la Cruz	Prugger
17:25	Naumann	Jax	Ibrahim	Melosik

Tuesday, September 8, 2015

	R 3.07	*R 1.04*	*R 1.26*	*R 1.27*
8:30	Leok			
9:20	Grote			
10:10	–Break–			
10:40	Romero			
11:30	–Short Break–			
11:40	Simeon	Debrabant	Braś	Fiedler
12:05	Paschkowski	Heuer	Martínez	Marszalek
12:30	–Lunch–			

	Minisymposium *Nonlinear evolution equations*	Minisymposium *Local and global error control issues*
14:00	Caliari	Kulikov
14:30	Henningsson	Kulikova
15:00	Hell	Lima
15:30	–Break–	
16:00	Einkemmer	Lang
16:30	Luan	Chistyakova
17:00	Krämer	Weiner
17:30	Bürger	Beigel

Wednesday, September 9, 2015

	R 3.07	*R 1.04*	*R 1.26*	*R 1.27*
8:30	–Opening–			
8:40	Butcher			
9:10	–Break–			
9:40	Führer	Kocsis	Perminov	Pulch
10:05	Arnold	Németh	Usman	Thalhammer
10:30	Mehrmann	Mohammadi	Pandit	Ableidinger
10:55	Tischendorf	Bezglasnyi	Rahimkhani	Ngnotchouye
11:20	–Lunch–			
12:30	Departure for the excursion to the BWM Plant Leipzig.			

Thursday, September 10, 2015

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9:20	Sandu			
10:10	–Break–			
10:40	Knoth	März	Pade	Høiseth
11:05	Faleichik	Estévez Schwarz	Schneider	Kraus
11:30	Bourchtein, A.	Altmann	Meyer	Natale
11:55	Bourchtein, L.	Burger	Klöppel	Khorshidi
12:20	–Lunch–			

	Minisymposium *Geometric integration of partial differential equations*	Minisymposium *Numerical PDEs in financial mathematics*
14:00	Cohen	Christara
14:30	Bader	Toivanen
15:00	Frank	von Sydow
15:30	–Break–	
16:00	Alonso-Mallo	in 't Hout
16:30	Duran	Wyns
17:00	Ostermann	Düring
17:30	Cano	Hendricks

Friday, September 11, 2015

	R 3.07
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9:20	Pareschi
10:10	Wensch
11:00	–Break–
11:20	Horváth
12:10	Grimm
13:00	–Closing–

2 Scientific Programme

Monday, September 7, 2015

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9:00 –Opening–

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Exponential Krylov subspace time integration for nanophotonics applications

Room R 3.07

10:40 **Celledoni**, Elena
Geometric methods for differential equations in applications of computer animation

11:30 **Hesthaven**, Jan
High-order accurate methods for fractional differential equations

Room R 3.07

14:00 **Kumar**, Vikas
Numerical solutions of time-dependent KdV type system via the Lie group method

14:25 **Wieloch**, Victoria
Variable step size implementation of a generalized-α Lie group integrator

14:50 **Hante**, Stefan
Lie Group time integration of a nonlinear geometrically exact Cosserat rod model

15:15 **Kolpakov**, Alexander
Influence of defect between closely placed disks on their capacity

Room R 1.04

14:00 **Schmitt**, Bernhard A.
Efficient A-stable peer two-step methods

14:25 **Podhaisky**, Helmut
Effective order Runge–Kutta methods with free output

14:50 **Schröder**, Dirk
Space adaptive linearly implicit two-step peer methods for time-dependent PDEs

15:15 **Soleimani**, Behnam
A class of implicit peer methods

Room R 1.26

14:00 **Anwar**, Mohamed-Naim
Delayed SIR Epidemic Model with a Saturated Incidence Rate

14:25 **Ha**, Phi
On the numerical solutions of linear delay differential-algebraic equations

14:50 **Rihan**, Fathalla
Stabilized Numerical Schemes for Singularly Perturbed Delay Differential Equations

15:15 **Unger**, Benjamin
Regularization of linear time-varying delay differential-algebraic equations

Room R 1.27

14:00 **Soll**, Tino
Sample Selection Approaches in Parameterized Model Order Reduction

14:25 **Feng**, Lihong
Model Reduction of Quadratic Bilinear Descriptor Systems using Parametric Reduction Techniques with Error Estimation

14:50 **Ahmad**, Mian Ilyas
Implicit Volterra Series Interpolation for Model Reduction of Bilinear Systems

15:15 **Hachtel**, Christoph
On Coupled MOR-Multirate Schemes: Derivation and Error Analysis

Room R 3.07

16:10 **Baum**, Ann-Kristin
A flow-on-manifold formulation of DAEs. Application to positive systems.

16:35 **Köbis**, Markus
Newmark type time integration methods for strongly damped mechanical systems

17:00 **Niroomand Rad**, Helia
Operator Index Reduction in Electromagnetism

17:25 **Naumann**, Andreas
Extended defect corrected averaging for highly oscillatory PDEs

Room R 1.04

16:10 **Gonzalez-Pinto**, Severiano
Some families of W-methods to stabilize standard explicit Runge-Kutta methods for stiff problems

16:35 **Rang**, Joachim
Adaptive timestep control for high order implicit Runge-Kutta methods

17:00 **Klinge**, Marcel
Explicit peer methods with variable nodes

17:25 **Jax**, Tim
Generalized ROW-Type Methods for Solving Semi-Explicit DAEs of Index-1

Room R 1.26

16:10 **Göckler**, Tanja
A convergence analysis for the shift-and-invert Krylov method

16:35 **Kandolf**, Peter
The backward error of the Leja method

17:00 **de la Cruz**, Hugo
On the construction of explicit exponential-based schemes for stiff Stochastic Differential Equations

17:25 **Ibrahim**, Fatma
Stabilized Extended One-Step Schemes for Stiff and Non-Stiff Delay Differential Equations

Room R 1.27

16:10 **D'Ambrosio**, Raffaele
Trigonometrically fitted numerical methods for reaction-diffusion problems

16:35 **Reguera**, Nuria
How to avoid order reduction when Lawson methods are used to solve linear initial boundary value problems

17:00 **Prugger**, Martina
On the parallel implementation of numerical schemes for the hyperbolic Euler equations

17:25 **Melosik**, Michal
On the 0/1 test for chaos for continuous ODEs: resonance, oversampling and frequency properties.

Tuesday, September 8, 2015

Room R 3.07

8:30 **Leok**, Melvin
Space-Time Finite-Element Exterior Calculus and Variational Discretizations of Gauge Field Theories

9:20 **Grote**, Marcus
High-Order Explicit Local Time-Stepping Methods For Wave Propagation

10:40 **Romero**, Ignacio
Structure-preserving integrators for smooth and non-smooth thermomechanical problems

Room R 3.07

11:40 **Simeon**, Bernd
Non-smoooth contact dynamics for the large-scale simulation of granular material

12:05 **Paschkowski**, Manuela
Unique solutions of initial value problems for mechanical systems with redundant unilateral constraints

Room R 1.04

11:40 **Debrabant**, Kristian
High order finite difference schemes for obstacle problems

12:05 **Heuer**, Christof
High-order compact schemes for parabolic problems with mixed derivatives in multiple space dimensions with application to basket options

Room R 1.26

11:40 **Braś**, Michał
Implicit–explicit general linear methods with inherent Runge–Kutta stability

12:05 **Martínez**, Vicente
A numerical technique for applying time splitting methods in shallow water equations.

Room R 1.27

11:40 **Fiedler**, Robert
Hydrodynamic force elements: A PDAE approach

12:05 **Marszalek**, Wieslaw
Jounce Newtonian equations for oscillating memristive circuits

Room R 3.07

Minisymposium organised by E. Hansen and A. Ostermann: Nonlinear evolution equations

14:00 **Caliari**, Marco
Splitting methods for the Schrödinger equation with vector potential

14:30 **Henningsson**, Erik
Convergence analyses of the Peaceman–Rachford and Douglas–Rachford Schemes for Semilinear Evolution Equations

15:00 **Hell**, Tobias
Improvement of dimension splitting methods

15:30 –Break–

16:00 **Einkemmer**, Lukas
Overcoming order reduction in diffusion-reaction splitting

16:30 **Luan**, Vu Thai
Parallel exponential Rosenbrock methods

17:00 **Krämer**, Patrick
Efficient time integration of the Maxwell-Klein-Gordon equation in the non-relativistic limit regime

17:30 **Bürger**, Raimund
Linearly implicit methods for a class of degenerate convection-diffusion problems

Room R 1.04

Minisymposium organised by G. Kulikov and R. Weiner:
Local and global error control issues in time stepping methods

14:00 **Kulikov**, Gennady
Embedded Nested Implicit Runge-Kutta Pairs of Gauss and Lobatto Types with Global Error Control for Stiff Ordinary Differential Equations

14:30 **Kulikova**, Maria
Global Error Control in Nonlinear Kalman Filtering Algorithms

15:00 **Lima**, Pedro
An Algorithm with Global Error Control for the Numerical Solution of the Generalized Density Profile Equation

15:30 –Break–

16:00 **Lang**, Jens
On Global Error Estimation and Control for Stiff Initial Value Problems

16:30 **Chistyakova**, Elena
Error Control in Solving Differential Algebraic Equations of High Order

17:00 **Weiner**, Rüdiger
Global error control with peer methods

17:30 **Beigel**, Dörte
Efficient goal-oriented global error estimation for BDF-type methods

Wednesday, September 9, 2015

Room R 3.07

Special session to celebrate the 75th birthday of Roswitha März

8:30 –Opening–

8:40 **Butcher**, John
The construction of high order G-symplectic methods

9:10 –Break–

Room R 3.07

9:40 **Führer**, Claus
Algebraic Variables in Higher Index DAEs

10:05 **Arnold**, Martin
Coupled error propagation in terms of vector valued error terms

10:30 **Mehrmann**, Volker
The Index of DAEs, Science or Religion

10:55 **Tischendorf**, Caren
Perturbation Analysis of hyperbolic PDAEs

Room R 1.04

9:40 **Kocsis**, Tihamér Albert
Optimal second-order diagonally implicit SSP Runge–Kutta methods

10:05 **Németh**, Adrián
Existence and optimality of SSP linear multistep methods: a duality-based approach

10:30 **Mohammadi**, Fatemeh
A Family of Runge-Kutta Restarters for Discontinuous ODEs

10:55 **Bezglasnyi**, Sergey
Analytic and numerical solutions to the problem of double pendulum stabilization

Room R 1.26

9:40 **Perminov**, Valeriy
Numerical solution of three dimensional conjugate problems of forest fires spread

10:05 **Usman**, Mustapha
Numerical solution of Euler-Bernoulli beam subjected to concentrated load

10:30 **Pandit**, Sapna
Haar Wavelet Operational Matrix Method for Solving a System of Fractional Differential Equations with nonlinear uncertain parameters

10:55 **Rahimkhani**, Parisa
Application of Bernoulli polynomials for solving fractional Riccati differential equations

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9:40 **Pulch**, Roland
The Hankel norm for quadrature methods applied to random dynamical systems

10:05 **Thalhammer**, Andreas
Computational mean-square stability analysis for linear systems of SODEs

10:30 **Ableidinger**, Markus
Variance reduction techniques for the numerical simulation of the stochastic heat equation

10:55 **Ngnotchouye**, Jean Medard
Weak convergence for a stochastic exponential integrator and finite element discretization of SPDE for multiplicative and additive noise

Thursday, September 10, 2015

Room R 3.07

8:30 **Descombes**, Stéphane
Locally implicit and implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media

9:20 **Sandu**, Adrian
Multi-methods for time discretization of evolutionary PDEs

Room R 3.07

10:40 **Knoth**, Oswald
Split-explicit methods with a large number of explicit stages

11:05 **Faleichik**, Boris
Accelerating convergence of Generalized Picard Iterations

11:30 **Bourchtein**, Andrei
Time-Splitting Scheme for Nonhydrostatic Atmospheric Model

11:55 **Bourchtein**, Ludmila
On grid generation for numerical schemes of atmospheric models

Room R 1.04

10:40 **März**, Roswitha
New answers to an old question: Essential underlying ODE versus inherent explicit ODE

11:05 **Estévez Schwarz**, Diana
Consistent initialization of DAEs using a specific minimum-norm correction

11:30 **Altmann**, Robert
Operator DAEs with Noise Appearing in Fluid Dynamics

11:55 **Burger**, Michael
Function Space Optimal Control Methods for Tracking Problems in Vehicle Engineering

Room R 1.26

10:40 **Pade**, Jonas
Cosimulation Convergence Criteria for Hessenberg DAEs of Index 2

11:05 **Schneider**, Fabio
Influence of spatial discretization of flexible structures on the stability of coupled simulations

11:30 **Meyer**, Tobias
Error estimation approach for controlling the comunication step size for semi-implicit co-simulation methods

11:55 **Klöppel**, Michael
A parallelization approach for the simulation of large scale multibody systems

Room R 1.27

10:40 **Høiseth**, Eirik Hoel
Structure preserving discretization of port-Hamiltonian systems

11:05 **Kraus**, Michael
Geometric Integration of Degenerate Lagrangian Systems

11:30 **Natale**, Andrea
Nonholonomic mechanics for perfect fluids

11:55 **Khorshidi**, Korosh
Exact PDE close-form solution of the vibrating rectangular nanoplates using non-local trigonometric shear deformation plate theory

Room R 3.07
Minisymposium organised by B. Cano:
Geometric integration of partial differential equations

14:00 **Cohen**, David
Multi-symplectic discretisation of wave map equations

14:30 **Bader**, Philipp
Volume Preservation by Runge-Kutta Methods

15:00 **Frank**, Jason
Enforcing power-law kinetic energy spectra under conservative discretizations of fluids

15:30 –Break–

16:00 **Alonso-Mallo**, Isaias
Geometric integration and absorbing boundary conditions

16:30 **Duran**, Angel
On the numerical solution of generalized Ostrovsky equations

17:00 **Ostermann**, Alexander
A splitting approach for the KdV and KP equations

17:30 **Cano**, Begoña
Avoiding order reduction when integrating nonlinear Schroedinger equation

Room R 1.04
Minisymposium organised by K. in't Hout:
Numerical PDEs in financial mathematics

14:00 **Christara**, Christina
PDE pricing of financial instruments with stochastic correlation

14:30 **Toivanen**, Jari
IMEX Schemes for Pricing Options under Jump-Diffusion Models

15:00 **von Sydow**, Lina
Forward option pricing using Gaussian RBFs

15:30 –Break–

16:00 **in 't Hout**, Karel
Convergence of ADI schemes for two-dimensional convection-diffusion equations with mixed derivative term

16:30 **Wyns**, Maarten
Convergence analysis of the Modified Craig-Sneyd scheme for two-dimensional convection-diffusion equations with nonsmooth initial data

17:00 **Düring**, Bertram
High-order compact finite difference schemes for option pricing in stochastic volatility models

17:30 **Hendricks**, Christian
High-Order-Compact ADI schemes for pricing basket options in the combination technique

Friday, September 11, 2015

Room R 3.07

8:30 **Buckwar**, Evelyn
Stochastic Numerics and Stability Issues

9:20 **Pareschi**, Lorenzo
Asymptotic-preserving methods and differential algebraic equations

10:10 **Wensch**, Jörg
TVD-based Finite Volume Methods for Sound-Advection-Buoyancy Systems

Room R 3.07

11:20 **Horváth**, Zoltán
Classical and novel analysis of positive invariance and strong stability preserving time integrators

12:10 **Grimm**, Volker
Resolvent Krylov subspace approximation to C_0-semigroups and their discretisations

13:00 –Closing–

3 Abstracts

Variance reduction techniques for the numerical simulation of the stochastic heat equation

Markus Ableidinger, Evelyn Buckwar, Andreas Thalhammer, *Wed 10:30 R 1.27*

We consider the finite dimensional stochastic heat equation (obtained by spatial discretisation)

$$\begin{aligned} du(t) &= \Delta_{h,0} u(t)dt + \sigma u(t)dW(t) \\ u(0) &= u_0, \end{aligned}$$

where $\Delta_{h,0}$ denotes the discrete Laplacian with homogeneous Dirichlet boundary conditions and $W(t)$ is a Q-Wiener process. For growing diffusion parameter $\sigma \in \mathbb{R}^+$ the equilibrium solution of the system eventually gets mean-square unstable, however it takes an unreasonably large number of numerical trajectories to see this instability in Monte-Carlo simulation. We will discuss the practicability and the influence of variance reduction techniques, namely importance sampling via Girsanov's theorem and control variates, on the Monte-Carlo estimation. This talk is based on joint work with E. Buckwar and A. Thalhammer and connected with the talk *Computational mean-square stability analysis for linear systems of SODEs* by A. Thalhammer, which treats the interplay of different stability concepts in numerical simulation.

Implicit Volterra Series Interpolation for Model Reduction of Bilinear Systems

Mian Ilyas Ahmad, Ulrike Baur and Peter Benner, *Mon 14:50 R 1.27*

We propose a new interpolatory framework for model reduction of large-scale bilinear systems. The input-output representation of a bilinear system in frequency domain involves a series of multivariate transfer functions, each representing a subsystem of the bilinear system. If a weighted sum of these multivariate transfer functions associated with a reduced bilinear system interpolates a weighted sum of the original multivariate transfer functions, we say that the reduced system satisfies Volterra series interpolation [1]. These interpolatory conditions can also ensure the necessary conditions for $\mathcal{H}_2$ optimal model reduction [1, 2]. We observe that, by carefully selecting the weights of the series, the Volterra series interpolatory conditions reduce to the problem of interpolating a linear system with an affine parameter dependence. Such linear parametric systems can then be reduced by some method for parametric model order reduction.

Linear systems where the affine parameter dependence produces low-rank variation in the state matrix can be mapped into a nonparameterized multi-input multi-output linear system. This allows us to utilize the standard (nonparametric) linear IRKA [3] for the problem of parameterized/bilinear interpolation. Numerical results show that the approximations are of comparable accuracy to those obtained from the bilinear iterative rational Krylov algorithm [2]. The proposed approach however has the advantage that it reduces the computational cost as it involves computations associated with linear systems only.

References

[1] G. Flagg and S. Gugercin. Multipoint Volterra Series Interpolation and $\mathcal{H}_2$ Optimal Model Reduction of Bilinear Systems. Accepted to appear in SIAM J. Matrix Anal. Appl., 2015. Available as arXiv:1312.2627.

[2] P. Benner and T. Breiten. Interpolation-based $\mathcal{H}_2$-model reduction of bilinear control systems. SIAM J. Matrix Anal. Appl., 33-3 (2012), 859–885.

[3] S. Gugercin, A.C. Antoulas, and C. Beattie. $\mathcal{H}_2$ model reduction for large-scale dynamical systems. SIAM J. Matrix Anal. Appl.,30-2 (2008), 609–638.

Geometric integration and absorbing boundary conditions

Isaias Alonso-Mallo, A.M. Portillo, *Thu 16:00 R 3.07*

This talk is about the confluence of two subjects of the numerical solution of time evolution PDEs: numerical methods that preserve geometric properties of the flow and absorbing boundary conditions to reduce the computation to a finite domain. This confluence is studied with special attention to the time stability of the resulting full discretization. Since geometric methods are not always A-stable, it is necessary a suitable behaviour of the real part of the eigenvalues of the spatially discretized problem to avoid in practice any time instability. We study the case of the one dimensional wave equation discretized with finite differences. Coupled wave equations are also considered.

Operator DAEs with Noise Appearing in Fluid Dynamics

Robert Altmann, T. Levajkovic, H. Mena (University of Innsbruck), *Thu 11:30 R 1.04*

We consider operator DAEs (or constrained PDEs) as they appear in applications from fluid dynamics. Thus, the constraint is given by the divergence operator and the system has the form

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

with (consistent) initial condition $u(0) = u_0$. In applications such as the Stokes equations, u would be the velocity of the fluid and p would denote the pressure.
In this talk, we consider additional Gaussian white noise in the right-hand sides. Because of the differential-algebraic structure, noise terms may result in instabilities such that a regularization is necessary. We present such a regularization and show the resulting advantages.

Delayed SIR Epidemic Model with a Saturated Incidence Rate

Mohamed-Naim Anwar, Fathalla A. Rihan, *Mon 14:00 R 1.26*

In this contribution, we consider a delayed SIR epidemic model in which the susceptibles are assumed to satisfy the logistic equation and the incidence term is of saturated form with the susceptible. We investigate the qualitative behaviour of the model and find the conditions that guarantee the asymptotic stability of corresponding steady states. We present the conditions in the time lag τ in which the DDE model is stable. Hopf bifurcation analysis is also addressed. Numerical simulations are provided in order to illustrate the theoretical results and gain further insight into the behaviour of this system.
Keywords: Delay, Hopf bifurcation, SIR, Stability, Stiff differential equation

Coupled error propagation in terms of vector valued error terms

Martin Arnold, *Wed 10:05 R 3.07*

Projectors are a useful tool to study certain components of a differential-algebraic equation separately from the other ones. We use them to analyse the convergence of generalized-α time integration methods for constrained mechanical systems with rank-deficient mass matrix. This convergence analysis is based on a coupled error propagation in terms of nine different vector valued error terms that may be investigated by a novel error recursion scheme for vector valued error terms.
The global error of generalized-α methods is seen to be composed of a second order error term resulting from the accumulation of local truncation errors and an additional error term that describes the influence of starting values. This additional error term may be of lower order but will be damped out after a short transient phase. It is characterized by powers of a 7×7 error amplification matrix $\mathbf{T}_z$ that is block-triangular with diagonal blocks of size 3×3, 2×2, 1×1 and 1×1. The sequence $(\mathbf{T}_z^n)_{n \geq 0}$ tends to zero since all eigenvalues of $\mathbf{T}_z$ are inside the unit circle in the complex plane. Nevertheless, $\|\mathbf{T}_z^n\|_2$ may be much larger than one in a transient phase since the 3×3 and 2×2 diagonal blocks are non-normal matrices.

Volume Preservation by Runge-Kutta Methods

Philipp Bader, D. I. McLaren, M. Webb, GRW Quispel, *Thu 14:30 R 3.07*

It is a classical theorem of Liouville that Hamiltonian systems preserve volume in phase space. Any symplectic Runge-Kutta method will respect this property for such systems, but it has been shown that no B-Series method can be volume preserving for all volume preserving vector fields (BIT 47 (2007) 351-378 and IMA J. Numer. Anal. 27 (2007) 381-405). We show that despite this result, symplectic Runge-Kutta methods can be volume preserving for a much larger class of vector fields than Hamiltonian systems, and discuss how some Runge-Kutta methods can preserve a modified measure exactly.

A flow-on-manifold formulation of DAEs. Application to positive systems.

Ann-Kristin Baum, *Mon 16:10 R 3.07*

We generalize the concept of the flow from ordinary differential equations (ODEs) to differential-algebraic equations (DAEs). Using the framework of derivatives arrays and the strangeness-index, we identify those DAEs that are uniquely solvable on a particular set of initial values and define a flow, the mapping that uniquely relates a given initial value with the solution through this point. The flow allows to study system properties like invariant sets, stability, monotonicity or positivity. For DAEs, the flow further provides insights into the manifold onto which the system is bound to and into the dynamics on this manifold. Using a projection approach to decouple the differential and algebraic components, we give an explicit representation of the flow that is stated in the original coordinate space. This concept allows to study DAEs whose dynamics are restricted to special subsets in the variable space, like a cone or the nonnegative orthant. We give a uniform description of flow invariance for constrained and unconstrained systems and specialize this result for positive systems, i.e., systems leaving the nonnegative orthant invariant. Positive systems arise in every application, in which the analyzed values represent real matter, like the amount of goods, individuals or the density of a chemical or biological species. Simulating these processes, the loss of positivity leads to sever stepsize restrictions or failures in the simulation. Having conditions on the flow, when the system is positive provides the basis to study positive preserving discretization for DAEs.

Efficient goal-oriented global error estimation for BDF-type methods

Dörte Beigel, *Tue 17:30 R 1.04*

The backward differentiation formulae (BDF) method is a state-of-the-art method to solve large-scale, highly nonlinear and stiff initial value problems (IVPs) in ordinary differential equations, as they may arise from solving instationary partial differential equations by the method of lines. So far, efficient realizations control only local error quantities, but in fact the global error of the numerical approximation should be controlled. To this end, the global error has to be estimated, which requires adjoint information. This information can be obtained either by solving the adjoint IVP or from adjoint internal numerical differentiation (IND) of the integration scheme. The latter discrete approach is highly desirable in terms of computational complexity and discrete consistency. However, for multistep BDF methods there is no apparent relation between the values from adjoint IND and the solution of the adjoint IVP. This contribution sheds light on this relation and shows how the global error is efficiently and accurately estimated with the help of discrete IND adjoints.
First, we present our recently developed functional-analytic framework based on the duality pairing of continuous functions and normalized functions of bounded variation. We show the equivalence of BDF schemes and their adjoint IND schemes to Petrov-Galerkin finite element (FE) discretizations.
With this FE formulation, we derive a novel goal-oriented global error estimator for BDF methods which uses, for the first time in the context of multistep methods, discrete IND adjoints. Our derivation makes use of the dual weighted residual methodology. We prove asymptotic correctness of the novel error estimator for constant BDF methods and confirm this numerically. Moreover, we give promising numerical results for the estimation accuracy in variable BDF-type methods with changing orders and stepsizes as used in practice. Finally, we give strong evidence that our estimator outperforms another estimator based on the solution of the adjoint IVP in terms of both efficiency and accuracy. The presented error estimation approach opens the way for the development of variable BDF-type methods with goal-oriented global error control.

Analytic and numerical solutions to the problem of double pendulum stabilization

Sergey Bezglasnyi, *Wed 10:55 R 1.04*

The paper is about one passive control problem. This is the problem of controlling plane motions of two-mass parametric pendulum in a uniform gravitational field. The pendulum is modeled by two equivalent weightless rods with two equivalent point masses moving along a circle. Our control parameter is the angle between the rods of the pendulum. So it is a function depending on the representative point of the gravity center of the pendulum in the phase plane. In this paper, we construct two control laws for excitation and damping the pendulum near the lower equilibrium position by means of the swing principle. The formulated problem is solved then by the method of Lyapunov's functions of the classical stability theory, and this solution is derived in the class of continuous functions in closed form. As an application of our result, we consider the problem of gravitational stabilization of two diametrically opposite relative equilibrium positions of a satellite in a circular orbit with in-plane perturbations. The theoretical outcome of this research is confirmed by numerical simulations in MATHEMATICA and in agreement with practical experimentation.

Exponential Krylov subspace time integration for nanophotonics applications
Mike Botchev, *Mon 9:20 R 3.07*

Behavior of light in nanophotonics structures such as photonic crystals or layers of strongly scattering materials is often described by the time dependent Maxwell equations. The equations are usually supplied with the nonreflecting boundary conditions, e.g., the so-called perfectly matched layers (PML). The method of choice for solving these problems by physicists and engineers is the finite difference time domain method. This method is based on the staggered finite differences in space and staggered leap-frog in time.
In this talk we demonstrate that exponential time integration with Krylov subspace evaluations of the matrix exponential actions can be efficient in these applications. We discuss how the following techniques can be employed to achieve this efficiency [2].

1. To keep the Krylov subspace dimension moderate, the rational shift-and-invert (SAI) Krylov subspaces are used [4, 5]. This means that instead of the regular Krylov subspace $\mathcal{K}_m(A, v) = \{v, Av, \ldots, A^{m-1}v\}$, we work with $\mathcal{K}_m((I + \gamma A)^{-1}, v)$ for some $\gamma > 0$.

2. In three space dimensions, the actions of $(I + \gamma A)^{-1}$ should be carried out by iterative linear solvers and we briefly discuss some preconditioning strategies to do this.

3. In our (limited) experience, it is crucial to employ the Krylov subspace in such a way that one (or just several) Krylov subspace(s) suffice for the whole time interval. For non-autonomous problems this leads to block Krylov subspaces [1].

In some cases these techniques result in a method exhibiting an optimal performance in the sense that the number of Krylov subspace outer (for the matrix exponential actions) and inner (for $(I + \gamma A)^{-1}$ actions) iterations do not grow as the spatial mesh gets finer. Finally, we comment on how this approach is related to a general across-time waveform relaxation framework [3]. This facilitates an across-time parallelization of the method, which is a topic of our current research.

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Time-Splitting Scheme for Nonhydrostatic Atmospheric Model
Andrei Bourchtein, Ludmila Bourchtein, *Thu 11:30 R 3.07*

Complete three-dimensional models of the atmosphere have solutions of different space and time scales. The fastest atmospheric waves are the acoustic ones, which do not contain any significant part of the atmospheric energy. The slower gravity waves are more energy valuable, while slow advective processes and Rossby waves carry the main part of the atmospheric energy. In this study, a time-splitting semi-implicit scheme is proposed for the nonhydrostatic atmospheric model, which approximates implicitly the fast acoustic and gravity waves, while slow processes are treated explicitly. Such time approximation requires solution of three-dimensional elliptic equations at each time step. Efficient elliptic solver is based on decoupling in the vertical direction and splitting in the horizontal directions. Stability analysis of the scheme shows that the time step is restricted only by the maximum velocity of advection. The performed numerical experiments show computational efficiency of the designed scheme and accuracy of the predicted atmospheric fields.

On grid generation for numerical schemes of atmospheric models
Ludmila Bourchtein, Andrei Bourchtein, *Thu 11:55 R 3.07*

Simulation of large-scale atmospheric and ocean processes, such as weather phenomena, regional and global circulations, and climate dynamics, imply the formulation of the corresponding mathematical models in spherical geometry. The properties of numerical schemes, used to find approximate solutions of atmospheric models, are defined, at certain degree, by the choice of the computational grids. Discretizations based on uniform grids in natural spherical coordinates suffer from highly non-uniform physical resolution, especially in polar regions. On the other hand, general homeomorphic mappings of spherical domains, which can provide quite uniform physical resolution, are not usually applied due to the complex form of the governing equations in such general coordinates. One of the widespread approaches to circumvent this problem is the application of conformal mappings from a sphere onto a plane, which preserve a simpler form of the governing equations and assure local isotropy and smoothness of the variation of physical mesh size on the computational grid. In this study the problem of generation of the conformal mappings with the most possible uniformity is considered. A construction of conformal mappings with the minimum distortion for spherical domains of different extension and form is analyzed, and the obtained results for the practical computational grids are compared with the theoretical evaluations.

Implicit–explicit general linear methods with inherent Runge–Kutta stability
Michał Braś, Giuseppe Izzo, Zdzislaw Jackiewicz, *Tue 11:40 R 1.26*

We consider the initial value problem for the system of ordinary differential equations of the form

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

where $f\colon \mathbb{R}^m \to \mathbb{R}^m$ represents non-stiff part and $g\colon \mathbb{R}^m \to \mathbb{R}^m$ stiff part of the system.
For efficient integration of such systems we consider the class of implicit-explicit (IMEX) methods, where the non-stiff part $f(y)$ is integrated by explicit method, and stiff part $g(y)$ is integrated by implicit method.
In this talk we present extrapolation based approach to construct IMEX general linear methods. We begin with implicit general linear methods with inherent Runge–Kutta stability (IRKS) of

order p, stage order q, with s internal stages and r external approximations. Here, we assume that $p = q = s - 1 = r - 1$. Next, we extrapolate the implicit values in non-stiff terms using available quantities from previus step and current step. The dimensions of coefficient matrices and degree of stability polynomial are doubled.

Our aim is to find IMEX methods with large regions of absolute stability of explicit part assuming that implicit part of the method is A- or L- stable. It is done by numerical search in the space of free parameters of the method and free parameters of extrapolation. We provide examples of such methods that have larger regions of absolute stability than in similar classes of general linear methods. Numerical examples are also given which illustrate good performance of these schemes.

Stochastic Numerics and Stability Issues

Evelyn Buckwar, *Fri 8:30 R 3.07*

Stochastic Differential Equations (SDEs) have become a standard modelling tool in many areas of science, e.g., from finance to neuroscience. Many numerical methods have been developed in the last decades and analysed for their strong or weak convergence behaviour. In this talk we will provide an overview on current directions in the area of stochastic numerics and report on recent progress in the analysis of stability properties of numerical methods for SDEs, in particular for systems of equations. We are interested in developing classes of test equations that allow insight into the stability behaviour of the methods and in developing approaches to analyse the resulting systems of equations.

Function Space Optimal Control Methods for Tracking Problems in Vehicle Engineering

Michael Burger, *Thu 11:55 R 1.04*

We discuss the use of optimal control methods to derive excitation and input quantities for numerical system simulation in vehicle engineering. In particular, in the field of durability testing, it is a typical task to compute such excitation signals that reproduce certain reference quantities during simulation in an optimal way. For instance, for an axle test-rig model with axle, control quantities (e.g. actuator displacements) are searched that reproduce best given wheel forces. The considered system, i.e., test-rig and specimen, is modeled as mechanical multibody system and mathematically described as differential-algebraic equation(DAE). The resulting model equations are usually complex and highly-nonlinear. The mentioned task is formulated as a tracking optimal control problem. The unknown excitations are control inputs and one aims at minimizing the deviation between simulation outputs and given references quantities. Thus, one is faced with a nonlinear DAE optimal control problem. We present some function space methods (in time domain) to solve such a problem: classical methods from optimization applied in an appropriate function space. We present and discuss extensions of specific ODE methods to the DAE case. We discuss the applicability of such methods in connection with commercial software tools for simulation and modeling(where the availability of information about the equations is limited). Finally, we present some numerical examples.

The construction of high order G-symplectic methods

John Butcher, *Wed 8:40 R 3.07*

A general linear method

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix}$$

is "G-symplectic" if for some non-singular symmetric matrix G and diagonal matrix D,

$$\begin{bmatrix} DA + A^{\mathsf{T}}D - B^{\mathsf{T}}GB & DU - B^{\mathsf{T}}GV \\ U^{\mathsf{T}}D - V^{\mathsf{T}}GB & G - V^{\mathsf{T}}GV \end{bmatrix} = 0.$$

Many examples of these methods are known and their behaviour is now well understood, both theoretically and experimentally. The focus is now on deriving high order methods in the anticipation that they will provide accurate and efficient integration schemes for mechanical and other problems. One of the starting points is an analysis of the order conditions (Butcher, J., Imran G.,Order conditions for G-symplectic methods, BIT, DOI 10.1007/s10543-014-0541-x (2015.)). It was shown that the order conditions are related to unrooted trees in a similar way to what is known for symplectic Runge–Kutta methods (Sanz-Serna J. M., Abia L., Order conditions for canonical Runge-Kutta schemes, SIAM J. Numer. Anal. 28, 1081–1096 (1991)). Starting from the order conditions, simplifications can be made by assuming time-reversal symmetry and enhanced stage order. Even after high order methods have been found, the construction of suitable starting schemes is an essential step before working algorithms can be built.

Linearly implicit methods for a class of degenerate convection-diffusion problems

Raimund Bürger, Stefan Diehl (Lund University, Sweden), Camilo Mejías (Universidad de Concepción, Chile) , *Tue 17:30 R 3.07*

This contribution is concerned with semi-implicit numerical schemes for the discretization of strongly degenerate parabolic equations of the type

$$u_t + f(u)_x = A(u)_{xx}, \quad A(u) = \int_0^u a(s)\,\mathrm{d}s, \tag{1}$$

posed on some finite x-interval along with initial and boundary conditions, and where the function a is piecewise continuous and satisfies $a(u) \geq 0$ for all u. In particular, $a(u) = 0$ is possible on u-intervals of positive length, so (1) may turn into a first-order hyperbolic conservation law where the location of the type-change interface is unknown a priori. Thus, solutions of (1) are in general discontinuous. Consequently, the well-posedness theory and numerical analysis of (1) are based on the framework of entropy (weak) solutions.
Applications of (1) include a model of sedimentation of suspensions in mineral processing and wastewater treatment [4, 5] (after suitable simplifications). The efficient numerical solution of (1) is therefore of substantial theoretical and practical interest. Explicit monotone difference approximations to (1) go back to [7], are easily implemented, and provably converge to the entropy solution. However, the restrictive CFL condition makes explicit schemes unacceptably slow. An alternative are nonlinearly implicit semi-implicit schemes that treat the diffusive term implicitly and allow for a less restrictive CFL condition. Such methods are also supported by a convergence theory [2] and have turned out to be more efficient than their explicit counterparts

in terms of error reduction versus CPU time [6]. However, their implementation requires the use of nonlinear solvers (e.g., Newton-Raphson method) which may fail to converge.
It is the purpose of this contribution to propose linearly implicit methods for the approximation of solutions of (1) as an alternative. These methods go back to Berger et al. [1], are based on a particular separate discretization of the diffusive term, enjoy a favorable CFL condition, and require the solution of a linear system at every time step, which is an advantage in practical applications. Preliminary results [3] show that these methods are competitive with the known explicit and nonlinearly implicit schemes in terms of accuracy and efficiency. It is demonstrated that these schemes are monotone, which is the key property required to demonstrate convergence to an entropy solution. The full convergence analysis is currently in preparation.

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Splitting methods for the Schrödinger equation with vector potential

Marco Caliari, Alexander Ostermann and Chiara Piazzola, *Tue 14:00 R 3.07*

This talk is about splitting methods for the Schrödinger equation with vector potential

$$i\partial_t u = \frac{1}{2}(i\nabla + A)^2 u + Vu,$$

where u is the quantum mechanical wave function, A the vector potential and V the scalar potential. After imposing the Coulomb gauge, the equation can be split into the kinetic part, the potential part and a pure convection part. For the latter, different semi-Lagrangian methods, based on the method of characteristics, are analyzed and compared, in particular from the point of view of mass conservation.

Avoiding order reduction when integrating nonlinear Schroedinger equation
Begoña Cano, *Thu 17:30 R 3.07*

In this talk a technique will be given to integrate nonlinear Schrödinger equation with nonhomogeneous Dirichlet boundary conditions using Strang method for the time integration. We will show that this procedure is second-order convergent. Moreover, we will state how to conserve the symmetry of the method although that will not assure a better long term behaviour.

Geometric methods for differential equations in applications of computer animation
Elena Celledoni, M. Eslitzbichler, *Mon 10:40 R 3.07*

Motion of virtual characters in video games is usually represented using a skeletal animation. The underlying skeleton consists of bones connected by joints. Animation of virtual characters relies on collections of data obtained by recording the movements of actors. The data consists of curves tracking the positions of the bones throughout the motion, and these curves can be processed by mathematical methods to produce new motions. In practice, the data consists of curves in $SO(3)^N$, where N is the number of bones in the skeleton. In the existing literature these curves are represented using Euler angles and neglecting the underlying Lie group structure, [7], [2]. We here report on the results we obtained by appropriately including the underlying geometric structure in the mathematical models and their numerical discretizations. The intrinsic geometric formulation is robust and works very well in problems of motion blending and curve closing, where earlier the same performance could be obtained only by using ad hoc strategies, e.g. keeping track of carefully chosen feature points along the curves.
We will briefly discuss how techniques from shape analysis on Lie groups can be successfully applied to computer animation treating character animations as points in an infinite dimensional manifold. This manifold is in fact an infinite dimensional Lie group where we are interested in computing distances and geodesics. As expected by smimilar experience in the case of shapes on Euclidean spaces [1], the choice of metrics on these infinite dimensional manifolds are a trade off between ease of computation and the needs dictated by the application at hand. In particular we will discuss elastic metrics and their relation to the L_2 norms for curves on the Lie algebra. Furthermore the extension to higher order Sobolev type norms will be considered. Working with curves of animation data, we are interested in particular in two mathematical problems: computing geodesics on the infinite dimensional Lie group; and projecting open curves onto the submanifold of closed curves. We will discuss the modeling of these problems by designing appropriate gradient flows. We will finally address the numerical discretization of these PDEs and show the advantages of the proposed approach in animation of character motion.

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Error Control in Solving Differential Algebraic Equations of High Order

Elena Chistyakova, V.F. Chistyakov, *Tue 16:30 R 1.04*

Consider a linear system of ordinary differential equations

$$A_k(t)x^{(k)}(t) + A_{k-1}(t)x^{(k-1)}(t) + \ldots + A_0(t)x(t) = f(t),\ t \in T := [0,1] \tag{1}$$

where $A_i(t)$ are $(n \times n)$-matrices, $i = \overline{1,k}$, $x(t)$ and $f(t)$ are the desired and the given vector-functions, correspondingly, with the initial data

$$x^{(j)}(0) = a_j,\ j = \overline{0,k-1}, \tag{2}$$

It is assumed that the input data is smooth enough and the following condition holds

$$\det A_k(t) = 0\ \forall t \in T. \tag{3}$$

In this talk, we introduce the notion of an index for systems (1) with the condition (3). Then, in terms of matrix polynomials, we obtain a criterion for the index of (1) not to exceed k. Provided that the criterion is fulfilled, we consider a difference scheme for solving (1),(2) and demonstrate that for the perturbation

$$\tilde{f}(t) = f(t) + \mu(t), \|\mu(t)\|_{\mathbf{C}} \leq \delta,$$

where δ is a small real number, the function of error depends both on the integration step and the level of perturbation.

This work has been supported by the Russian Foundation for Basic Research, grant No. 15-01-03228-a.

PDE pricing of financial instruments with stochastic correlation

Christina Christara, Nat Chun-Ho Leung, *Thu 14:00 R 1.04*

Correlation between financial quantities plays an important role in pricing financial derivatives. Existing popular models assume that correlation either is constant, or exhibits some deterministic behaviour. However, market observations suggest that correlation is a stochastic process.

We are interested in deriving the Partial Differential Equation (PDE) problems for pricing financial derivatives assuming stochastic correlation, solving them by accurate and efficient numerical methods, and studying the effect of the model to the prices. We present the PDE, the numerical solution, and comparison of the PDE results to a Monte-Carlo simulation. We also discuss the relevant numerical challenges.

Multi-symplectic discretisation of wave map equations
David Cohen, Olivier Verdier, *Thu 14:00 R 3.07*

We present a new multi-symplectic formulation of constrained Hamiltonian partial differential equations, and we study the associated local conservation laws. A multi-symplectic discretisation based on this new formulation is exemplified by means of the Euler box scheme. When applied to the wave map equation, this numerical scheme is explicit, preserves the constraint and can be seen as a generalisation of the SHAKE algorithm for constrained mechanical systems. Furthermore, numerical experiments show excellent conservation properties of the numerical solutions.

Trigonometrically fitted numerical methods for reaction-diffusion problems
Raffaele D'Ambrosio, Angelamaria Cardone, Beatrice Paternoster, *Mon 16:10 R 1.27*

It is the purpose of this talk to present novel finite difference schemes for reaction-diffusion problems, which generate traveling waves as fundamental solutions. Such problems have been widely employed as mathematical model for life science phenomena exhibiting the generation of periodic waves along their dynamics (e.g. cell cycles, frequently behaving if they are driven by an autonomous biochemical oscillator; intracellular calcium signalling, since calcium shows many differrent types of oscillations in time and space, in response to various extracellular signals).
The periodic character of the problem suggests to propose a numerical solution which takes into account this behavior, i.e. by tuning the numerical solver to accurately and efficiently follow the oscillations appearing in the solution, since classical numerical methods would require the employ of a very small stepsize to accurately reproduce the dynamics.
For this reason, we propose an adaptation of classical finite difference schemes which will take into account the qualitative nature of the solutions, in a problem-oriented setting. We may say that a three-fold level of adaptation to problem will be carried out: along time and space, by suitable semidiscretization with problem-based finite differences and analog time solvers for the semi-discrete problem, and along the problem by taking into account the peculiarity of the vector field, for instance by proposing suitable novel implicit-explicit schemes.
The corresponding numerical method will depend on variable coefficients, which are functions of the parameters characterizing the solution (e.g. the frequency of the oscillations). A theoretical study of the error associated to the overall numerical scheme gives us the possibility to propose an accurate estimate of the unknown parameters on which the numerical method depends.
Practical constructive aspects and accuracy analysis will be treated, as well as numerical experiments showing the effectiveness of the approach will be provided.

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On the construction of explicit exponential-based schemes for stiff Stochastic Differential Equations
Hugo de la Cruz, *Mon 17:00 R 1.26*

Currently there are diverse discretization methods for stochastic differential equations (SDEs) having in common the explicit use of exponentials in obtaining an approximate solution. However, the majority of them have been designed for semi-linear SDEs and hence, in different cases, their numerical implementation is not always feasible or is of limited use when applied to general stiff SDEs. In this work we consider a computational feasible alternative for constructing stable exponential-based numerical schemes for the computational integration of multidimensional non-autonomous stiff SDEs. A comparative study with other exponential methods is presented, showing the benefits of the schemes proposed in relation to these ones.

High order finite difference schemes for obstacle problems
Kristian Debrabant, Olivier Bokanowski, *Tue 11:40 R 1.04*

New finite difference schemes based on Backward Differentiation Formulae in time are proposed for the approximation of one-dimensional non-linear diffusion equations with an obstacle term. Stability estimates are obtained for one of the schemes. Numerical experiments illustrate the convergence of the proposed schemes, and they are applied to the American option problem in mathematical finance.

Locally implicit and implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media
Stéphane Descombes, Lanteri, Moya, Christophe, *Thu 8:30 R 3.07*

We are concerned with the numerical simulation of electromagnetic wave propagation in dispersive media i.e. when the electromagnetic material characteristics depend of the frequency. In the time-domain, this translates in a time dependency of these parameters that can be taken into account through an additional differential equation for, e.g, the electric polarization, which is coupled to the Maxwell's equations which is a PDE system.
We propose and analyze two efficient time integration methods for dealing with grid induced stiffness when using non-uniform (locally refined) meshes and use these methods to study the interaction of electromagnetic waves with biological tissues.
On the one hand the first method is a fully implicit method in time with a hybridizable discontinuous Galerkin method to decrease the number of degrees of freedom and on the other hand the second method is a locally implicit method blending the second order leap-frog scheme and the second order Crank-Nicolson scheme. A particular attention is payed to show that this method retains its second-order ODE convergence under stable simultaneous space-time grid refinement $\Delta t \backsim h$, $h \to 0$ towards the exact PDE solution.
This is a joint work with Stéphane Lanteri, Ludovic Moya and Alexandra Christophe, Inria research centre, Sophia Antipolis Méditerranée.

On the numerical solution of generalized Ostrovsky equations
Angel Duran, *Thu 16:30 R 3.07*

Presented in this talk is a numerical study of solitary waves of the Ostrovsky equation and generalized versions. From the point of view of the numerical analysis, the talk is focused on the improvement of the methods to generate traveling waves, on the performance of experiments

of perturbations of the traveling waves and on the analysis of convergence of a fully discrete code considered to make these experiments. From the experimental point of view, the study attempts to shed some light on the dynamics of these waves in the classical and generalized versions of the equation, for classical and generalized solitary waves and for small and large perturbations.

High-order compact finite difference schemes for option pricing in stochastic volatility models

Bertram Düring, *Thu 17:00 R 1.04*

We present high-order compact finite difference schemes for option pricing in stochastic volatility models. The schemes are fourth-order accurate in space and second-order accurate in time. We discuss analytical results on the (unconditional) stability and present results of numerical experiments.

Overcoming order reduction in diffusion-reaction splitting

Lukas Einkemmer, Alexander Ostermann, *Tue 16:00 R 3.07*

For diffusion-reaction equations employing a splitting procedure is attractive as it reduces the computational demand and facilitates a parallel implementation. Moreover, it opens up the possibility to construct second-order integrators that preserve positivity independent of the time step size used. However, for boundary conditions that are neither periodic nor of homogeneous Dirichlet type order reduction limits its usefulness. In the situation described the Strang splitting procedure is no more accurate than Lie splitting.
In this talk, we introduce a modified Lie/Strang splitting procedure that, while retaining all the favorable properties of the original method, does not suffer from order reduction. That is, the modified Strang splitting is second order accurate in time. Furthermore, for time independent boundary conditions the required modification can be precomputed and thus no additional computational cost is incurred.
We demonstrate our results by presenting numerical simulations in one and two space dimensions with inhomogeneous and time-dependent Dirichlet boundary conditions. In addition, a mathematically rigorous convergence analysis is presented that explains the results observed in the numerical simulations.
This talk is based on *L. Einkemmer, A. Ostermann. Overcoming order reduction in diffusion-reaction splitting. Part 1: Dirichlet boundary conditions. To appear in SIAM J. Sci. Comput., 2015*

Consistent initialization of DAEs using a specific minimum-norm correction

Diana Estévez Schwarz, René Lamour, *Thu 11:05 R 1.04*

We present a new approach to compute consistent initial values and consistent Taylor series for higher index DAEs. The consistent Taylor series result from the constraints and a specification that, for given values, minimizes the correction for the differentiated components and can be described using suitable orthogonal projections. The constraints and the projections are obtained by an analysis of the derivative array provided by automatic differentiation. Computing these projections we simultaneously check whether singularities appear. Our prototype implemented in Python is demonstrated for linear and nonlinear higher index DAEs of moderate size. We place particular emphasis on the differences to methods that are based on a structural analysis.

Accelerating convergence of Generalized Picard Iterations

Boris Faleichik, Ivan Bondar, *Thu 11:05 R 3.07*

Generalized Picard Iterations (GPI) is a family of iterated Runge–Kutta methods aimed to matrix-free solution of stiff systems [1]. Originally based on artificial time integration these methods can be regarded as a special iterative processes for solving nonlinear systems during the implementation of implicit RK methods. The convergence rate of GPI in case of linear ODE system $y' = Jy$, where J is a square matrix with spectrum from left complex half-plane, is determined by the magnitude of $\rho(J)\rho(J^{-1})$.
In the talk we are going to discuss some properties of GPI as a representatives of explicit RK family and suggest a way of accelerating the convergence of GPI by means of damping the components of residual vector corresponding to small eigenvalues of J. Some numerical experiments justifying the efficiency of suggested approach will be presented.

[1] B. Faleichik, I. Bondar, V. Byl: Generalized Picard iterations: A class of iterated Runge–Kutta methods for stiff problems. Journal of Computational and Applied Mathematics, Volume 262, 15 May 2014, Pages 37-50, ISSN 0377-0427, http://dx.doi.org/10.1016/j.cam.2013.10.036.

Model Reduction of Quadratic Bilinear Descriptor Systems using Parametric Reduction Techniques with Error Estimation

Lihong Feng, Mian Ilyas Ahmad, Peter Benner, *Mon 14:25 R 1.27*

We propose an interpolation based projection framework for model reduction of quadratic bilinear descriptor systems. The approach represents the bilinear part of the original quadratic bilinear descriptor system into a linear system with affine parameter dependance and identifies projection matrices from the linear parametric system. Two different approaches are used to map the bilinear system into a linear parametric system. One is based on simply treating the input as a parameter and the other is linked to the selection of weights in the Volterra series interpolation [1]. The main purpose of mapping a bilinear system as a linear parametric system is to utilize the error estimation techniques derived recently in [2]. This allows us to select a good choice of interpolation points and parameter samples for the construction of the projection matrices by employing the error estimator in a greedy type framework. The results are compared with the standard quadratic bilinear projection methods [3, 4] and it is observed that the approximations through the proposed methods are comparable to the standard method. An advantage of the proposed method is that the computations associated with the quadratic term in the construction of the projection matrices can be saved.

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Hydrodynamic force elements: A PDAE approach

Robert Fiedler, Martin Arnold, *Tue 11:40 R 1.27*

The simulation of mechanical systems results often in multi-component phenomena with different time scales or different solution strategies which influence each others problem characteristics. In our case we have a flexible multibody system coupled with special force elements. The modelling of elastohydrodynamic bearings in combustion engines leads to a coupled system of partial differential algebraic equations, which is represented by a flexible multibody system model of crankshaft and bearing and by the Reynolds equation that describes the non-linear effects in the fluid film. The hydrodynamic forces depend strongly on the position and the elastic deformation of crankshaft and bearing shell. Therefore a fine spatial discretisation is needed.
The influence of the spatial discretisation on accuracy and numerical effort will be discussed. Since a fine one substantially slows down the numerical solution, we propose an asymptotic analysis with methods from singular perturbation theory to speed-up time integration. The interplay of this semi-analytical approach with index reduction techniques for the multibody part is studied for the fourbar test problem.
Numerical tests for a realistic benchmark problem illustrate the advantages of this approach.

Enforcing power-law kinetic energy spectra under conservative discretizations of fluids

Jason Frank, Keith Myerscough (Leuven) and Ben Leimkuhler (Edinburgh),
Thu 15:00 R 3.07

As noted by Ascher and McLachlan, inviscid fluid fluid dynamics presents a challenge to geometric integration. Firstly, although continuum formulations of inviscid fluid dynamics possess a well-known Poisson structure, it has proven particularly challenging to preserve such structure under discretization. Secondly, although the viscous length scale encountered in practical applications such as large scale atmosphere and ocean flows is well below the grid scale, justifying an inviscid assumption, the effect of viscous dissipation on these scales implies a power law distribution of kinetic energy in the presence of large scale forcing. Such a kinetic energy distribution will not be observed when energy and enstrophy preserving schemes are used. Consequently, in practice some form of artificial viscosity is typically employed. In this talk we describe a method for preserving an observed steady state kinetic energy spectrum by applying Nosé-Hoover thermostats to energy shells in Fourier space. The new technique is computationally cheap and leads to only weak perturbation of large scale dynamics, point-wise autocorrelation functions, and ensemble dispersion.

Algebraic Variables in Higher Index DAEs

Claus Führer, *Wed 9:40 R 3.07*

Higher index differential algebraic equations are ill-posed problems [3, 426]. Nevertheless one is attempted to solve them with DAE software like Sundial's BDF code IDA, [2]. In the index-3 case the application of variable step-size variable order codes requires a special treatment of algebraic variables. In the talk we review the definition of these variables and the problems which arise, when these variables are not treated separately in the error control. Numerical tests of various implementation alternatives within the ODE software wrapper Assimulo [1] will be presented.

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Some families of W-methods to stabilize standard explicit Runge-Kutta methods for stiff problems

Severiano Gonzalez-Pinto, D. Hernandez-Abreu, S. Perez-Rodriguez, *Mon 16:10 R 1.04*

A technique to stabilize standard explicit Runge-Kutta methods, by converting them in W-methods, is proposed. The main point to get the associated family of W-methods for a given explicit Runge-Kutta method is to use some smart simplification to reduce the large number of order conditions that must be sasitsfied for a W-method to reach a pre-fixed order (8 order conditions for order three, 21 conditions for order four, 58 conditions for order five, see e.g. Hairer and Wanner [1, Chap. IV.7]).
Based on this idea, for any given 4-stage explicit Runge-Kutta method, two uni-parametric families of third order W-methods are obtained. The free parameter (namely θ) can be used to increase the stability regions of the associated W-methods. In fact, it is possible to find L-stable ROW-methods (i.e., Rosenbrock-Wanner methods) in the family for some specific values of the parameter θ.
The new family of W-methods are also equiped with the splitting provided by the Approximate Matrix Factorization (AMF) [3], which converts the W-method in some kind of ADI-method (Alternating Direction Implicit method, see e.g. [2, Chap. IV]). This kind of methods is mainly used to solve large time-dependent PDE systems (2D or 3D spatial variables) discretized in space by using finite differences or finite volumes. For the case of d-splittings ($d = 1, 2, 3$), some stability properties of the family of W(AMF)-methods are analyzed.
Some numerical experiments, by applying the W(AMF)-methods, on a few interesting stiff problems coming from PDE discretizations are presented. The goal is to illustrate the relevance of the stability properties and the order reached by the methods and to see how they perform when compared with others proposed in the literature.

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Resolvent Krylov subspace approximation to C_0-semigroups and their discretisations

Volker Grimm, *Fri 12:10 R 3.07*

The recent success of exponential integrators and splitting methods for evolution equations triggers a very strong demand for efficient approximations of C_0-semigroups and related operator/matrix functions applied to given initial data. For fine space discretisations, this corresponds to the approximation of a matrix exponential for a huge and sparse matrix times a vector. An important finding is, that methods that work for the approximation of the semigroup in the continuous case render approximations that are independent of the space discretisation in the discretised case. These methods are therefore more appropriate for large problems resulting from a fine spatial grid. In time integration, this is nothing but the observation that certain implicit time-integration schemes are much more efficient for large stiff systems of ODEs. Despite the fact that rational approximations are known to achieve faster convergence rates in this case, the PDE community often sticks to approximations like the backward Euler and the Crank-Nicolson method that are comparatively easy to compute for fine space discretisations of evolution equations. Higher order Runge-Kutta methods and higher order rational approximations are deemed too costly and too cumbersome to implement.
A fascinating new finding is that there are methods that converge faster than the backward Euler and the Crank-Nicolson method for approximately the same computational cost. In fact, the programs computing the resolvents in the backward Euler method or the Crank-Nicolson scheme can be reused without essential changes. The idea is to approximate the semigroup with infinitesimal generator A in the resolvent Krylov subspace

$$\mathcal{K}_m((\gamma I - A)^{-1}, b) = \mathrm{span}\{b, (\gamma I - A)^{-1}b, \ldots, (\gamma I - A)^{-m+1}b\}, \qquad \gamma > 0\,.$$

The corresponding Krylov subspace method automatically converges faster for smoother initial data b. Moreover, the convergence is independent of the grid in space for the discretised evolution equation. No method at comparable computational cost is known that shares these favourable properties. The obtained results will be illustrated by numerical experiments with different space discretisations.

High-Order Explicit Local Time-Stepping Methods For Wave Propagation

Marcus Grote, Julien Diaz, Michaela Mehlin, Teodora Mitkova, *Tue 9:20 R 3.07*

In the presence of complex geometry, adaptivity and mesh refinement are certainly key for the efficient numerical simulation of wave phenomena. Locally refined meshes, however, impose severe stability constraints on any explicit time-marching scheme, where the maximal time-step allowed by the CFL condition is dictated by the smallest elements in the mesh. When mesh refinement is restricted to a small subregion, the use of implicit methods, or a very small time-step in the entire computational domain, are very high a price to pay.
Explicit local time-stepping schemes (LTS) overcome the bottleneck due to a few small elements by using smaller time-steps precisely where the smallest elements in the mesh are located. For wave equations without damping, leap-frog based LTS methods lead to high-order explicit LTS schemes, which also conserve the energy. For damped wave equations, Adams-Bashforth or Runge-Kutta based LTS methods lead to efficient LTS schemes of arbitrarily high accuracy. When combined with a finite element discretization in space with an essentially diagonal mass matrix, the resulting time-marching schemes are fully explicit and thus inherently parallel. Numerical experiments with continuous and discontinuous Galerkin finite element discretizations validate the theory and illustrate the usefulness of these local time-stepping methods.

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

Tanja Göckler, Volker Grimm, *Mon 16:10 R 1.26*

Time integration methods for stiff systems of ordinary differential equations often involve the action of a matrix function $f(A)$ on a vector b. The matrix A typically arises from a spatial discretization of a partial differential equation and has a huge field-of-values lying somewhere in the left complex half-plane. Refining the discretization, the norm of A becomes very large. Therefore, the efficient and reliable approximation of $f(A)b$ with a convergence rate independent of $\|A\|$ is a current topic of interest and research.
Recent advances have shown that rational Krylov subspace methods have a great advantage over standard Krylov subspace methods in this case. We thus approximate $f(A)b$ in the shift-and-invert Krylov subspace

$$\operatorname{span}\{b, (\gamma I - A)^{-1}b, (\gamma I - A)^{-2}b, \ldots, (\gamma I - A)^{-(m-1)}b\}\,, \quad \gamma > 0\,.$$

By transforming the left complex half-plane to the unit disk, we obtain convergence results that depend on the smoothness of a transformed function on the boundary of this disk. In particular, we establish sublinear error bounds for the matrix φ-functions being of central importance in exponential integrators. A remarkable aspect of our analysis is the independence of the error from the norm of the considered discretization matrix.
Moreover, we discuss suitable choices for the shift γ in the shift-and-invert Krylov subspace and illustrate our results by several numerical experiments.

On the numerical solutions of linear delay differential-algebraic equations

Phi Ha, *Mon 14:25 R 1.26*

Differential-algebraic equations (DAEs) have an important role in modeling practical systems, wherever the system needs to satisfy some algebraic constraints due to conservation laws or surface conditions. On the other hand, time-delays occur naturally in various dynamical systems, both physically, when the transfer phenomena (energy, signal, material) is not instantaneous, and artificially, when a time-delay is used in the controller. The combination of differential-algebraic equations and time-delays leads to a new mathematical object: "delay differential-algebraic equations (Delay-DAEs)", which is a source of many complex behavior.
In this talk, we address the computational problem for numerical solutions to general linear Delay-DAEs. First, we discuss the characteristic properties, which have not been mentioned in prior studies of numerical solutions to Delay-DAEs. Then, we propose an algorithm, which extends the classical (Bellman) method of steps, to determine the solution of general linear Delay-DAEs. The properties of the algorithm are studied and the theoretical results are illustrated with numerical examples.

On Coupled MOR-Multirate Schemes: Derivation and Error Analysis

Christoph Hachtel, Andreas Bartel, Michael Günther, *Mon 15:15 R 1.27*

A system of ODEs that fits well for multirate integration schemes often consists of at least one large scale subsystem with slow dynamic behaviour compared with the remaining subsystems. Such systems naturally occur in multiphysics coupled problems. It is an intuitive idea to apply a model order reduction (MOR) to the large scale, slow changing subsystem to save computational effort. Since the subsystems are coupled one has to apply MOR methods for coupled systems like in [1].

In this talk we will present a suitable definition of a reduced order, slow changing subsystem. We will focus on the definition of the coupling interface to the other subsystems so that the input-output behaviour of the reduced order slow subsytem and the resulting complete ODE system is well approximated.

A model order reduction of one or more subsystems will cause additional errors in a time domain simulation. Furthermore the multirate integration scheme requires some special error investigation because different time schales for different subsystems are used [2]. We will provide an extension to the existing error analysis for multirate θ-methods that includes the error of the model order reduction of the slow changing subsystem.

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Lie Group time integration of a nonlinear geometrically exact Cosserat rod model

Stefan Hante, Martin Arnold, *Mon 14:50 R 3.07*

Guided by the analysis in [1], we present a nonlinear geometrically exact Cosserat rod model, that can be obtained by applying a Lie group variational principle in time and space for linear, viscoelastic material behaviour. The rotational components are represented using unit quaternions $p \in \mathbb{S}^3$ (Euler parameters). By adding constraints, a second order partial differential algebraic equation with solution in the Lie group $\mathbb{R}^3 \times \mathbb{S}^3$ is obtained. Following the method of lines the equation is semidiscretized in space using a staggered grid (see [2]), yielding a second order differential algebraic equation of index three with solution in the Lie group $(\mathbb{R}^3 \times \mathbb{S}^3)^n \times \mathbb{R}^3$.

A general purpose Lie group generalized-α solver is then applied in order to solve the index-three DAE either directly or using a stabilized index-two formulation. As a test scenario we use the 'flying spaghetti' benchmark problem, in which forces and moments are applied to an unhitched straight rod, resulting in three-dimensional rotations.

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Improvement of dimension splitting methods

Tobias Hell, Alexander Ostermann, *Tue 15:00 R 3.07*

A *dimension splitting method* may suffer from a severe order reduction when applied to an inhomogeneous evolution equation of the form

$$u'(t) = \mathcal{L}u(t) + g(t), \quad u(0) = u_0$$

on $L^2(\Omega)$, where $\Omega = (0,1)^2$ and $\mathcal{L} = \partial_x(a\partial_x) + \partial_y(b\partial_y)$ is an uniformly strongly elliptic operator with $a, b \in \mathcal{C}^2(\overline{\Omega})$ and $D(\mathcal{L}) = H^2(\Omega) \cap H_0^1(\Omega)$. For instance, the *exponential Strang splitting* involving the split operators $\mathcal{A} = \partial_x(a\partial_x)$ and $\mathcal{B} = \partial_y(b\partial_y)$ converges, in general, with order $5/4 - \varepsilon$ in time for arbitrarily small $\varepsilon > 0$ due to arising corner singularities in the derivatives of the solution. However, one might modify the problem such that the full convergence order of 2 is achieved.
In this talk, regularity results for the corresponding stationary problem on $(0,1)^d$ with $d > 2$ are presented and their consequences for the improvement of dimension splitting methods in higher dimensions are discussed.

High-Order-Compact ADI schemes for pricing basket options in the combination technique

Christian Hendricks, Christof Heuer, Matthias Ehrhardt, Michael Günther, *Thu 17:30 R 1.04*

In this work we combine high order compact (HOC) and alternating direction implicit (ADI) schemes for pricing basket options in a sparse grid setting. HOC schemes exploit the structure of the underlying partial differential equation to obtain a high order of consistency while employing a compact stencil. In the time discretisation we propose an efficient ADI splitting to derive a stable scheme. The combination technique is used to construct the so called *sparse grid* solution, which leads to a significant reduction of necessary grid points and therefore to a lower computational effort.

Convergence analyses of the Peaceman–Rachford and Douglas–Rachford Schemes for Semilinear Evolution Equations

Erik Henningsson, Eskil Hansen, *Tue 14:30 R 3.07*

We analyse convergence of the Peaceman–Rachford and Douglas–Rachford time discretization schemes for semilinear evolution equations. The vector field of the equation is assumed to be the sum of two unbounded dissipative operators. A setting in which the Peaceman–Rachford and Douglas–Rachford splitting methods exhibit excellent stability properties.
Convergence orders are given when the vector field is the sum of a linear and a nonlinear operator. The full range of possible orders (including convergence without order) are given depending on the regularity of the solution. In contrast to previous convergence order studies we do not assume Lipschitz continuity of the nonlinear operator.
Taking the analysis further we combine these temporal discretizations with convergent spatial discretizations. We do this in the setting of linear evolution equations and prove optimal, simultaneous, space-time convergence orders. We observe how the results profit from the excellent local error structures of the Peaceman–Rachford and Douglas–Rachford schemes.
Applications include semilinear reaction-diffusion equations. The convergence orders are illustrated by numerical experiments.

Related articles:
E. Hansen and E. Henningsson.
A convergence analysis of the Peaceman–Rachford scheme for semilinear evolution equations.
SIAM J. Numer. Anal., 51(4):1900–1910, 2013.
E. Hansen and E. Henningsson.
A full space-time convergence order analysis of operator splittings for linear dissipative evolution equations.
Preprint, Lund University, `http://www.maths.lth.se/na/staff/erik/`, 2014.

High-order accurate methods for fractional differential equations

Jan Hesthaven, *Mon 11:30 R 3.07*

Fractional calculus is emerging as a popular tool for the modeling of a variety of problems across the sciences and engineering. However, even though fractional calculus is as old as classic calculus, the development of accurate and efficient computational tools is substantially less advanced in this area.
In this presentation, we first provide some background on fractional calculus, focusing on initial value problems and the problems being particular to such models. We then discuss the development of high-order accurate methods for solving fractional differential equations, illustrated with some examples, and conclude with a brief discussion of some of the many open problems.

High-order compact schemes for parabolic problems with mixed derivatives in multiple space dimensions with application to basket options

Christof Heuer, Bertram Düring, *Tue 12:05 R 1.04*

In this work we present a high-order compact finite difference approach for a class of parabolic partial differential equations with time and space dependent coefficients as well as with mixed second-order derivative terms in n spatial dimensions. We derive general conditions on the coefficients which allow us to obtain a high-order compact scheme which is fourth-order accurate in space and second-order accurate in time. As an application example we consider the pricing of European Power Put Options in the multidimensional Black-Scholes model for two and three underlying assets. Due to the low regularity of typical initial conditions we employ the smoothing operators of Kreiss et al. to ensure high-order convergence of the approximations of the smoothed problem to the true solution.

Classical and novel analysis of positive invariance and strong stability preserving time integrators

Zoltán Horváth, *Fri 11:20 R 3.07*

The state space of time dependent differential equations (ODEs, PDEs, DAEs) of applied mathematics often posses positively invariant subsets (which are subsets of the state space from which trajectories do not escape from the subset forward in time if they initiate from there) and have functionals that are decreasing along the solutions. For examples of positively invariant sets we refer to the positive orthant in many applications (for concentration like variables at modelling chemical or biological diffusion-advection-reaction systems) and regions of feasibility for the Euler equations of gas dynamics. Total variation, entropy, Lyapunov functions form some examples for functionals that are decreasing along the solutions of some PDEs or related semidiscretized ODEs modelling transport processes.

Under the numerical time discretization methods these properties are natural and in many cases necessary to be preserved (e.g. negative concentrations or increasing entropy have no physical meaning, furthermore diminition of total variation is a pillar of ensuring convergence of numerical methods in gas dynamics). However, it is not trivial at all what numerical methods and what time step sizes imply the preservations of invariant sets and decreasing functionals along numerical solutions; accuracy and stability of the numerical method together do not imply this. In the last decades an analysis is developed for general numerical time stepping schemes to determine the suitable time steps that fulfill the requirements of the preservation properties. The suitable step sizes are characterized in terms of the scheme coefficients and some simple characteristics of the problem. These are, respectively, the absolute monotonicity radius of the scheme and the largest step size under which the Explicit Euler method has the preservation property. Thus this classical analysis works under the condition that the Explicit Euler method fulfils the preservation property.
In this lecture we present the classical analysis with references. In addition, we shall give some examples when this can be applied to nontrivial situations (e.g. for semidiscretized hyperbolic conservation laws). However, some simple particular examples show that the numerical preservation property is present but the classical analysis can be applied since the Explicit Euler method does not respect the preservation property for any step sizes. Examples for these include, among others, FEM semidiscretizations of the heat equations, spectral difference semidiscretization for the advection equation, high order WENO schemes for advection and DAEs for transport. We shall present another condition on the problem and some different terms of the scheme coefficients that guarantee the numerical preservation properties for implicit methods. We shall apply them in the examples above to show the applicability of the novel analysis.

Structure preserving discretization of port-Hamiltonian systems

Eirik Hoel Høiseth, Elena Celledoni, *Thu 10:40 R 1.27*

Port-Hamiltonian systems are a generalization of Hamiltonian systems that allow for the inclusion of inputs and outputs. Port-Hamiltonian systems offer a simple paradigm for modelling complex physical systems by the energy- consistent interconnection of a (possibly large) number of simple subsystems. This approach can also be viewed as a technique for control design. The structure-preserving (and in particular passivity-preserving) integration of this generalization of Hamiltonian systems is of interest both from a theoretical perspective, and in engineering applications. We present some results on structure preserving discretization of port-Hamiltonian systems.

Stabilized Extended One-Step Schemes for Stiff and Non-Stiff Delay Differential Equations

Fatma Ibrahim, Fathalla A. Rihan and Stefan Turek, *Mon 17:25 R 1.26*

The importance of delay differential equations (DDEs), in modelling mathematical biological, engineering and physical problems, has motivated searchers to provide efficient numerical methods for solving such important type of differential equations. Most of these types of differential models are stiff, and suitable numerical methods must be introduced to simulate the solutions. In this paper, we provide a reliable computational technique, based on a class of extended one-step methods for solving stiff and non-stiff DDEs. The efficiency and stability properties of this technique are studied. Numerical results and simulations are presented to demonstrate the effectiveness of the methodology.

Convergence of ADI schemes for two-dimensional convection-diffusion equations with mixed derivative term

Karel in 't Hout, Maarten Wyns, *Thu 16:00 R 1.04*

Alternating Direction Implicit (ADI) schemes are well-known in the numerical solution of multidimensional time-dependent partial differential equations (PDEs) arising in financial mathematics. The Craig-Sneyd (CS), Modified Craig-Sneyd (MCS) and Hundsdorfer-Verwer (HV) schemes form three popular ADI schemes. A structural analysis of their fundamental properties, notably convergence, is of main interest. Up to now, however, a rigorous convergence result has only been derived in the literature for the HV scheme and only in the case of one-dimensional PDEs. In this talk we shall present new results revealing that, under natural stability and smoothness conditions, the CS, MCS and HV schemes all possess a temporal order of convergence equal to two, uniformly in the spatial mesh width, whenever they are applied to two-dimensional convection-diffusion equations with mixed derivative term. The obtained convergence results are illustrated by numerical experiments for contemporary stochastic volatility models.

Generalized ROW-Type Methods for Solving Semi-Explicit DAEs of Index-1

Tim Jax, Gerd Steinebach, *Mon 17:25 R 1.04*

Since being introduced in the sixties and seventies, semi-implicit Rosenbrock-Wanner (ROW) methods have become an important tool for the time-integration of ODE and DAE problems. Over the years, these methods have been further developed in order to save computational effort by regarding approximations with respect to the given Jacobian [5], reduce effects of order reduction by introducing additional conditions [2, 4] or use advantages of partial explicit integration by considering underlying Runge-Kutta formulations [1]. As a consequence, there is a large number of different ROW-type schemes with characteristic properties for solving various problem formulations given in literature today.
In order to combine the most relevant ROW-type representations, a new class of methods for computing semi-explicit DAE problems of index-1 is introduced. The generalized formulation covers many well-known ROW-type methods including schemes for problems with additive and partitioned splitting into stiff and non-stiff components. Thus, it enables to take the form of the most advantageous integration strategy with respect to characteristics of a given problem. Satisfying corresponding order conditions, all methods involved can be realized with just one single set of coefficients regarding appropriate approximations with respect to given Jacobian entries. In this context, new order conditions for using non-exact Jacobians when applying ROW methods to DAE problems are introduced by extending the theory of Roche [3].

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The backward error of the Leja method

Peter Kandolf, Marco Caliari, Alexander Ostermann, Stefan Rainer, *Mon 16:35 R 1.26*

The Leja method is a well established scheme for computing the action of the matrix exponential, see [2]. We present a new backward error analysis, see [3], that allows for a more efficient method. From a scalar computation in high precision we predict the necessary number of scaling steps based only on a rough estimate of the field of values or norm of the matrix and the desired backward error. We use the convergence behaviour of the scalar case on ellipses in the complex plane to get a bound for the matrix argument.
We focus on the development of the error estimation and present some numerical experiments to illustrate its behaviour. In comparisons focusing on the amount of matrix-vector products needed for the interpolation we can show that for a wide class of matrices the Leja method saves matrix-vector products in comparison to the Taylor method, see [1].

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Exact PDE close-form solution of the vibrating rectangular nanoplates using nonlocal trigonometric shear deformation plate theory

Korosh Khorshidi, Mohammad Khodadadi, *Thu 11:55 R 1.27*

In this study, exact close form solution for free flexural vibration of rectangular nanoplates presented based on nonlocal trigonometric shear deformation theory, with neglect in-plane displacements of the mid-plane to calculate the local and nonlocal natural frequency. As well nonlocal elasticity theory is employed to investigate effect of small scale on natural frequency of the plate. The novelty of the paper is that the analytical closed-form solution is developed without any use of approximation for a combination of six different boundary conditions; specifically, two opposite edges are hard simply supported and any of the other two edges can be hard simply supported, clamped or free. Governing equations of motion of the plate are derived by using the Hamilton's principle. The present analytical solution can be obtained with any required accuracy and can be used as benchmark. Numerical examples are presented to illustrate the effectiveness of the proposed method compared to other methods reported in the literature. Finally, the effect of boundary conditions, variations of aspect ratios, thickness ratios and small scale parameter on natural frequency parameters and vibration mode sequence are examined and discussed in detail.

Explicit peer methods with variable nodes
Marcel Klinge, R. Weiner, *Mon 17:00 R 1.04*

We consider a special class of explicit general linear methods, explicit peer methods with s stages as introduced in [2] of the form

$$U_{m,i} = \sum_{j=1}^{s} b_{ij} U_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, U_{m-1,j}) + h_m \sum_{j=1}^{i-1} r_{ij} f(t_{m,j}, U_{m,j}),$$
$$i = 1, \ldots, s$$

for the solution of nonstiff initial value problems. In general, these methods require s function calls per step. By using a special structure of the coefficients of the explicit peer method [1], we say an explicit peer method has n_s shifted stages and $s_e = s - n_s$ effective stages, it is possible to reduce the number of function evaluations per step to s_e. This implies for variable step sizes variable nodes, which depend on the step size ratio and the nodes of the previous step. In this talk we present methods with $s = 4, 5, 6$ stages and $n_s = 2, 3$ shifted stages of order $p = s$ (for constant step sizes superconvergent of order $p = s + 1$) which are tested in MATLAB and compared with `ode23` and `ode45`.

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A parallelization approach for the simulation of large scale multibody systems
Michael Klöppel, Martin Flehmig, Andreas Naumann, Volker Waurich, Marcus Walther, Jörg Wensch, *Thu 11:55 R 1.26*

Virtual prototyping plays an important role in the engineering disciplines. The possibility to model and simulate prototypes on a computer instead of building real-world ones saves time and money. Nowadays. engineers can rely on special tools like object oriented modeling languages, e.g., Modelica, to describe their models. These models can be automatically processed and simulated using standard DAE-solvers, like the BDF-code DASSL as well as its newer offsprings DASKR and DASRT. The advantage of this approach is that the practitioners can concentrate themselves on modeling, whereas the numerical intricacies of the simulation are handled by the software. On the other hand, such simulations are usually slower than implementations which are parallelized and optimized by hand.
In this contribution we concentrate on the DASSL-family of solvers and use a parallelism across the system approach. The novelty of this approach is that the parallelization is carried out automatically and does not require any a priori knowledge about the system. In addition, we increase the parallel potential by implementing a modification of the DASSL-code, which was already proposed by M. Arnold et al. for serial speed up. The implemented methods are demonstrated on engineering examples.

Split-explicit methods with a large number of explicit stages
Oswald Knoth, Marco Müller, *Thu 10:40 R 3.07*

Split-explicit methods are a common integration method in numerical weather prediction. They combine two explicit methods to integrate different parts of the right hand side with different time steps. Common combinations are for the slow part Leap-Frog, Runge-Kutta, or Adams-method and for the fast part a Verlet-type integration method. For Runge-Kutta methods as the slow integrator Wensch et.al give a generalization (MIS-method) and analyzed this new method in case of an exact integration of the fast part. To improve the efficiency of the method we propose an optimization strategy to find low order methods (up to order 3) with a large number of explicit stages. The goal is to enlarge the stability region with respect to the number of function evaluations for the large and small steps. Different methods are compared for two-dimensional test examples used in numerical weather prediction.

Optimal second-order diagonally implicit SSP Runge–Kutta methods
Tihamér Albert Kocsis, Adrián Németh, *Wed 9:40 R 1.04*

Optimal Strong Stability Preserving (SSP) Runge–Kutta methods have been widely investigated in the last decade and many open conjectures have been formulated. The iterated implicit midpoint rule has been observed numerically optimal in large classes of second-order methods, and was proven to be optimal for some small cases, but no general proof was known so far to show its optimality. In this talk we show a new approach to analytically investigate this problem and determine the unique optimal methods in the class of second order diagonally implicit Runge–Kutta methods.

Influence of defect between closely placed disks on their capacity
Alexander Kolpakov, S. I. Rakin, *Mon 15:15 R 3.07*

We study influence of defect between closely placed disks on their capacity. The capacity $C(D)$ is defined as minimal value of Dirichlet integral

$$C(D) = \min \int_D |\nabla \phi(x,y)| dxdy,\ \phi \in H_2^1(D),$$

over domain $D = R^2 \setminus D_1 \setminus D_2 \setminus D$. where D_1, D_2 are two closely placed disks, D is a domain between the discs (the model of defect).
We demonstrate that $C(D)$ monotonically decreases when D monotonically increases in the sense of domains inclusion.
Additional information may be obtained from the numerical experiments. Our experiments shows that the capacity $C(D)$ strongly depend on the length of the defect in the direction normal line connecting the centers of the disks and slow depends on the thickness of the defect. This result may be used to develop network models for high contrast densely packing particles imbedding into matrix with defects [1].

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Geometric Integration of Degenerate Lagrangian Systems

Michael Kraus, Omar Maj, Hiroaki Yoshimura, *Thu 11:05 R 1.27*

The talk aims at answering the question of how to derive long-time stable numerical methods for the integration of particle trajectories in fusion plasmas?

In numerical simulations of dynamical systems it is crucial to preserve certain structures of the equations in order to obtain accurate results, especially - but not only - in long-time simulations. Most systems encountered in plasma physics are Hamiltonian and therefore have a rich geometric structure, most importantly symplecticity and conservation of momentum maps. As most of these systems are formulated in noncanonical coordinates, they are not amenable to standard symplectic methods which are popular for the integration of canonical Hamiltonian systems. An alternative route towards the systematic derivation of structure-preserving numerical methods is provided by the Lagrangian frame. The discretisation of the variational formulation leads to so called variational integrators which can be seen as the Lagrangian equivalent to symplectic methods. However, for noncanonical Hamiltonian systems most often the Lagrangian is degenerate. This degeneracy gives rise to instabilities of the variational integrators which need to be overcome in order to make long-time simulations possible.

We will review basic ideas of geometric or structure-preserving numerical integration and introduce the method of variational integrators. The guiding-centre system, a particularly important system from plasma physics, will be used to exemplify the problems which arise for noncanonical Hamiltonian systems with degenerate Lagrangians. We will show how the resulting instabilities of the variational integrators can be eliminated by appropriate projection methods in order to obtain truly long-time stable numerical methods.

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

Patrick Krämer, Katharina Schratz, *Tue 17:00 R 3.07*

Solving the Maxwell-Klein-Gordon (MKG) equation in the non-relativistic limit regime is numerically very delicate as the solution becomes highly oscillatory in time. In order to resolve the oscillations, standard integration schemes require severe time step restrictions.
The idea to overcome this numerical challenge lies in the asymptotic expansion of the solutions, which allows us to filter out the high frequencies explicitly (see [1] for the case of the Klein-Gordon equation).
More precisely, this ansatz allows us to break down the numerical task to solving a non-oscillatory Schrödinger-Poisson system (SP), which can be carried out very efficiently without any additional time step restriction for example by applying splitting methods (cf. [2]). This formally derived non-relativistic limit of the MKG equation has already been studied from an analytical point of view in [3].
In my talk I want to present the ideas of the convergence proof for the MKG equation to the SP system and give some numerical results.

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Embedded Nested Implicit Runge-Kutta Pairs of Gauss and Lobatto Types with Global Error Control for Stiff Ordinary Differential Equations

Gennady Kulikov, *Tue 14:00 R 1.04*

The problem of efficient global error estimation and control is studied in embedded nested implicit Runge-Kutta pairs [1] of Gauss and Lobatto types applied to stiff ordinary differential equations (ODEs). Stiff problems may arise in many areas of application and their accurate numerical solution is an important issue of applied mathematics. The cheap global error estimation designed recently in the mentioned Runge-Kutta pairs can severely overestimate the global error when applied to stiff ODEs [2] and, hence, it reduces the efficiency of those solvers. Therefore we explain here the reason of that error overestimation and show how to improve the mentioned computation techniques for stiff problems. Such modifications not only boost the efficiency of numerical integration of stiff ODEs, but also make the embedded nested implicit Runge-Kutta pairs with the modified global error control far superior the stiff built-in Matlab ODE solvers with only local error control.

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Global Error Control in Nonlinear Kalman Filtering Algorithms

Maria Kulikova, G. Yu. Kulikov, *Tue 14:30 R 1.04*

The new *Accurate Continuous-Discrete Extended Kalman Filter* based on the combined use of the embedded Runge-Kutta pair `NIRK4(2)` (or `NIRK6(4)`) with global error control [1] and Mazzoni's scheme [2] is discussed, here. More precisely, the state expectation equation is solved by the `NIRK4(2)` (or `NIRK6(4)`) method with global error control because only this equation may be nonlinear and, hence, create more difficulty for the accurate numerical solution. On the other hand, the error covariance matrix equation is treated by the corresponding part of Mazzoni's scheme. We also do not calculate and control the error of the numerical scheme applied to this matrix differential equation because of its linearity. All this saves the execution time of the codes, considerably. To increase the accuracy and robustness of our complex computational technique for a finite-precision computer arithmetics, we develop the square-root variant of the designed hybrid ODE solver with the global error control. Then, we examine it in severe conditions of tackling a seven-dimensional radar tracking problem, where an aircraft executes a coordinated turn. The latter is considered to be a challenging one for testing nonlinear filtering algorithms. Our numerical results confirm that the presented technique is flexible and robust. It treats successfully (and without any additional tuning) the target tracking problem for various initial data and for a range of sampling times. A numerical comparison to other effective filters as the continuous-discrete cubature and unscented Kalman filters is also provided.

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Numerical solutions of time-dependent KdV type system via the Lie group method

Vikas Kumar, *Mon 14:00 R 3.07*

With the consideration of inhomogeneous media and non-uniform boundaries, the time-dependent KdV type system can be used to describe some complex and realistic phenomena. Lie group method, is one of the most powerful methods to determine exact solutions of nonlinear systems of partial differential equation. The Lie group analysis is based on reducing the number of independent variables by one. Using suitable similarity transformations, the given time-dependent KdV type system is reduced to a system of ordinary differential equations. During the procedure of reducing system of partial differential equation to systems of ordinary differential equation, we got some special highly nonlinear systems of ordinary differential equation which are not easily solvable for exact solutions. Therefore, Haar Wavelet based numerical method and classical fourth order Runge-Kutta method are applied to the reduced systems of ordinary differential equations for constructing numerical solutions of the KdV type system.

Newmark type time integration methods for strongly damped mechanical systems

Markus Köbis, Martin Arnold, *Mon 16:35 R 3.07*

The simulation of mechanical or biological structures often results in systems of ODEs with very strong dissipative forces. In this talk we will adress the prototypical equations

$$M(q^\delta)\ddot{q}^\delta = f(t, q^\delta, \dot{q}^\delta) - \frac{1}{\delta} G^\top(q^\delta) G(q^\delta)\dot{q}^\delta, \quad (0 < \delta \ll 1)$$

for a given vector-valued function $f\colon \mathbb{R} \times \mathbb{R}^{n_q} \times \mathbb{R}^{n_q} \to \mathbb{R}^{n_q}$, and matrix-valued functions $M\colon \mathbb{R}^{n_q} \to \mathbb{R}^{n_q \times n_q}$ (the symmetric positive definite mass matrix) as well as $G\colon \mathbb{R}^{n_q} \to \mathbb{R}^{n_g \times n_q}$, which defines an invariant manifold $\mathfrak{M} := \{(q, v) : G(q)v = 0\}$ and is supposed to have a full-rank for all arguments $q \in \mathbb{R}^{n_q}$. From a DAE viewpoint this system may be seen as a singular perturbation of the index two system

$$\begin{aligned} M(q^0)\ddot{q}^0 &= f(t, q^0, \dot{q}^0) - G^\top(q^0)\lambda^0, \\ 0 &= G(q^0)\dot{q}^0 \end{aligned}$$

well known in the context of multibody system dynamics. We will apply time integration methods of Newmark type to the above equations and investigate their convergence properties by extending results from the DAE case to this singularly perturbed setting. Numerical results for benchmarks of small and moderate size will be presented and confirm the theoretical findings.

On Global Error Estimation and Control for Stiff Initial Value Problems

Jens Lang, Alexander Rath, *Tue 16:00 R 1.04*

In [1] we have studied a classical global error estimation based on the first variational equation, and global error control, for which we have used the property of tolerance proportionality. We have found, using the linearly implicit Runge-Kutta-Rosenbrock method ROS3P as example integrator, that the classical approach is remarkably reliable. For parabolic PDEs, the ODE approach is combined with estimates for the spatial truncation errors based on Richardson extrapolation [2].

In spite of the fact that the asymptotic theory behind the first variational equation is classical in the sense that stiffness is not taken into account, the approach works also successfully for stiff equations. This gave us the motivation to derive global error estimates in the framework of B-convergence, where a one-sided Lipschitz condition is assumed. We will present first results for one-step methods of order $p \leq 3$.

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Space-Time Finite-Element Exterior Calculus and Variational Discretizations of Gauge Field Theories

Melvin Leok, John Moody, Joe Salamon, *Tue 8:30 R 3.07*

Many gauge field theories can be described using a multisymplectic Lagrangian formulation, where the Lagrangian density involves space-time differential forms. While there has been prior work on finite-element exterior calculus for spatial and tensor product space-time domains, less has been done from the perspective of space-time simplicial complexes. One critical aspect is that the Hodge star is now taken with respect to a pseudo-Riemannian metric, and this is most naturally expressed in space-time adapted coordinates, as opposed to the barycentric coordinates that Whitney forms are typically expressed in terms of.
We introduce a novel characterization of Whitney forms and their Hodge dual with respect to a pseudo-Riemannian metric that is independent of the choice of coordinates, and then apply it to a variational discretization of the covariant formulation of Maxwell's equations. Since the Lagrangian density for this is expressed in terms of the exterior derivative of the four-potential, the use of finite-dimensional function spaces that respects the de Rham cohomology results in a discretization that inherits the gauge symmetries of the continuous problem. This yields a variational discretization that exhibits a discrete Noether's theorem.

An Algorithm with Global Error Control for the Numerical Solution of the Generalized Density Profile Equation

Pedro Lima, G. Yu. Kulikov, M. L. Morgado, *Tue 15:00 R 1.04*

We are concerned with a generalization of the Cahn-Hilliard continuum model for multiphase fluids [1] where the classical Laplacian has been replaced by a degenerate one (i.e., so-called p-Laplacian). Using spherical symmetry, the model can be reduced to a boundary value problem

for a second order nonlinear ordinary differential equation. One searches for a monotone solution of this equation which satisfies certain boundary conditions.
The case of the classical Laplacian was studied in detail in [2] and [3], while the generalized equation was analysed in [4] and [5]. It was proved that the arising boundary value problem possesses a unique increasing solution, under certain restrictions on the parameters. The asymptotic behavior of the solution has been analysed at two singular points; namely, at the origin and at infinity. From the point of view of numerical approximation, this problem presents some challenges, due to the singularities and to the existence of an interior layer where the derivative of the solution may take very high values. An efficient numerical technique for treating such singular boundary value problems has been presented, based on the shooting method and on nested implicit Runge-Kutta formulas with global error control. The present talk will focus mainly on the latter approach. We will briefly describe the computational algorithm and present some numerical results, which are highly accurate and in agreement with the experimental ones.

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Parallel exponential Rosenbrock methods

Vu Thai Luan, Alexander Ostermann, *Tue 16:30 R 3.07*

Exponential Rosenbrock integrators have been shown to be very efficient in solving large stiff differential systems of ODEs. So far, such exponential methods have been derived up to order 5. In this talk we give a convergence result for methods of order up to 6 and construct new integrators of orders 4, 5, and 6. In contrast to the existing schemes of orders 4 and 5, the new schemes, which are called parallel stages methods, can be implemented on a multi-processor system or parallel computers. Moreover, the great advantage of the new schemes of orders 4 and 5, when compared to the old schemes of the same orders of accuracy, is that they use the same number of stages. This offers a significant improvement over the old schemes, which have the same orders, in terms of computational time when implemented in parallel. The numerical experiments show the efficiency of the new integrators as well as the comparative performance with the old ones.
Main references:

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Jounce Newtonian equations for oscillating memristive circuits

Wieslaw Marszalek, Zdzislaw Trzaska, *Tue 12:05 R 1.27*

The prediction made by L. O. Chua 40+ years ago (see: IEEE Trans. Circuit Theory, 18 (1971) 507-519 and also: Proc. IEEE, 100 (2012) 1920-1927) about the existence of a passive element (called memristor) that links the charge and flux variables has been confirmed by the HP lab group in its report (see: Nature, 453 (2008) 80-83) on a successful construction of such an element. This sparked an enormous interest in mem-elements, analysis of their unusual dynamical properties (i.e. pinched hysteresis loops, memory effects, etc.) and construction of their emulators.
In this talk we discuss certain properties of the memristive circuits yielding mixed-mode oscillations. Mathematical models of such circuits can be linked to the Newton's law $\phi'' - F(t, \phi, \phi')/m = 0$, with ϕ denoting the flux or charge variables, m is a positive constant and the nonlinear function F contains memory terms. This leads further to scalar fourth-order ODEs called the *jounce* Newtonian equations. The *jounce* equations are used to construct the $RC+$ op-amp simulation circuits in SPICE. Also, the linear RC and RL circuits with sinusoidal inputs are derived to match the *RMS* values of the memristive periodic circuits. SPICE and Matlab are used in the illustrative examples of periodic responses and calculations of their *RMS* and one-period energy values.

A numerical technique for applying time splitting methods in shallow water equations.

Vicente Martínez, *Tue 12:05 R 1.26*

In this talk we analyze the use of time splitting techniques for solving shallow water equations. We discuss some properties that these schemes should satisfy so that interactions between the source term and the shock waves are controlled. This work shows that these schemes must be well balanced in the meaning expressed by Greenberg and Leroux [3]. More specifically, we analyze in what cases it is enough to verify an Approximate C-property and in which cases it is required to verify an Exact C-property (see [1], [2]). We also discuss this technique in two dimensions and include some numerical tests in order to justify our reasoning.

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The Index of DAEs, Science or Religion

Volker Mehrmann, *Wed 10:30 R 3.07*

We discuss the different Index concepts for differential-algebraic systems. Being developed in many different scientific communities and with modifications over the years, it is a constant struggle for people entering the field of DAEs to figure out the subtle differences and similarities. We will put the different concepts in a common perspective and indicate that an index concept that allows to speak a common language between the different groups such as theory people and practioners, software developers and users, etc would be a real success story for the further development of the field.

On the 0/1 test for chaos for continuous ODEs: resonance, oversampling and frequency properties.

Michal Melosik, Wieslaw Marszalek (DeVry University), *Mon 17:25 R 1.27*

The 0/1 test for chaos developed several years ago (see: G. A. Gottwald and I. Melbourne, A new test for chaos in deterministic systems, Proc. R. Soc. London, vol. 460, pp. 603-611, 2003; also G.A. Gottwald and I. Melbourne, On the implementation of the 0/1 test for chaos, SIAM J. Appl. Dynamical Syst., vol. 8, pp. 129-145, 2009) is an alternative way to the Lyapunov exponents approach to test both discrete and continuous systems for the presence of chaos. The 0/1 test is based on the statistical methods of regression and correlation. It is known that in the continuous case the phenomena of resonance and oversampling may impact the results of the test and lead to incorrect findings.
In this paper we discuss in detail the resonance and oversampling features of the 0/1 test for chaos for continuous systems of ODEs and propose methods to avoid those undesired features. Our method is based on certain frequency properties of the 0/1 test for chaos. The results of our approach are compared with those obtained by using the first minimum approach of the mutual information approach. Several numerical results for typical chaotic systems (including memristive circuits) are included.

Error estimation approach for controlling the comunication step size for semi-implicit co-simulation methods

Tobias Meyer, Bernhard Schweizer, *Thu 11:30 R 1.26*

This contribution presents an approach for controlling the macro-step size in connection with co-simulation methods [1, 3]. The investigated step-size controller is tailored for semi-implicit co-simulation techniques. Concretely, we consider predictor/corrector co-simulation approaches [2]. By comparing variables from the predictor and the corrector step, an error estimator for the local error can be constructed. Making use of the estimated local error, a step-size controller for the macro-step size can be implemented. Different numerical examples are presented, which show on the one hand the applicability of the method and on the other hand the benefit of a variable macro-grid with respect to simulation time.

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A Family of Runge-Kutta Restarters for Discontinuous ODEs

Fatemeh Mohammadi, Carmen Arévalo, Claus Führer, *Wed 10:30 R 1.04*

In this talk we present an extended idea of Runge–Kutta methods designed to restart multistep methods applied to ODEs with frequent discontinuities [3,4].
Multistep methods use information from previous steps to approximate the next value. A single step of these Runge–Kutta methods provides sufficiently accurate initial values to start a high order multistep method, whereas classical algorithms either apply a Runge–Kutta method several times or start with a variable order implementation. Both classical schemes can lead to inefficiency when the integration has to be interrupted frequently due to discontinuities.
We demonstrate the advantage of this approach by an extension of Assimulo [1] together with Sundials [2].

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New answers to an old question: Essential underlying ODE versus inherent explicit ODE

Roswitha März, *Thu 10:40 R 1.04*

In the context of differential-algebraic equations (DAEs) one finds different associated explicit ordinary differential equations (ODEs): completion ODEs, underlying ODEs, essential underlying ODEs and inherent ODEs. Each of them is occasionally considered to control the flow of the DAE. However, how are they related to each other? This question has been asked long time ago, also in early NUMDIFF-conferences, but it has been partly answered only.
We will put straight the notions and then take a closer look to essential underlying ODEs (EU-ODEs) and inherent explicit regular ODEs (IERODEs). The latter arise within the projector

based decoupling of DAEs. The former has been introduced by U. Ascher and L.R. Petzold for Hessenberg-form index-2 DAEs in 1992 by means of special transformations. We extend this notion to general arbitrary-index linear DAEs, no matter in which form, without or with properly involved derivative.
Any regular linear differential-algebraic equation (DAE) features a unique IERODE living in the given space. In contrast, there are several EUODES living in a transformed space with possible minimal dimension. In 2005 it has been pointed out by K. Balla and Vu Hoang Linh that, for index-2 Hessenberg-form DAEs, an EUODE is a condensed IERODE. We show that this applies also in general.
The understanding of the relation between the IERODE and the EUODEs enables us to uncover the stability behavior of the DAE flow. We discuss several questions concerning Lyapunov stability, Lyapunov spectra, Lyapunov regularity, and Perron identity.

Nonholonomic mechanics for perfect fluids

Andrea Natale, Colin J. Cotter, *Thu 11:30 R 1.27*

Perfect fluid models, such as the incompressible Euler equations, possess a remarkable geometric structure which can be described using the classical Lagrangian and Hamiltonian formalism. This structure is responsible for the numerous properties of the solutions, including conservation of energy and circulation, which directly descend from the symmetries of the system. Although powerful numerical techniques have been derived to tackle this class of problems, two main difficulties arise when dealing with fluids. Firstly, the infinite-dimensional nature of the problem requires a truncation that would preserve its variational nature. Secondly, numerical integrators should be designed in the Eulerian setting in order to avoid complications related to moving or deforming meshes. [1] addressed both issues by approximating the Lie algebra of divergence-free vector fields by its action on piecewise constant functions defined on a triangulation of the computational domain and imposing a nonoholonomic constraint to obtain a sparse matrix algorithm. In this talk, we build on their results to develop a high order finite element geometric formulation of perfect incompressible fluids. The main idea of the method is to reinterpret the spatial discretization of the velocity fields as a nonholonomic constraint, and to define an isomorphism with a suitable Lie algebra. We present some preliminary results obtained with this formulation and we set the scene for further developments of the algorithm.

References

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Extended defect corrected averaging for highly oscillatory PDEs

Andreas Naumann, Michael Klöppel, Jörg Wensch, *Mon 17:25 R 3.07*

We consider parabolic partial differential equations where the support of the sources or of the inhomogenous Neumann boundary conditions undergoes an oscillatory motion. The timescale of this oscillation is much smaller than the characteristic time scale of diffusion, which is of main interest. Resolution of the smallest timescale constitutes a strong restriction on the stepsize of time integration method. Averaging techniques like stroboscopic averaging, or the heterogenous multiscaling methods, have been developed to overcome this restriction. Especially time- and space varying stiffness coefficients lead to strong timestep restrictions. We will present an

extension to the defect corrected averaging with time varying periodic coefficients, that allows to use macro timesteps in the range of several periods. Both schemes make use of krylov subspace methods for the coarse scale problem and are speed up by the application of preconditioners.

Weak convergence for a stochastic exponential integrator and finite element discretization of SPDE for multiplicative and additive noise

Jean Medard Ngnotchouye, Antoine Tambue, *Wed 10:55 R 1.27*

We consider a finite element approximation of a general semi-linear stochastic partial differential equation (SPDE) driven by space-time multiplicative and additive noise. We examine the weak convergence of an exponential integrator in the case where the linear operator is not necessarily self adjoint. As usual we found that the rate of weak convergence is twice the strong rate of convergence. Our convergence result is in agreement with some numerical results presented for a linear diffusion equation in two dimensions as well as a nonlinear example of a two-dimensional stochastic advection diffusion reaction equation motivated from realistic porous media flow.

Operator Index Reduction in Electromagnetism

Helia Niroomand Rad, *Mon 17:00 R 3.07*

Electromagnetic disturbances among elements in an electrical circuit and their influences on dynamics of the circuit, the so-called crosstalk phenomenon, can be modeled by bilateral coupling of the set of partial differential equations (PDEs), namely the Maxwell equations, with the set of differential-algebraic equations (DAEs), the so-called circuit equations. Our approach to numerically treating such a model is by semi-discretization of the Maxwell equations in space, where the circuit equations are incorporating into the boundary conditions via the coupling relations. This allows us to obtain a set of DAEs corresponding to the original PDEs, which in turn leads to a large DAE system as a model equation for the crosstalk.
Semi-discretization of the Maxwell equations by finite element method results in a system of high index DAEs. On the other hand, the high index may create instabilities and inconsistencies in the numerical treatment of DAEs, and therefore it is necessary to regularize the system by an index reduction technique before the time integration.
In this talk, we introduce the operator based Maxwell equations and show that with the certain choice of spaces for the operators, the semi-discretized Maxwell equations has index 1.

Existence and optimality of SSP linear multistep methods: a duality-based approach

Adrián Németh, David Ketcheson, *Wed 10:05 R 1.04*

We investigate strong stability preserving linear multistep methods and prove the existence of explicit LMMs of any order with positive SSP coefficients. Our approach is based on formulating a linear programming problem and establishing infeasibility of the dual problem. This yields a number of other theoretical advances.

A splitting approach for the KdV and KP equations

Alexander Ostermann, Lukas Einkemmer, *Thu 17:00 R 3.07*

We consider a splitting approach for the time integration of partial differential equations containing a Burgers-type nonlinearity. Typical examples comprise the Korteweg–de Vries (KdV) and the Kadomtsev–Petviashvili (KP) equation. Whereas the linear part in both equations is efficiently integrated by fast Fourier techniques, the nonlinearity is handled with the method of characteristics.
For the Burgers-type nonlinearity we propose a semi-Lagrangian approach based on polynomial interpolation. It is shown that the necessary interpolation procedure can be efficiently implemented. The error made by our splitting scheme is compared to exponential integrators which have been shown in Klein and Roidot (SIAM J. Sci. Comput., 2011) to perform best for stiff solutions of the KP equation. In addition, the conservation properties of the numerical schemes under consideration are investigated.
The talk is based on the paper *L. Einkemmer and A. Ostermann, A splitting approach for the Kadomtsev–Petviashvili equation*, arXiv:1407.8154 (2014).

Cosimulation Convergence Criteria for Hessenberg DAEs of Index 2

Jonas Pade, Caren Tischendorf, *Thu 10:40 R 1.26*

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

Haar Wavelet Operational Matrix Method for Solving a System of Fractional Differential Equations with nonlinear uncertain parameters

Sapna Pandit, *Wed 10:30 R 1.26*

In this paper, we develop a frame work to obtain approximate numerical solutions of systems of ordinary differential equations (ODEs) involving fractional order derivatives in the Caputo derivative sense using uniform Haar wavelets operational method. A truncated Haar wavelet series together with the wavelet operational matrix are utilized to reduce the fractional differential equations to system of algebraic equations. Numerical experiments have been conducted on test problems to illustrate the merits of the proposed method. The absolute errors are reported to show that the proposed method is working well and produces satisfactory results.

Asymptotic-preserving methods and differential algebraic equations

Lorenzo Pareschi, *Fri 9:20 R 3.07*

Many applications involve PDEs with multiple space-time scales. Numerically resolving such scales may be computationally prohibitive and therefore one resorts on the use of some asymptotic analysis in order to derive reduced models which are valid in the small scales regime. The derivation of numerical schemes which are capable to describe correctly such asymptotic behavior without resolving the small scales has attracted a lot of attention in the recent years leading to the so-called asymptotic-preserving methods. In this talk we survey some of these techniques in the case of hyperbolic and kinetic PDEs and emphasize the close relationship with singular perturbed systems and differential algebraic equations.

Unique solutions of initial value problems for mechanical systems with redundant unilateral constraints

Manuela Paschkowski, Martin Arnold, *Tue 12:05 R 3.07*

Making use of Langrange multiplier methods the dynamics of interconnected rigid or flexible bodies under certain inequality constraints can be modeled as a system of second order differential equations coupled with a complementarity problem

$$\begin{aligned} M(q)\ddot{q} &= f(q,\dot{q},t) + G^T(q)\lambda, \\ 0 \leq \lambda &\perp g(q) \geq 0. \end{aligned}$$

Here, the mass matrix $M(q) \in \mathbb{R}^{n\times n}$ is supposed to be symmetric, positive definite. A common assumption is furthermore that the active constraints $g(q) \geq 0$ are independent which means that the Jacobian matrix $G(q) := \frac{\partial}{\partial q}\, g(q) \in \mathbb{R}^{m\times n}$ has full rank. But many application models (e.g. of vehicle construction, biomechanics or robotics) deal with dependent (redundant) constraints. One option is to identify and eliminate these terms. However, if the complexity and the computational effort of the implementation should be optimized, the use of redundant constraints cannot be avoided. Using existence results for generalized complementarity problems and measure differential inclusions we generalize the proof of existence of solutions to the case with redundant unilateral constraints. Furthermore we will discuss existence and uniqueness of solutions in the case of singular mass matrices.

Numerical solution of three dimensional conjugate problems of forest fires spread

Valeriy Perminov, *Wed 9:40 R 1.26*

The mathematical model simulating the heat and mass transfer processes taking place during the crown forest fire spread is developed to take into account atmosphere boundary layer. The aim of the present paper is to solve the system of three dimensional non-stationary equations describing the behavior of crown forest fires propagating through crown canopy and to study the mutual influence of crown forest fires and boundary layer of atmosphere using numerical simulation with a physics-based model. It is a coupled atmosphere/crown fire behavior model and is based on the laws of conservation of mass, momentum, species and energy. The paper gives a new mathematical setting and method of numerical solution to this problem. The three-dimensional Reynolds equations are solved numerically for turbulent flow using diffusion equations for chemical components and equations of energy conservation for gaseous and condensed phases. The method of finite volume is used to obtain discrete analogies. Using finite volume method, the solution domain is subdivided into a finite number of small control volumes by a grid. The grid defines the boundaries of the control volumes while the computational node lies at the center of the control volume. The advantage of finite volume method is that the integral conservation is satisfied exactly over the control volume. The boundary-value problem is solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions was calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting was then integrated. Difference equations that arise in the course of sampling were resolved by the method of SIP. The accuracy of the program was checked by the method of inserted analytical solutions. The time step was selected automatically. This approach allows investigating dynamics of forest fire initiation and spreading under influence of various external conditions: a) meteorology conditions (air temperature, wind velocity etc.), b) type (various kinds of forest combustible materials) and their state (load, moisture etc.). Fields of

temperature, velocity, component mass fractions, and volume fractions of phases were obtained numerically. The results of calculation are agreed with the laws of physics and experimental data.

Effective order Runge–Kutta methods with free output

Helmut Podhaisky, John Butcher, *Mon 14:25 R 1.04*

The concept of effective order was introduced in 1969. It makes it possible to reduce the number of order conditions for explicit Runge–Kutta methods considerably; for example, for p=5, from 17 to 10. In particular, it is possible to construct methods of effective order five with only five stages. It might be asked why efficient codes based on these methods are not available and widely used. One possible reason is that a finishing method, with additional cost, is needed whenever an output of the solution needs to be computed.
In this talk we will show that it is possible to construct methods for which essentially free output is available at the end of any step. This is achieved by re-using the stage values of the main method to provide an in-built finishing method. The main tool for this investigation is the composition of B-series.

On the parallel implementation of numerical schemes for the hyperbolic Euler equations

Martina Prugger, *Mon 17:00 R 1.27*

The modeling of fuids usually results in a number of partial diferential equations that relate the change of local properties (such as density, velocity, temperature,...) in time to the corresponding change in space. Among the equations used, the Euler equations (for inviscid fow) and the Navier-Stokes equations (for viscid fow) are probably the most prominent examples and are used in a variety of applications. Mathematically speaking, the proper discretization of conservation laws is of importance to obtain physically relevant results that can be used in applications ranging from the analysis of aircrafts to transport phenomena in the sun.
These problems are challenging from a numerical point of view, since care has to be taken to propagate shock waves without diminishing the performance of the scheme.
MPI is the classical approach for scientific computation on a parallel architecture. However, with respect to the ongoing developement of HPC systems, a reduction of the communication overhead is desirable. The Partitioned Global Address Space (PGAS) programming model is a more convenient way to write a parallel program and it offers the potential of reducing the communication overhead.

The Hankel norm for quadrature methods applied to random dynamical systems

Roland Pulch, *Wed 9:40 R 1.27*

We consider linear dynamical systems in form of ordinary differential equations. The Hankel norm represents a bound for the ratio between the energy of outputs and inputs in the system. For modelling uncertainties, we replace physical parameters of the system by random variables. The random process, which satisfies the dynamical system, is expanded into a series with orthogonal basis functions. We define a Hankel norm for a truncated expansion, although it does not solve some dynamical system. The unknown coefficients of the truncated expansion represent probabilistic integrals. Thus they can be computed approximately by a quadrature method like sparse grid techniques or quasi Monte-Carlo schemes, for example. We arrange all involved linear dynamical systems into a much larger system, which is coupled by the outputs

only. For the coupled linear system, the Hankel norm exists in the usual sense. We proof that these Hankel norms of the approximate systems converge to the Hankel norm associated to the exact truncated series provided that the quadrature method is convergent. Furthermore, numerical results of a test example are presented, where different quadrature techniques are involved.

Application of Bernoulli polynomials for solving fractional Riccati differential equations

Parisa Rahimkhani, Yadollah Ordokhani, *Wed 10:55 R 1.26*

In this paper, a collocation method based on the Bernoulli polynomials is presented for the nonlinear Riccati differential equations with fractional order. The fractional derivatives are described in the Caputo sense. The method is based upon Bernoulli polynomials approximations. First, the Bernoulli polynomials and some their properties are presented. Also, an operational matrix of fractional order integration is derived and is utilized to reduce the initial value problems to system of algebraic equations. The technique is applied to some problems to demonstrate the validity and applicability of the proposed method.

Adaptive timestep control for high order implicit Runge-Kutta methods

Joachim Rang, *Mon 16:35 R 1.04*

It is possible to construct fully implicit Runge–Kutta methods such as Gauß-Legendre, Radau-IA, Radau-IIA, Lobatto-IIIA, -IIIB, and -IIIC methods of arbitrary high order of convergence. The aim of this paper is to find a new adaptive time stepping for these classes. Adaptive time step control with embedding is well-known for Runge–Kutta methods, and therefore new embedded methods of order $s-1$ for the above classes of fully implicit Runge–Kutta methods are constructed.
Since these fully implicit methods need the solution of a huge non-linear system of equations different approaches for non-linear equations are discussed and compared. It can be observed that non-linear solvers such as the usually used simplified Newton method have a step size restriction if they are used in the solution process of higher order FIRK methods.
We apply our new methods on some ODEs, DAEs and PDEs to show that this approach can be a more efficient approach than using lower order methods (see [1])

Literature:

[1] Rang, Joachim and Niekamp, Rainer. *A component framework for the parallel solution of the incompressible Navier-Stokes equations with Radau-IIA methods.* Int. J. Numer. Meth. Fluids 78 (5), pp. 304-318, 2015.

How to avoid order reduction when Lawson methods are used to solve linear initial boundary value problems

Nuria Reguera, Isaías Alonso-Mallo and Begoña Cano, *Mon 16:35 R 1.27*

The advantages of exponential methods for integrating in time partial differential equations are well known. Nevertheless, these methods can present a severe order reduction when they are used for integrating stiff problems. In this talk, we will show how it is possible to avoid this order reduction when integrating linear initial boundary value problems with Lawson exponential methods, even in the case of nonvanishing boundary conditions.

Stabilized Numerical Schemes for Singularly Perturbed Delay Differential Equations

Fathalla Rihan, *Mon 14:50 R 1.26*

There is general agreement among scientists that delay differential equations have a richer mathematical framework, and better consistency with observations, compared with corresponding models without memory or after-effects. However, many problems that modeled by delay differential equations – especially in the study of chemical kinetics, or immune system interactions – are 'stiff', in the sense that they have properties that make them slow and expensive to solve using explicit numerical methods. The efficient use of reliable numerical methods (based in general on implicit formulae) for dealing with stiff models involves a degree of sophistication not necessarily available to nonspecialists. In this paper, we suggest the so called mono-implicit continuous Runge-Kutta schemes, a subclass of semi-implicit continuous Runge-Kutta schemes, for numerical approximations of delay differential equations. The schemes are suitable for both stiff and non-stiff initial value problems. Stability properties of the methods are investigated. Some examples are considered to show the efficiency of the numerical methods.

Structure-preserving integrators for smooth and non-smooth thermomechanical problems

Ignacio Romero, *Tue 10:40 R 3.07*

There has been a large amount of work on structure-preserving numerical methods in mechanics, mostly applied to Hamiltonian problems. However, many problems of interest in this field are not Hamiltonian, since they include dissipative mechanisms.

For a general class of dissipative problems though, the ones possessing a thermodynamic structure, it is possible to devise numerical methods that preserve it, yielding approximations that are strictly energy-conserving and entropy non-decreasing, for closed systems. The solutions obtained in this fashion give accurate pictures of the dynamics of the underlying problem, and often result in robust numerical schemes.

In this talk we will describe this kind of numerical approximations in the context of smooth problems [1] and present new results for non-smooth ones. The latter can be employed, for example, to construct thermodynamically consistent integrators for thermoplasticity, but are general enough to encompass other cases of interest.

References

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Multi-methods for time discretization of evolutionary PDEs

Adrian Sandu, *Thu 9:20 R 3.07*

Many applications involve large scale simulations of systems modeled by time dependent partial differential equations (PDEs). These systems are typically driven by multiple physical processes and their dynamics is characterized by multiple scales.

The time discretization defines the overall data dependencies in a simulation, as well as the way the simulation progresses across the nodes of a distributed platform. No single time stepping

method can effectively solve multiphysics multiscale applications, where different physical processes have different dynamical characteristics (e.g., stiff and non-stiff), and different variables evolve at vastly different time scales (e.g., from milliseconds for reactive chemical species to decades for temperature averages in a climate application).
We discuss multi-methods where different processes are treated with different numerical discretizations (e.g., implicit-explicit) and different time steps are used for different components (multirate). Specifically, the focus of the talk is on partitioned general linear methods and on generalized-structure additive Runge-Kutta methods.

Efficient A-stable peer two-step methods

Bernhard A. Schmitt, Rüdiger Weiner, *Mon 14:00 R 1.04*

Efficient peer methods for stiff intitial value problems should satisfy different criteria like a large angle of $A(\alpha)$-stability, uniform zero-stability for time-adaptive grids and small error constants or superconvergence. We present a new algebraic criterion for A-stability, which requires semi-definiteness of a certain matrix. In fact, A-stable and superconvergent peer methods with s stages can be characterized by a set of $O(s^2)$ nonlinear equations. Also, a new criterion for uniform zero stability is formulated leading to a finite set of inequalities. Hence, peer-methods satisfying all 3 criteria can be constructed by solving a set of nonlinear inequalities with standard methods. Peer methods found with this procedure are compared with existing ones on a few test problems.

Influence of spatial discretization of flexible structures on the stability of coupled simulations

Fabio Schneider, Michael Burger, *Thu 11:05 R 1.26*

In advanced system simulation, the numerical simulation of several coupled subsystems, i.e. the co-simulation, becomes more and more important. Especially, the simulation of kinematically coupled subsystems is widespread, e.g. in automotive engineering.
Recently, we developed a new approach, which kinematically couples mechanical subsystems in an efficient and robust way. In our approach, we use algebraic coupling constraints to formulate a force-displacement coupling and, thus, we do not introduce an artificial coupling stiffness into the system. Moreover, the algebraic constraints allow very general coupling joints, leading to a wide range of possible applications for the approach.
Our main application is the coupled simulation of rigid multibody systems and flexible structures. In general, the flexible structure is described mathematically as partial differential equation and is transformed into an ordinary differential equation via spatial discretization. Consequently, we analyze how the spatial discretization of the flexible structure influences the stability of our co-simulation approach. We will see that a subsystem mass ratio is decisive for stable co-simulation and can be improved by refining the discretization.
To illustrate the presented coupling approach, we first apply our method and the stability considerations on a test problem. Afterwards, to show the potential of the new approach, a complex nonlinear cable model is coupled with a multibody system.

Space adaptive linearly implicit two-step peer methods for time-dependent PDEs

Dirk Schröder, Jens Lang, Alf Gerisch, *Mon 14:50 R 1.04*

In [GLPW(2009)] linearly-implicit two-step peer methods are sucessfully applied in the numerical solution of time-dependent partial differential equations. The computations were performed adaptive in time, but on a fixed spatial grid. However problems like the propagation of flame fronts are solved more efficiently when solved both adaptive in time and space.

This talk addresses the fully adaptive solution of PDEs with linearly-implicit peer methods. We first discretize in time with linearly implicit peer methods and than discretize in space with linear finite elements. The error in time is estimated by an embedded solution of lower order, while the spatial error is estimated by the DLY error estimator based on hierarchical bases. We address the question of efficiency of the spatial error estimator and compare the performance of linearly implicit peer methods to Rosenbrock methods.

References

[GLPW(2009)] Alf Gerisch and Jens Lang and Helmut Podhaisky and Rüdiger Weiner High-order linearly implicit two-step peer-finite element methods for time-dependent PDEs *Applied Numerical Mathematics*, 59:624–638, 2009.

Non-smoooth contact dynamics for the large-scale simulation of granular material

Bernd Simeon, Jan Kleinert, *Tue 11:40 R 3.07*

Non-smooth contact dynamics provides a powerful simulation framework for granular material that, in contrast to classical discrete element methods, is stable for arbitrary time steps and produces visually acceptable results in very short computing time. Yet when it comes to the prediction of the forces that interact with a solid modeled as continuum, non-smooth contact dynamics is typically not accurate enough. We therefore propose to combine the method class with an interior point algorithm for higher accuracy. Our specific algorithm is based on so-called Jordan algebras and exploits the relation to symmetric cones in order to tackle the conical constraints that are intrinsic to frictional contact problems. In every interior point iteration a linear system has to be solved. We analyze how the interior point method behaves when it is combined with Krylov subspace solvers and incomplete factorizations. Numerical experiments demonstrate that preconditioners and efficient linear solvers are essential for the method to be applicable to large-scale problems.

A class of implicit peer methods

Behnam Soleimani, *Mon 15:15 R 1.04*

We present a class of s-stage implicit two step peer methods for the solution of stiff differential equations using in addition also the function values from the previous step. This allows to increase the order to $p = s$. Corresponding s-stage methods for $s \leq 5$ of order $p = s$ with optimal zero stability are presented. Numerical tests and comparison with ode15s show the high potential of this class of implicit peer methods. Under special conditions, we prove that an optimally zero-stable subclass of these methods is superconvergent of order $p = s + 1$.

Sample Selection Approaches in Parameterized Model Order Reduction

Tino Soll, Roland Pulch, *Mon 14:00 R 1.27*

Modeling of scientific or industrial applications often yields high-dimensional dynamical systems due to techniques of computer-aided-design, for example. Thus a model order reduction is required to decrease the dimensionality to enable an efficient numerical simulation. In addition, methods of parameterized model order reduction (pMOR) shall preserve the physical parameters as independent variables in the reduced order models. We consider linear dynamical systems in the form of ordinary differential equations. In the domain of the parameters, often samples are chosen to construct a reduced order model. For each sample point an ordinary technique for model order reduction can be applied to compute a local basis. Moment matching techniques or balanced truncation schemes are feasible, for example. A global basis for pMOR can be constructed from the local bases by a singular value decomposition. We investigate approaches for an appropriate selection of the finite set of samples. Our focus is on moment matching techniques using the Arnoldi procedure. Hence the transfer function of the dynamical system is examined in the frequency domain. We use a sensitivity analysis of the transfer function with respect to the parameters as a tool to select sample points. Simulation results are shown for illustrative examples.

Computational mean-square stability analysis for linear systems of SODEs
Andreas Thalhammer, Markus Ableidinger, Evelyn Buckwar, *Wed 10:05 R 1.27*

We consider the mean-square stability analysis for linear SODEs from a computational point of view. The criteria for deciding whether the equilibrium solution of a linear system of SODEs is stable or unstable in the mean-square sense, is theoretically well understood. However, the numerical simulations obtained by Monte-Carlo techniques are strongly influenced by the path-wise behaviour of the numerical trajectories. In the case of almost sure stable but mean-square unstable systems, the mean-square instability depends on very rare exploding trajectories which renders the computational cost of the standard Monte-Carlo approach prohibitively high. We will illustrate this behaviour by numerical studies for linear SODE systems obtained e.g. by the spatial discretisation of SPDEs. This talk is based on a joint work with M. Ableidinger and E. Buckwar and is connected with the talk *Variance reduction techniques for the numerical simulation of the stochastic heat equation* by M. Ableidinger, where the numerical simulation of the spatially discretised stochastic heat equation is treated.

Perturbation Analysis of hyperbolic PDAEs
Caren Tischendorf, Christoph Huck, *Wed 10:55 R 3.07*

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

IMEX Schemes for Pricing Options under Jump-Diffusion Models
Jari Toivanen, *Thu 14:30 R 1.04*

Partial-integro differential (PIDE) formulations are often used to price options under jump-diffusion models. Their discretizations lead to dense matrices or matrix blocks. With implicit-explicit (IMEX) time discretizations, solutions with these dense matrices can be avoided. We describe three second-order accurate IMEX schemes and show them to be stable under fairly mild stability conditions. Numerical experiments demonstrate the efficiency of these methods under one-dimensional Merton model and two-dimensional Bates stochastic volatility model.

Regularization of linear time-varying delay differential-algebraic equations
Benjamin Unger, *Mon 15:15 R 1.26*

Differential-algebraic equations (DAEs) are a widely accepted tool for modeling and simulation of constrained dynamical systems. Applications, such as multibody systems, electrical circuit simulation or fluid dynamics, that may be modeled as DAE often feature hereditary effects caused by internal time delays or delayed feedback control. This leads to so called delay DAEs (DDAEs).
In this talk we show that DDAEs are essentially ill-posed in general and hence require a suitable regularization prior to the numerical treatment. The ill-posedness for DAEs is typically classified by of one of many index concepts [1], e. g. the strangeness index [2]. While this translates to DDAEs, numerical algorithms may additionally suffer from hidden noncausal constraints. In this context, the shift index [3] characterizes the degree of noncausality of the DDAE. We present a novel regularization methodology for linear time-varying DDAEs, which is a generalization of the strangeness-free reformulation procedure to DDAEs and allows for an efficient computation of the strangeness and shift index. The resulting regularized system is well-posed and suitable for classical numerical algorithms like the Bellmann method of steps (cf. [4]).

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Numerical solution of Euler-Bernoulli beam subjected to concentrated load

Mustapha Usman, *Wed 10:05 R 1.26*

This paper investigate the numerical solution of Euler-Bernoulli beam subjected to concentrated load. the governing partial differential equation is solved using analytical-numerical method. The result of the analysis were depicted graphically. It was observe that as damping increases, the amplitude of the deflection increases keeping the fixed length of the beam constant and when there is no damping, the amplitude of deflection increases as the fixed length decreases. also with the fixed value of damping the amplitude of deflection decreases as the fixed length of the beam increases.

Forward option pricing using Gaussian RBFs

Lina von Sydow, Jamal Amani Rad, Josef Höök, Elisabeth Larsson, *Thu 15:00 R 1.04*

We will present a method to numerically price options by solving the Fokker-Planck equation. The solution to this partial differential equation (PDE) describes the evolution of the conditional probability density $p(s,t)$ for the value s of the underlying asset at time t, given that the value is s_0 at time t_0. This enables the pricing of several contracts with pay-offs $\phi(s,K,T)$ (with strike-price K and time of maturity T) by simply integrating the conditional probability density function at time of maturity with the pay-off function for each contract.
This means that our method only requires the solution of one PDE to price several contracts. This is useful in practical applications where it is common to price many contracts simultaneously for the same underlying diffusion model.
From a numerical perspective the initial condition for the Fokker-Planck equation $p(s_0,t_0)$ is particularly challenging since it is a Dirac delta function. In [1] a closed-form expansion for the conditional probability density was introduced that is valid for small time-steps. We use this for the computation of $p(s,\Delta t)$ the first time-step. For the remaining time-steps we discretize the Fokker-Planck equation using BDF-2 in time and Radial Basis Function (RBF) approximation in space with Gaussian basis functions.
We will demonstrate the good qualities of our proposed method for European call options and barrier options.

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Global error control with peer methods

Rüdiger Weiner, *Tue 17:00 R 1.04*

In common ode methods the step size control is based on the estimation of the local error, and decreasing the tolerances will lead to a reduction of the global error. However, the proportionality factor between local and global error is unknown, often the global error exceeds the local tolerance by several magnitudes. In these cases a global error control is desirable.
We consider global error control with peer triples, both explicit for nonstiff and implicit for stiff problems. In the nonstiff case we combine two methods of orders 5 and 6. In the stiff case the methods have to be chosen carefully to use the same coefficient matrices in the Newton iteration and to have good stability properties. We present methods of orders 2 and 3 which are superconvergent of orders 3 and 4 for constant step sizes. Numerical tests show the reliability of our approach, the prescribed global accuracy is met in all problems. Furthermore, comparison with the built-in MATLAB codes shows the efficiency of our methods.

TVD-based Finite Volume Methods for Sound-Advection-Buoyancy Systems

Jörg Wensch, *Fri 10:10 R 3.07*

The simulation of atmospheric dynamics is an important issue in Numerical Weather Prediction. It relies on the numerical solution of the Euler equations. These equations exhibit phenomena on different temporal scales. In the lower troposphere sound waves propagate approximately ten times faster than the advective waves. After remarks on the historical development of numerical weather prediction we present multirate infinitesimal step (MIS) schemes based on a finite volumes spatial discretization with different treatment of slow and fast processes in the time discretization. An approach to overcome the CFL restriction caused by sound waves are split-explicit methods. Through multirate techniques the terms relevant for sound waves are integrated by small time steps with a cheap time integration procedure, whereas the slow processes are solved by an underlying Runge-Kutta method using a larger macro step size.
The analysis of these methods is based on the interpretation as an exponential or Lie group integrator. By assuming an exact solution of the fast waves with frozen coefficients for the slow waves order conditions for our multirate infinitesimal step methods are derived. Stability is discussed with respect to the linear acoustics equation.
We construct methods based on TVD-RK schemes by different search and optimization procedures. For the established RK3 time stepping scheme the stability bound with respect to the sound CFL number is approximately 3. For our methods this bound extends up to 12. Numerical simulation results for established benchmark problems are presented. The theoretically predicted properties are confirmed by the experiments.

Variable step size implementation of a generalized-α Lie group integrator

Victoria Wieloch, Martin Arnold, *Mon 14:25 R 3.07*

Step size selection is an efficient method to improve the result accuracy and to keep the costs low.
In this presentation, such a step size control shall be developed for the generalized-α method in its Lie group formulation, which is a second order time integration method for differential-algebraic equations. However, an order reduction may appear when the step size is varied. An adaption of velocity and acceleration variables must be carried out to prevent this. Afterwards, local truncation errors can be estimated with which the time step control is carried out. The error estimates are investigated for differential-algebraic equations in index-3 and in stabilized index-2 formulation. The variable step size implementation is tested for the Heavy top benchmark in the Lie groups $\mathbb{R}^3 \times SO(3)$ and $SE(3)$.

Convergence analysis of the Modified Craig-Sneyd scheme for two-dimensional convection-diffusion equations with nonsmooth initial data

Maarten Wyns, *Thu 16:30 R 1.04*

In this paper we consider the Modified Craig–Sneyd (MCS) scheme which forms a prominent time stepping method of the Alternating Direction Implicit type for multidimensional time-dependent convection-diffusion equations with mixed spatial derivative terms. When the initial function is nonsmooth, which is often the case in for example financial mathematics, application of the MCS scheme can lead to spurious erratic behaviour of the numerical approximations. We prove that this undesirable feature can be resolved by replacing the very first MCS timesteps by several (sub)steps of the implicit Euler scheme. This technique is often called Rannacher time stepping. We derive a useful convergence bound for the MCS scheme combined with Rannacher time stepping when it is applied to a model two-dimensional convection-diffusion equation with mixed-derivative term and with Dirac-delta initial data. Ample numerical experiments are provided that show the sharpness of our obtained error bound.

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