The seminar NUMDIFF–12 is jointly organized by the *Institute of Mathematics, Martin Luther University Halle-Wittenberg*, and the *Center for Mathematics and Computer Science* (CWI) in Amsterdam.

Scientific Committee:

- Martin Arnold (Halle)
- Rüdiger Weiner (Halle)
- Ben P. Sommeijer (Amsterdam)
- Jan G. Verwer (Amsterdam)

Local organizers:
Martin Arnold, Alf Gerisch, Karin Helbich, Helmut Podhaisky, Rüdiger Weiner.

Acknowledgements

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Contents

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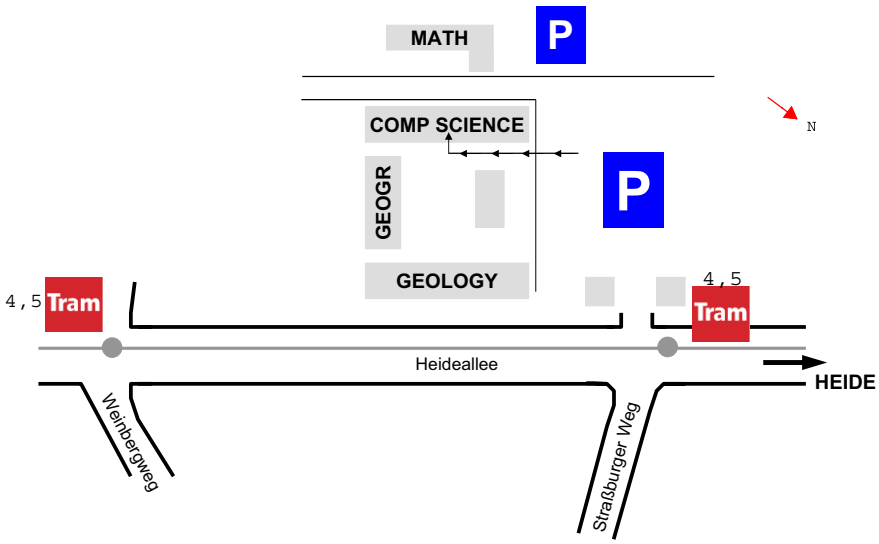
1 General Information

1. **Conference Site and Duration**
   The conference will take place in the lecture rooms of the Computer Science Building situated within the Weinberg Campus at Von-Seckendorff-Platz 1. There is a sufficiently large number of free parking spaces available.



   The conference will begin at 8:30 on Monday, 14 September 2009, and finish around 13:15 on Friday, 18 September 2009. Lectures will start each day at 8:30.

   To reach the conference site from the InterCity Hotel Halle-Neustadt we recommend to use the tram leaving in front of the hotel towards the city (direction "Hauptbahnhof" for line 9 and line 10 and direction "Beesen" for line 2). Then, get off at the third stop "Rennbahnkreuz" and change to a tram leaving from the track perpendicular to the arriving track (100 meter walk). You can use line 4 and line 5 (direction "Kröllwitz"). Get off at the third stop "Straßburger Weg".

2. **Conference Office and Registration**
   The conference office will be open on Sunday, 13 September 2009, from 17:00 to 20:00 in the lobby of the InterCity Hotel Halle-Neustadt. 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, 14 September 2009.

Please register at the conference office after your arrival. You will then also receive your conference documents. 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 3.28. For the minisymposia and the contributed talk sessions the following lecture rooms will be used in addition: 1.23, 1.26, 1.27, 1.29. All lecture rooms are in the building Von-Seckendorff-Platz 1 and will be clearly signposted.

   All lecture rooms will be equipped with laptop and data projector. The laptops will be prepared for presentations in PDF and Powerpoint format. Speakers should load their talk onto the conference laptop of their lecture room before the beginning of their allocated session. Any speaker requiring an overhead projector and/or other equipment should contact the organisers as soon as possible.

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 and as a guest you can pay in cash. Please ask local participants or the staff in the conference office for further information. A cafeteria is located at the ground floor of the conference site.

6. **Computer and Internet Access**
   Wireless internet access as well as computer terminals with internet access will be available for participants at the conference site. The necessary login information will be provided in the conference office.

7. **Conference Dinner**
   The conference dinner will be held in the InterCity Hotel Halle-Neustadt on Thursday, 17 September at 19:00. One dinner ticket is included in the conference fee; accompanying persons pay EUR 30. The fee for the dinner is payable in cash when registering in the conference office.

8. **Guided Tour on Wednesday afternoon**
   You are invited to an excursion to the city of Lutherstadt Wittenberg on Wednesday, 16 September (included in the conference fee). Busses will leave from the conference site at 13:00 and will return to Halle at around 19:30. In Wittenberg we will enjoy a guided tour through the historic city centre including a visit to the *Schlosskirche* (Castle Church). You will also have some time to visit one or two other attractions in Wittenberg or have a coffee, tea, or beer in one of the restaurants or cafés. *If you are interested then please register for the excursion at the conference office.*

9. **Conference Proceedings**
   The proceedings of NUMDIFF-12 will be published as a special issue of the IMACS Journal *Applied Numerical Mathematics*. Guest editors are M. Arnold, W. Hundsdorfer, J.G. Verwer and R. Weiner.

Every speaker of NUMDIFF-12 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.elsevier.com/locate/apnum`

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 2009. Manuscripts should be submitted electronically (in PDF or PS format and only a manuscript file) to

`Jan.Verwer@cwi.nl`

2 Programme Overview

Monday, September 14, 2009

	Room 3.28
8:30– 8:50	**Opening**
8:50– 9:40	Verwer
9:40–10:30	Bock
10:50–11:40	Guglielmi
11:40–12:30	Gerisch

	Room 3.28	**Room 1.26**	**Room 1.23**	**Room 1.29**
14:00–14:25	Steinebach	Garrappa	Farago	Busch
14:25–14:50	Jebens	Chistyakova	Forghani	Schierz
14:50–15:15	Bajars	Schiller	Saravi	Savcenco
15:15–15:40	Bourchtein, L.	Zegeling	Rahimpour	
16:10–16:35	Perez-Rodriguez	Horvath	Linel	Rößler
16:35–17:00	Portero	Bourchtein, A.	Guibert	Ferro
17:00–17:25	Beck	Zharovsky	Isaev	Augustin
17:25–17:50	Rang	Schlegel	Perminov	

Tuesday, September 15, 2009

	Room 3.28
8:30– 9:20	Leimkuhler
9:20–10:10	Jackiewicz

	Room 3.28	**Room 1.26**	**Room 1.23**	**Room 1.29**	**Room 1.27**
10:40–11:05	Hernandez-Abreu	Podhaisky	Mitsui	Ordokhani	Banifatemi
11:05–11:30	Arnold	d'Ambrosio	Weiner	Tsybulin	Yousefi
11:30–11:55	Hesch	Paternoster	Weiß	Kolpakov	Lutoshkin
11:55–12:20	Estevez Schwarz	Izzo	Chan	Govorukhin	Mittal

	Room 3.28	**Room 1.26**
	Minisymposium: *Adaptivity in Space and Time*	Minisymposium: *Numerical methods in weather & climate*
14:00-14:30	Dörfler	Bokhove
14:30-15:00	Veeser	Reich
15:00-15:30	Apel	Dubinkina
16:00-16:30	Huang	Wensch
16:30-17:00	Debrabant	Gaßmann
17:00-17:30	Vexler	Rhebergen
17:30–18:00		Horenko

Wednesday, September 16, 2009

	Room 3.28
8:30– 9:20	Hochbruck
9:20– 9:50	Butcher

	Room 3.28	**Room 1.26**	**Room 1.23**	**Room 1.29**	**Room 1.27**
10:20–10:45	Hill	Conte	Lang	Geiser	Schweitzer
10:45–11:10	Schmitt	Lopez-Fernandez	Zakharov	Günther	Shapeev
11:10–11:35	Mozartova	El Azab	Rakin	Huisinga	Sarmany

The busses for the excursion to Wittenberg will depart at 13:00 from the conference site.

Thursday, September 17, 2009

	Room 3.28
8:30– 9:20	Ascher
9:20–10:10	de Sterck

	Room 3.28	**Room 1.26**	**Room 1.23**	**Room 1.29**	**Room 1.27**
10:40–11:05	Ostermann	Pham	Brunk	Islam	Hollevoet
11:05–11:30	Hansen	Kuznetsov	Baumanns	Cardone	Bartoszewski
11:30–11:55	Emmrich	Weber	Marszalek	Jiwari	Pulch
11:55–12:20	Kramer	Mohaghegh	Jansen	Arabzadeh	Barikbin

	Room 3.28	**Room 1.26**
	Minisymposium: *Time integration in technical mechanics*	Minisymposium: *Stochastic differential equations*
14:00–14:30	Brüls	Buckwar
14:30–15:00	Krause	Kværnø
15:00–15:30	Schindler	Jentzen
16:00–16:30	Hartmann	Larsson
16:30–17:00	Acary	Ritter
17:00–17:30		Stanciulescu

Friday, September 18, 2009

	Room 3.28
8:30– 9:20	Iserles
9:20–10:10	Sanz-Serna
10:30–11:20	Oosterlee
11:20–12:10	Beyn
12:10–13:00	Simeon
13:00	**Closing**

3 Scientific Programme

Monday, September 14, 2009

Room 3.28

8:30– 8:50 **Opening**

8:50– 9:40 **Jan Verwer**
On the time integration of Maxwell's equations

9:40–10:30 **Hans-Georg Bock**
Realizing On-Line Optimal Control of Engineering Processes Based on Detailed DAE Models by the "Real-Time Iteration" Approach

10:30–10:50 **—— Break ——**

10:50–11:40 **Nicola Guglielmi**
Regularization of discontinuous ODEs with application to neutral delay differential equations

11:40–12:30 **Alf Gerisch**
Peer-Methods for Time-Dependent Finite Element Computations

12:30–14:00 **—— Lunch ——**

Room 3.28

14:00–14:25 **Gerd Steinebach**
Peer methods for the one-dimensional shallow water equations with CWENO space discretization

14:25–14:50 **Stefan Jebens**
Implicit Peer Methods for the Compressible Euler Equations

14:50–15:15 **Janis Bajars**
Structure-preserving discretization of internal wave attractors

15:15–15:40 **Ludmila Bourchtein**
On correct boundary conditions in numerical schemes for the shallow water equations

15:40–16:10 **—— Break ——**

16:10–16:35 **Soledad Perez-Rodriguez**
A variable time step–size code for advection-diffusion-reaction PDEs

16:35–17:00 **Laura Portero**
Variable step-size fractional step Runge-Kutta methods for time-dependent partial differential equations

17:00–17:25 **Steffen Beck**
Numerical Test of Krylov-Solvers in MATLAB

17:25–17:50 **Joachim Rang**
Adaptive time step control for the incompressible Navier-Stokes equations

Room 1.26

14:00–14:25 **Roberto Garrappa**
Numerical solution of semilinear systems of Fractional Differential Equations

14:25–14:50 **Elena Chistyakova**
Regularizing Properties of Difference Schemes for Singular Integral-Differential Equations

14:50–15:15 **Hagen Schiller**
Convergence of continuous approximations for discontinuous ODEs

15:15–15:40 **Paul Zegeling**
Analysis and Computation of Non-monotonous Travelling Waves in a Non-equilibrium Richard's Equation

15:40–16:10 **—— Break ——**

16:10–16:35 **Róbert Horváth**
Unconditionally stable time integration with operator splitting

16:35–17:00 **Andrei Bourchtein**
Semi-Lagrangian semi-implicit time splitting scheme for atmospheric model

17:00–17:25 **Evgeniy Zharovsky**
On the Numerical Solution of the Fokker-Planck Equation on Geodesic Grids

17:25–17:50 **Martin Schlegel**
Numerical Solution of Multiscale Problems in Atmospheric Modeling

Room 1.23

14:00–14:25 **István Faragó**
Mathematical modelling of fuel-cells with heterogenous parameter distribution

14:25–14:50 **Amir Ahmad Forghani**
Theoretical Modeling of a New Membrane Dual -Type Fischer-Tropsch Reactor in GTL Technology

14:50–15:15 **Masoud Saravi**
Numerical solution of Linear Ordinary Differential Equations in Quantum Chemistry by Spectral Methods

15:15–15:40 **M. R. Rahimpour**
Reduction of CO_2 Emission in FT Synthesis Using a Novel Combination of Fixed and Fluidized Hydrogen-permselective Membrane Reactor-Separator loop

15:40–16:10 **—— Break ——**

16:10–16:35 **Patrice Linel**
Parallel time integration of ODEs by symmetrization of the time interval

16:35–17:00 **David Guibert**
Parallel iterative time domain decompositions based on deferred correction methods for solving ODE systems

17:00–17:25 **Vadim Isaev**
On the Collocations and Least Squares Method Capabilities

17:25–17:50 **Valeriy Perminov**
Numerical solution of forest fire initiation problem

Room 1.29

14:00–14:25 **Martin Busch**
Co-Simulation Strategies for Coupled Multibody and Finite Element Models Incorporating Semi-Implicit Coupling Techniques

14:25–14:50 **Tom Schierz**
Stabilized modular time integration of coupled DAEs

14:50–15:15 **Valeriu Savcenco**
Partitioning strategies for multirate time stepping for DAEs

15:40–16:10 **—— Break ——**

16:10–16:35 **Andreas Rößler**
Multi-level Monte Carlo methods with higher order schemes for the weak approximation of the solution of SDEs

16:35–17:00 **Maria Ferro**
An Extension of Albrecht's Approach for Stochastic Differential Equations

17:00–17:25 **Florian Augustin**
Numerics of the Wiener-Askey calculus for ordinary differential equations with uncertain parameters

17:25–17:50

Tuesday, September 15, 2009

Room 3.28

8:30– 9:20 **Benedict Leimkuhler**
Stochastic-Dynamical Methods for Controlled Variables

9:20–10:10 **Zdzislaw Jackiewicz**
Search for Highly Stable General Linear Methods for Ordinary Differential Equations

10:10–10:40 **—— Break ——**

Room 3.28

10:40–11:05 **Domingo Hernández-Abreu**
An efficient family of strongly A-stable Runge-Kutta collocation methods for stiff systems and DAE's. Convergence results

11:05–11:30 **Martin Arnold**
Newmark like time integration methods for second order DAEs

11:30–11:55 **Christian Hesch**
A Uniform Framework for DAE Integrators in Flexible Multibody Dynamics

11:55–12:20 **Diana Estevez Schwarz**
Consistent initialization for structured DAEs

Room 1.26

10:40–11:05 **Helmut Podhaisky**
General linear methods with inherent Runge-Kutta stability for stiff problems

11:05–11:30 **Raffaele D'Ambrosio**
Highly stable two step collocation methods for stiff differential systems

11:30–11:55 **Beatrice Paternoster**
Two-step modified collocation methods with structured coefficient matrices for ordinary differential equations

11:55–12:20 **Giuseppe Izzo**
Continuous two-step peer methods for ODEs

Room 1.23

10:40–11:05 **Taketomo Mitsui**
"Look-Ahead" Linear Multistep Methods

11:05–11:30 **Rüdiger Weiner**
Efficient Global Error Estimation and Control in Explicit Parallel Peer Methods

11:30–11:55 **Daniel Weiß**
Stability of rational approximations to the exponential function with restricted denominator

11:55–12:20 **Tina Ming-Hua Chan**
Hopf algebra and the B-series with a new aspect

Room 1.29

10:40–11:05 **Yadollah Ordokhani**
Direct Walsh-Hybrid Method for Variational Problems

11:05–11:30 **Vyacheslav Tsybulin**
One-parameter family of steady states in the model of population dynamics
11:30–11:55 **Aleksandr Kolpakov**
Numerical procedure for solutions of a strongly nonlinear problem
11:55–12:20 **Vasily Govorukhin**
Calculation of vortex patch dynamics in inviscid incompressible fluid

Room 1.27

10:40–11:05 **Ehsan Banifatemi**
Numerical solution of Fredholm integral equations by using CAS wavelets
11:05–11:30 **Sohrab Ali Yousefi**
Ritz Legendre Multiwavelet Method for the Damped Generalized Regularized Long-Wave (DGRLW) Equation
11:30–11:55 **Igor Lutoshkin**
The parameterization method for numerical solution of delay singular differential equations
11:55–12:20 **Ramesh Chand Mittal**
Higher Order Method for Burger's Equation

Room 3.28

Minisymposium: Adaptivity in Space and Time
14:00-14:30 **Willy Dörfler**
Convergence and optimality results in adaptive FEM
14:30-15:00 **Andreas Veeser**
Convergence of space-adaptive algorithms
15:00-15:30 **Thomas Apel**
Anisotropic finite elements for singularly perturbed model problems
15:30-16:00 **—— Break ——**
16:00-16:30 **Weizhang Huang**
An anisotropic mesh adaptation method for the finite element solution of variational problems
16:30-17:00 **Kristian Debrabant**
On global error control for parabolic PDEs
17:00-17:30 **Boris Vexler**
Goal Oriented Space-Time Adaptivity for Simulation and Optimization of Parabolic Systems

Room 1.26

Minisymposium: Numerical methods in weather & climate
14:00–14:30 **Onno Bokhove**
Simulations of hybrid Rossby-shelf modes in a laboratory ocean
14:30–15:00 **Sebastian Reich**
Data assimilation using continuous ensemble Kalman filters
15:00–15:30 **Svetlana Dubinkina**
Statistically accurate simulations for atmospheric flows

15:30–16:00 **—— Break ——**

16:00–16:30 **Jörg Wensch**
Simulation of an isentropic layer model by particle methods

16:30–17:00 **Almut Gaßmann**
Nonhydrostatic atmospheric modeling on icosahedral grids

17:00–17:30 **Sander Rhebergen**
Discontinuous Galerkin finite element method for shallow two-phase flows

17:30–18:00 **Illia Horenko**
Computational Time Series Analysis of Multidimensional Non-Stationary Data

Wednesday, September 16, 2009

Room 3.28

8:30– 9:20 **Marlis Hochbruck**
Time integration meets inverse problems

9:20– 9:50 **John Butcher**
Long term integration using general linear methods

9:50–10:20 **—— Break ——**

Room 3.28

10:20–10:45 **Adrian Hill**
G-matrices for algebraically stable general linear methods

10:45–11:10 **Bernhard A. Schmitt**
On algebraic stability of general linear methods and peer methods

11:10–11:35 **Anna Mozartova**
Monotonicity and boundedness properties of general linear methods.

Room 1.26

10:20–10:45 **Dajana Conte**
Two-step diagonally–implicit collocation–based methods for Volterra Integral Equations

10:45–11:10 **María López-Fernández**
A Quadrature Based Method for Evaluating the Exponential-Type Functions for Exponential Methods

11:10–11:35 **Tamer El-Azab**
Exponential Peer Methods

Room 1.23

10:20–10:45 **Holger Lang**
Numerical aspects in the dynamic simulation of geometrically exact rods

10:45–11:10 **Alexander Zakharov**
Numerical modeling of kinetics of radiation defect clusters nucleation and radiation-induced swelling in graphite

11:10–11:35 **Sergei Rakin**
Numerical analysis of homogenized tunability of composite material

Room 1.29

10:20–10:45 **Jürgen Geiser**
Iterative Splitting Schemes as time integration methods: Theory and Application

10:45–11:10 **Michael Günther**
Exponential Smoothing Splines for Spot Market Price Simulation

11:10–11:35 **Wilhelm Huisinga**
Global Sensitivity Analysis of Ordinary Differential Equations via solution of the associated PDE problem

Room 1.27

10:20–10:45 **Julia Schweitzer**
Numerical Simulation of Relativistic Laser-Plasma Interaction

10:45–11:10 **Vasily Shapeev**
Three Dimensional Numerical Simulation of Thin Metal Plates Laser Welding

11:10–11:35 **Domokos Sarmany**
DG vs Nedelec in the finite element time-domain computations of the second-order Maxwell equations

Thursday, September 17, 2009

Room 3.28

8:30– 9:20 **Uri Ascher**
Surprising computations

9:20–10:10 **Hans De Sterck**
Efficient numerical simulation of stationary Euler fluid flows with critical points and shocks

10:10–10:40 **—— Break ——**

Room 3.28

10:40–11:05 **Alexander Ostermann**
Operator splitting methods: analysis and convergence

11:05–11:30 **Eskil Hansen**
High order splitting methods for semigroups

11:30–11:55 **Etienne Emmrich**
Time discretisation of nonlinear evolution problems

11:55–12:20 **Felix Kramer**
Strang Splitting for Reaction-diffusion Equations

Room 1.26

10:40–11:05 **Duc Toan Pham**
Proper Orthogonal Decomposition in Decoupling Large Dynamical Systems

11:05–11:30 **Evgenii Kuznetsov**
Numerical solution of DAE's using method of continuation with respect to a parameter

11:30–11:55 **Steffen Weber**
Quasistatic approximations for stiff second-order differential equations

11:55–12:20 **Kasra Mohaghegh**
Model order reduction for differential algebraic equations using the direct approach.

Room 1.23

10:40–11:05 **Markus Brunk**
Positivity preserving discretization of time dependent semiconductor model equations

11:05–11:30 **Sascha Baumanns**
Consistent initialization of partial-differential-algebraic equations for circuit simulation

11:30–11:55 **Wieslaw Marszalek**
Mixed-Mode Oscillations in a Modified Chua's Circuit

11:55–12:20 **Lennart Jansen**
Effective numerical circuit simulation regarding the variation in parameters

Room 1.29

10:40–11:05 **Md. Shafiqul Islam**
Numerical solutions of differential equations on using Bernoulli polynomials

11:05–11:30 **Angelamaria Cardone**
Multistep collocation methods for Volterra Integro-Differential Equations

11:30–11:55 **Ram Jiwari**
Construction of Higher Order Numerical Method

11:55–12:20 **Bahman Arabzadeh**
Numerical solution of variational problems using the hybrid of Block-pulse and Hartly functions

Room 1.27

10:40–11:05 **Davy Hollevoet**
Exponential fitting and deferred correction for BVPs

11:05–11:30 **Zbigniew Bartoszewski**
Numerical solution of boundary value problems for differential equations with deviating argument by ε-fixed points

11:30–11:55 **Roland Pulch**
Polynomial Chaos for Boundary Value Problems of Dynamical Systems

11:55–12:20 **Zahra Barikbin**
Bernstein Ritz method for solving boundary value variational problems

Room 3.28

Minisymposium: Time integration in technical mechanics

14:00-14:30 **Olivier Brüls**
Lie group vs. classical time integrators in multibody dynamics: formulations and numerical benchmarks

14:30-15:00 **Rolf Krause**
Preserving accuracy and stability in the numerical integration of dynamic contact problems

15:00-15:30 **Thorsten Schindler**
Spatial Simulation of Pushbelt CVTs with Timestepping Schemes

15:30-16:00 **—— Break ——**

16:00-16:30 **Stefan Hartmann**
High-order time integration in structural finite element analysis based on material non-linearities

16:30-17:00 **Vincent Acary**
Higher order schemes for nonsmooth mechanical systems

17:00-17:30

Room 1.26

Minisymposium: Stochastic differential equations

14:00–14:30 **Evelyn Buckwar**
Linear stability analysis for stochastic Theta-methods applied to systems of SODEs

14:30–15:00 **Anne Kværnø**
B-series analysis of stochastic Taylor methods

15:00–15:30 **Arnulf Jentzen**
Taylor expansions for stochastic partial differential equations

15:30–16:00 **—— Break ——**

16:00–16:30 **Stig Larsson**
Finite element approximation of the stochastic wave equation

16:30–17:00 **Klaus Ritter**
Multi-level Algorithms for Stochastic Heat Equations

17:00–17:30 **Vasile Stanciulescu**
Numerical solution of the Dirichlet problem for linear parabolic stochastic partial differential equations based on averaging over characteristics

Friday, September 18, 2009

Room 3.28

8:30– 9:20	**Arieh Iserles** Asymptotic numerics of highly oscillatory equations
9:20–10:10	**J. M. Sanz-Serna** Analytical averaging, numerical ordinary differential equations and multiscale methods
10:10–10:30	**—— Break ——**
10:30–11:20	**Cornelis W. Oosterlee** Numerical Mathematics Aspects of Computational finance
11:20–12:10	**Wolf-Jürgen Beyn** The freezing method for dynamical patterns in equivariant PDEs
12:10–13:00	**Bernd Simeon** Solving Transient Saddle Point Problems in Computational Mechanics
13:00	**Closing**

4 Abstracts

Higher order schemes for nonsmooth mechanical systems
Vincent Acary

The work is devoted to the study of new high resolution and higher order time integration methods for nonsmooth multibody systems. The term "high resolution" applies to methods that are at least first order methods when non smooth events are encountered and of higher order on smooth solutions. We focus our work on event-capturing methods where accurate findings of events are not performed. Most well-known instances of Nonsmooth Multibody Systems are the mechanical systems subjected to perfect unilateral constraints, systems subjected to unilateral contact with Coulomb's friction or systems with impacts. In this work, we will focus on Lagrangian dynamical systems with unilateral constraints and impacts, i.e.

$$\begin{cases} M(q)\dot{v}(t) = F(t,q(t),v(t)) + \nabla_q g(t,q(t))\lambda, \\ \dot{q}(t) = v(t), \\ y = g(t,q(t)), \\ 0 \leq y \perp \lambda \geq 0, \\ v^+(t) = \mathcal{F}(v^-(t),q(t),t). \end{cases} \tag{1}$$

In this work, we propose adaptive time–step strategies for standard time-stepping schemes (Moreau's time stepping scheme) and we derive a new time-stepping scheme based on rough localization of events. The performance of these new schemes will be shown on standard academic examples such as a bounding ball with accumulation of impacts, linear impacting oscillator and double pendulum with impacts. This work paves the way to new schemes for an efficient numerical time integration of non smooth mechanical and raises some open problems about the order of accuracy of standard time–stepping schemes for general non smooth systems.

Highly stable two step collocation methods for stiff differential systems
Raffaele D'Ambrosio, Z. Jackiewicz

We describe a class of two-step continuous methods for the numerical integration of initial-value problems based on stiff ordinary differential equations (ODEs). These methods generalize the class of two-step Runge–Kutta methods. The coefficients of these formulas were obtained by relaxing some of the collocation conditions to derive methods with desirable stability properties. We restrict our attention to methods of order $p = m$ and stage order $q = p$ to avoid order reduction phenomenon for stiff equations, and determine some of the parameters to reduce the contribution of high order terms in the local discretization error. Moreover, we enforce the methods to be A-stable and L-stable.
We derive methods with $p = q = m$ for $m = 1, 2, 3, 4$ and estimate the local error and terms of order $O(h^{p+2})$. These estimates and their filtered versions will aid the implementation of these methods in variable step size-variable order environment. The results of some numerical experiments which indicate the effectiveness of two-step collocation methods and reliability of local error estimation will also be presented.

References

[1] R. D'Ambrosio, M. Ferro, Z. Jackiewicz, B. Paternoster, *Two-step almost collocation methods for ordinary differential equations*, in press on Numerical Algorithms (doi: 10.1007/s11075-009-9280-5)

[2] R. D'Ambrosio, Z. Jackiewicz, *Continuous two–step Runge–Kutta Methods for ordinary differential equations*, submitted

[3] R. D'Ambrosio, Z. Jackiewicz, *Construction and implementation of highly stable two-step collocation methods for stiff differential systems*, in preparation.

Anisotropic finite elements for singularly perturbed model problems

Thomas Apel

Anisotropic meshes are characterized by elements with large or even asymptotically unbounded aspect ratio. Such meshes are known to be particularly effective for the resolution of directional features of the solution, like edge singularities and boundary layers.
In the talk we survey a posteriori error estimates for discretizations with anisotropic meshes. We focus on results obtained by and with collaborators for singularly perturbed model problems: a linear reaction-diffusion equation, an anisotropic diffusion model equation, and a simplified shell model.

Numerical solution of variational problems using the hybrid of Block-pulse and Hartly functions

Bahman Arabzadeh

A numerical method for solving variational problems is presented in this paper. The method is based upon hybrid of Hartly functions approximations. The properties of hybrid functions which are the combinations of block-puls functions and Hartly functions are first presented. The operational matrix of integration is then utilized to reduce the variational problems to the solution of algebraic equations. Illustrative examples are included to demonstrate the validity and applicability of the technique.

Newmark like time integration methods for second order DAEs
Martin Arnold

Newmark like time integration methods exploit the second order structure of the equations of motion in structural dynamics. The most popular time integration methods of Newmark type are the HHT method and the generalized-α method that are unconditionally stable in the linear case and converge with order $p = 2$ in all solution components if the method coefficients are defined appropriately.
Recently, these methods were extended to constrained mechanical systems that are represented by second order DAEs of index 3. The generalization to mixed first and second order systems with additional algebraic equations is straightforward.
Standard techniques of DAE theory like index reduction and a convergence analysis based on coupled error recursions in differential and algebraic components may be used successfully to define and to analyse these Newmark like DAE integrators. Second order convergence is shown for the equations of motion in index-3 form and in an appropriate extension of the Gear-Gupta-Leimkuhler formulation that is tailored to constrained mechanical systems in multidisciplinary applications.

Surprising computations
Uri Ascher

Computer simulations for differential equations (DEs) often require complex numerical methods. It is important and often difficult to devise efficient methods for such purposes and to prove their properties. The resulting computations usually produce expected results, at least qualitatively, which in itself does not diminish the importance of the numerical methods.
Occasionally, however, one comes across a (correct) computation that yields surprising results. In the process of writing a textbook on numerical methods for time dependent DEs I have encountered some such, and this talk describes several instances including solving Hamiltonian systems, KdV and NLS, and applying WENO methods for nonlinear conservation laws. What can be qualified as "surprising" is of course a subjective matter, nonetheless the combined effect of this talk hopefully sheds light on using marginally stable methods for solving marginally stable problems.

Numerics of the Wiener-Askey calculus for ordinary differential equations with uncertain parameters
Florian Augustin, P. Rentrop

In the last two decades the Wiener-Askey calculus for solving ordinary differential equations with uncertain parameters has drawn considerable attention. To handle uncertainties Monte-Carlo methods are often applied. Although these sampling based methods are easy to perform they may suffer from bad convergence, especially in the approximation of higher moments. In contrast, the Wiener-Askey calculus is based on the functional dependence between the solution process and the uncertain parameters. Dependent on the distribution of the random data, the solution process is decomposed into a series of orthogonal polynomials. Thereby the orthogonality is induces by the inner product in L_2 with respect to the probability measure of the data. By using a Galerkin projection the random dependent ordinary differential equation is reduced to a system of deterministic ordinary differential equations. But the application of this method reveals to be capricious in many cases. The discussion of the possibilities and drawbacks of the Wiener-Askey calculus will be the scope of this talk.

Numerical solution of Fredholm integral equations by using CAS wavelets
Ehsan Banifatemi

A numerical method for solving the Fredholm integral equations is presented. The method is based upon CAS wavelet approximations. The properties of CAS wavelet are first presented. CAS wavelet approximations method are then utilized to reduce the Fredholm integral equations to the solution of algebraic equations. Illustrative examples are included to demonstrate the validity and applicability of the technique.

Structure-preserving discretization of internal wave attractors
Janis Bajars

Internal waves in stratified fluids exhibit the phenomenon of wave attractors, whereby the energy is focused on a low-dimension manifold. To distinguish the relevant physical processes, we consider structure/symmetry preserving discretizations in forced-dissipative case. We discuss relevant structure, and give numerical illustrations.

Bernstein Ritz method for solving boundary value variational problems
Zahra Barikbin, S. A. Yousefi

A direct method for solving boundary value variational problems using a modified Bernstein polynomial basis is presented. The approximation of the problem is based on the modified Bernstein polynomial basis. The properties of Bernstein polynomials are first presented. The method expands the desired solution in terms of a set of continuous polynomials over a closed interval and then makes use of the Ritz method to determine the expansion coefficients to construct a solution. However, accuracy and efficiency are dependent on the size of the set of Bernstein polynomials. The current procedure is implemented to solve variational problems in three cases, when functionals depending on several functions and their first derivatives, functionals depending on higher-order derivatives and functionals depending on functions of several independent variables. Illustrative examples are included to demonstrate the validity and applicability of the technique.

Numerical solution of boundary value problems for differential equations with deviating argument by ε-fixed points
Zbigniew Bartoszewski

The talk will be devoted to certain approximation of a continuous operator mapping the metric space into itself by means of operators transforming finite dimensional metric spaces into themselves as well as to approximations of fixed-points of this operator by so called ε-fixed-points of finite dimensional operators. Examples of applications of this kind of approximations to construction of numerical methods of solution of boundary value problems for differential equations with deviating argument will be presented.
The convergence of the resulting methods under assumption that the right-hand sides of the differential equations are continuous and the problems have unique solutions is proved. Numerical results for a number of examples and a comparison with the results obtained with other numerical methods applied to these examples will also be given.

Consistent initialization of partial-differential-algebraic equations for circuit simulation

Sascha Baumanns, Monica Selva Soto, Caren Tischendorf

Modeling circuits that contain semiconductor devices may lead to a coupled system of differential-algebraic equations (DAEs) and partial-differential equations (PDEs), i. e. a system of partial-differential-algebraic equations (PDAEs) describes the circuit in this case.
The spatial discretization of the PDEs in the coupled system leads to a DAE that may be formulated with a properly stated leading term. For a successful numerical integration of this DAE a consistent initialization is needed. Under certain topological conditions it can be shown that the tractability index does not exceed two.
Exploiting the special DAE structure and using an index reduction, we can compute a consistent initialization within two steps. Firstly, we start up from a possibly inconsistent initialization by determining an operation point. Secondly, a linear system is solved for correcting the operation point such that the hidden constraints in the index two case are also satisfied.
Here we present the coupled PDAE system and uncover some structural properties of the resulting DAE after spatial discretization. An algorithm for the calculation of a consistent initialization for that DAE is proposed and some examples are computed.

Numerical Test of Krylov-Solvers in MATLAB

Steffen Beck, Rüdiger Weiner

We discuss the application of peer methods with Krylov techniques to large stiff systems of ordinary differential equations. Peer methods are characterized by a high stage order and therefore they do not suffer from order reduction for very stiff systems. This makes them well suited for semi-discretized partial differential equations. The methods are implemented and tested in MATLAB. We present numerical results for 2D-MOL-systems and compare them with the MATLAB codes ROWMAP (Podhaisky/Weiner/Schmitt/Beck) and EXP4 (Hochbruck/Lubich/Selhofer).

The freezing method for dynamical patterns in equivariant PDEs

Wolf-Jürgen Beyn, Vera Thümmler, J. Lorenz

Typical examples of dynamical patterns occuring in reaction diffusion systems are traveling waves in one, spiral waves in two, and scroll waves in three space dimensions. We consider the solution of Cauchy problems on unbounded domains that converge asymptotically to such spatio-temporal patterns. We introduce the freezing method that aims at computing a time-dependent coordinate frame in which the solution converges to a stationary spatial pattern. Using equivariance with respect to the action of a Lie group the underlying PDE is transformed into a partial differential algebraic equation (PDAE) which is subsequenty solved by truncating to a bounded domain and by discretizing in space and time. Several features of this approach are discussed, such as the longtime behavior of the PDAE near stable patterns, the relation to spectral properties, and the extension of the method to hyperbolic equations and to systems with multiple structures.

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Realizing On-Line Optimal Control of Engineering Processes Based on Detailed DAE Models by the "Real-Time Iteration" Approach

Hans-Georg Bock

One of the most promising control approaches in process engineering is the idea to use detailed, possibly first principle differential equation models to predict the performance of a process under perturbations over a certain horizon, and to compute on-line an optimal decision and control strategy, subject to constraints. However, even the fastest "all-at-once" optimization BVP solvers available today are much too slow to provide a quick enough optimal control response for fast processes. The lecture will report on recent progress in dedicated real-time optimization algorithms that have produced a speed-up in response time, which gains several orders of magnitude over standard approaches.
Starting from an "all-at-once" off-line approach based on the direct multiple shooting method, inexact SQP or Gauss-Newton methods, and a perturbation embedding, a "real-time iteration" (RTI) approach is presented, that uses the latest process data at each iteration of the optimization process. Through precomputation of Hessians, gradients and QP factorizations the response time to perturbations of states and systems parameters is minimized. It is shown how this approach is further drastically accelerated by special algorithmic schemes for on-line feasibility and optimality improvement (FOI), and a primal-dual on-line active set strategy (OASeS). The new methods are capable of solving constrained optimal (closed-loop) control problems even of very fast processes modeled by DAE on-line. Theoretical results as well as applications to real-life problems in engineering will be presented.

Simulations of hybrid Rossby-shelf modes in a laboratory ocean

Onno Bokhove

Idealized laboratory experiments reveal the existence of forced dissipative hybrid Rossby shelf modes. The laboratory ocean consists of a deeper ocean accommodating basin/ocean scale Rossby modes, and a coastal step shelf accommodating trapped shelf modes. Planetary Rossby modes are mimicked in the laboratory via a uniform topographic slope in the North-South direction. Hybrid modes are found as linear modes in numerical calculations and similar streamfunction patterns exist in streak photography of the rotating tank experiments. These numerical calculations are based on depth-averaged potential vorticity dynamics with Ekman forcing and damping. Nonlinear calculations explore the deficiencies observed between reality and the linear solutions. The aim of the work is twofold: to show that idealized hybrid Rossby shelf modes are at least laboratory reality, and to contribute in a general sense to the discussion on the coupling and energy exchange associated with hybrid modes between shallow coastal seas and deep ocean basins. Discontinuous Galerkin finite element methods have been used for the simulations. The corresponding energy and entrophy conservative and stable numerical discretization will be discussed.

Semi-Lagrangian semi-implicit time splitting scheme for atmospheric model

Andrei Bourchtein, Ludmila Bourchtein

A semi-Lagrangian semi-implicit finite difference scheme with time splitting corresponding to multi-scale nature of the atmospheric dynamics is developed for the nonhydrostatic atmospheric model. The principal elements of the scheme are solution of the trajectory equations for advective part, separation of the vertical normal modes in fast and slow parts with respect to gravity wave propagation speed of each mode, explicit and simpler approximation of slower vertical modes and implicit time differencing for faster modes. This approach allows choosing time step based on accuracy considerations and replacing the 3D elliptic problem inherent for semi-implicit differencing by a set of 2D elliptic problems. The performed numerical experiments show computational efficiency of the proposed scheme and accuracy of the predicted atmospheric fields.

On correct boundary conditions in numerical schemes for the shallow water equations

Ludmila Bourchtein, Andrei Bourchtein

In the atmosphere-ocean regional models, the initial conditions are supplied by data assimilation schemes and boundary conditions are usually provided by a global model. Therefore, the values of almost all prognostic fields are usually available on the domain boundary and there are many options for specification of boundary conditions.
In this study our concern is a non-physical growth of solutions leading to numerical blow-up in the cases when the choice of boundary conditions seems to be physically justifiable and the initial boundary value problem for the primitive differential systems is well posed. This growth can be observed in both conditionally and absolutely stable numerical schemes and it can be eliminated by reducing the time step. Since the periodic numerical problem is conditionally or absolutely stable, such behavior points out that instability of computations is related to used boundary conditions.
We study this problem in a simplified model of one-dimensional gravity waves, which allows us to perform complete analysis of the stated problem and reveal the causes of such instability. Based on performed analysis and numerical experiments, some recommendations for choosing the boundary conditions are given to avoid this non-physical behavior of numerical solutions.

Lie group vs. classical time integrators in multibody dynamics: formulations and numerical benchmarks

Olivier Brüls, Alberto Cardona

The dynamics of flexible multibody systems with large rotations is often described using large sets of index-3 differential-algebraic equations. In this context, the Lie group structure of the dynamic system may be exploited in order to provide an elegant solution to the rotation parameterization problem.
The talk discusses an original Lie-group extension of the classical generalized-alpha method, which can be used to solve index-3 differential-algebraic equations in multibody dynamics. Second-order accuracy is demonstrated at least in the unconstrained case and the performance is illustrated on several critical benchmarks with high rotational speeds. The remarkable simplicity of the new algorithms opens some interesting perspectives for real-time applications, model-based control and optimization of multibody systems.

Positivity preserving discretization of time dependent semiconductor model equations

Markus Brunk, Anne Kværnø

In simulation of integrated circuits the inclusion of distributed models for semiconductor devices becomes desirable, as they allow for more accurate results by inclusion of thermal or quantum effects, for instance.
For those models discretization schemes are preferred which keep physical properties also for the discrete solutions. For a class of drift-diffusion-like models we employ a mixed finite element scheme leading to a positive DAE or ODE system for particle densities.
Index results for the corresponding system and the coupled system of network and device equations are stated.
Finally, for time integration of the device system we introduce a simple splitting technique based on one-step methods, exponential integration and a Gummel-type iterative solver. For adequate mesh size this allows for efficient second order positivity preserving time integration of the transient semiconductor model equations.

Linear stability analysis for stochastic Theta-methods applied to systems of SODEs

Evelyn Buckwar, Conall Kelly, Thorsten Sickenberger

An important issue arising in the analysis of numerical methods for approximating the solution of a differential equation is concerned with the ability of the methods to preserve the asymptotic properties of equilibria. For stochastic ordinary differential equations investigations in this direction have mainly focussed on scalar equations so far. In this talk I will first examine the structure of stochastic perturbations that are known to a.s. stabilise or destabilise the equilbrium solutions of systems of differential equations. These perturbation structures, encoded in the diffusion coefficient matrix of a linear system, will provide the basis for choosing test equations. Then I will present a mean-square and a.s. stability analysis of the Theta-discretisations of these test equations. The talk is based on joint work with Conall Kelly and Thorsten Sickenberger.

Co-Simulation Strategies for Coupled Multibody and Finite Element Models Incorporating Semi-Implicit Coupling Techniques

Martin Busch, Bernhard Schweizer

Standard coupling methods - e.g. explicit multirate approaches with equidistant communication time grids - may entail enormous CPU times or may practically even fail, because very small communication time steps have to be chosen in order to obtain a stable solution.
To stabilize the solution process, a semi-implicit coupling approach is presented, which also allows the application of a non-equidistant communication time grid. In this context, a straightforward strategy for controlling the macro time steps is discussed.
The semi-implicit coupling technique is used for coupling a commercial MBS-Code with a commercial FEA-Code. As a practical example, we consider a hybrid nonlinear rotor/bearing model of a high-speed turbine. The rotor is modeled as a flexible multibody system. For calculating the bearing reactions, a finite element discretization is applied. Both codes are coupled via interprocess communication (IPC). A time-efficient semi-implicit implementation is achieved by a parallel approach on multiple CPUs.

Long term integration using general linear methods

John Butcher

For one-step methods, the ability to perform reliable integrations for extended time periods, at least for appropriate problem classes, depends on a number of attributes, such as time-symmetry and the symplectic property. In the case of general linear methods, similar requirements are

needed with symplectic behaviour generalized to G-symplectic behaviour. An additional complication is the possible presence of parasitic terms which inevitably corrupt the numerical results for time-symmetric linear multistep methods. However, it is possible to eliminate this effect in the case of general linear methods. This talk will discuss these issues and the possible construction of implementable high-order methods which work well over extended time intervals.

Multistep collocation methods for Volterra Integro-Differential Equations

Angelamaria Cardone, Dajana Conte, Beatrice Paternoster

Volterra Integro-Differential Equations (VIDEs) are models of evolutionary problems with memory in many applications. Generally, the numerical treatment of such equations leads to an high computational cost, especially due to the computation of the "lag–term", which contains the past history of the phenomenon. As it is well known, a collocation method is based on the idea of approximating the exact solution of a given equation with a suitable function belonging to a chosen finite dimensional space, usually a piecewise algebraic polynomial, which satisfies the equation exactly on a certain subset of the integration interval (called the set of collocation points). Multistep collocation methods and two-step Runge-Kutta methods have been already developed in the context of Ordinary Differential Equations [3] and Volterra Integral Equations [1,2]. In this talk we describe the derivation of multistep collocation methods for VIDEs, where the numerical solution depends on the approximation of the solution in a fixed number of previous time–steps, instead of only one step, as in the standard collocation. This approach allows to increase the order of classical one–step methods, without any increase of the computational cost. We analyze the order of convergence of the proposed methods and provide the stability analysis.

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Hopf algebra and the B-series with a new aspect

Tina Ming-Hua Chan

In this paper, the links between Hopf algebra and the B-series are presented. In Butcher's approach, the composition rules and the inverse operators are generated recursively using the dual space of the tree space. The non-commutative feature of the tree product by Butcher 1972 is the main reason for generating these important operators on the dual space. This causes the complexity of generating these operators. In Hopf algebra approach, the co-product, and anti-pode are two operators which generate the composition rules and the inverse operators. However, these operators are not presented recursively in Hopf algebra. The authors propose to generate the tree space using the forest space. The product on the forest is commutative which breaks the limitation of the tree product. By applying linear operators defined on the forest space and the tree space to the Banach space, we are able to derive recursive formulas of composition rules and inverse operators in an explicit way. The new aspect of applying linear operators on the forest space and the tree space to Banach space is found to have wilder applications on deriving results of integration methods.

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Regularizing Properties of Difference Schemes for Singular Integral-Differential Equations

Elena Chistyakova

We consider systems of integral-differential equations with a singular matrix multiplying the derivative of the desired vector-function. Such systems appear in many applications, in particular, when modelling electric and hydraulic circuits. These systems are ill-posed problems, i.e. small perturbations (noise) in the initial data lead to significant changes in the solution. It has been proved that some difference schemes, applied to the specified class of the systems considered, possess the property of self-regularization. This means that the numerical process is stable with respect to perturbation of the initial data if we take a corresponding step of discretization.

Two-step diagonally–implicit collocation–based methods for Volterra Integral Equations

Dajana Conte, R. D'Ambrosio, B. Paternoster

It is the purpose of this talk to introduce a family of diagonally–implicit continuous methods for the numerical integration of Volterra Integral Equations, which are obtained as a modification of the class of two-step collocation methods introduced in [1, 2]. The derived methods result from the choice of suitable conditions to be satisfied by the collocation polynomial and from the application of special quadrature formulae for the approximation of the increment term, in such a way that the coefficient matrix of the nonlinear system for the computation of the internal stages is lower triangular. The constructed methods have an high uniform order of convergence together with strong stability properties (e.g A-stability). Moreover, the structured shape of the coefficient matrix can be suitably exploited in order to get an efficient implementation in a parallel environment. We present the constructive technique, discuss the order of convergence and provide numerical experiments that confirm the theoretical expectations.

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On global error control for parabolic PDEs

Kristian Debrabant, Jens Lang

In this talk we will report on some joint activities with Jan Verwer (CWI) regarding efficiency and reliability questions for finite difference approximations of parabolic problems. First, systems of ODEs are considered. Existing popular codes focus on efficiency by adaptively optimizing time grids in accordance to local error control. The reliability question, that is, how large are the global errors, has received much less attention. We have implemented 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 Runge-Kutta-Rosenbrock method ROS3P as example integrator, that the classical approach is remarkably reliable. For finite difference approximations of parabolic PDEs, the ODE approach is combined with estimates for the spatial truncation errors based on Richardson extrapolation. Numerical examples are used to illustrate the reliability of the estimation and control strategies.

Sigma transformation and ALE formulation for three-dimensional free surface flows

Astrid Decoene

In three-dimensional free surface flows the movement of the domain is a critical feature. of the domain in three-dimensional Several techniques exist to deal with its treatment. Among them, the Arbitrary Lagrangian Eulerian (ALE) approach has been adopted by many authors because of its great adaptability. It consists in moving the mesh at an arbitrary velocity which should be different from the fluid velocity, allowing for a continuous updating of the mesh. Another widely used technique, especially in the atmospheric and oceanographic communities, is referred to as the sigma transformation or topography-following coordinate system. It consists in performing a transformation of the vertical coordinate – the z-coordinate – allowing to adopt a vertical discretization of the domain which at each time step follows the bathymetry and the free surface. Different systems have been developed on this approach, characterized by the choice of the discrete transformation function. To our knowledge, the link between both approaches is not clearly established in the literature. We establish the link between the sigma transformation approach and the ALE approach. For that purpose we introduce the ALE-Sigma (ALES) approach, which consists in an ALE interpretation of the sigma transformation. Taking advantage of this new approach, we propose a general ALES transformation, allowing for a great adaptability of the vertical discretization and therefore overcoming some drawbacks of the classical sigma transformation. We present numerical results, showing the advantages of this general coordinate system, as for example a better representation of horizontal stratifications.

Efficient numerical simulation of stationary Euler fluid flows with critical points and shocks
Hans De Sterck

In this presentation we will discuss efficient numerical methods for ODE and PDE systems that describe stationary compressible Euler fluid flows in which transitions from subsonic to supersonic flow occur. It is well-known that flow solutions of this type are hard to compute numerically using the stationary form of the
equations. Therefore, time marching methods with explicit or implicit time integration are normally employed. However, the computational complexity of the time marching approach is far from optimal, because convergence tends to be slow and tends to slow down even more as resolution increases.
In this talk we explore the alternative of solving the stationary equations directly, which is a viable approach when the solution topology is known in advance. We first present a solution method for one-dimensional flows with critical points. The method is based on a dynamical systems formulation of the problem and uses adaptive integration combined with a two-by-two Newton shooting method. Example calculations show that the resulting method is fast and accurate. A sample application area for this method is the calculation of transonic hydrodynamic escape flows from extrasolar planets and the early Earth, and the method is also illustrated for quasi-one-dimensional nozzle flow and black hole accretion. The method can be extended easily to handle flows with shocks, using a Newton method applied to the Rankine-Hugoniot relations. Extension to flows with heat conduction is also discussed. The presentation will conclude with some thoughts on how the approach presented can be generalized to problems in higher dimensions.

Convergence and optimality results in adaptive FEM
Willy Dörfler

An Adaptive Finite Element Method can be seen as an iterative solver for a PDE for a prescribed tolerance. This process includes the solution of the discrete problem, the a posteriori error estimation, the selection of the elements for local refinement and the construction of a new mesh. The problem of convergence of such an iteration has now been solved in various situations. Independent of that, it is important to know, whether the resulting meshes are in some sense the best one can get. Answers to this questions have been found in the last years.

Statistically accurate simulations for atmospheric flows
Svetlana Dubinkina, Jason Frank

A Hamiltonian particle-mesh method for quasi-geostrophic potential vorticity flow is proposed. The microscopic vorticity field at any time is an area- and energy-conserving rearrangement of the initial field. We construct a statistical mechanics theory to explain the long-time behavior of the numerical solution. The statistical theory correctly predicts the spatial distribution of particles as a function of their point vorticity. A nonlinear relation between the coarse grained mean stream function and mean vorticity fields is predicted, consistent with the preservation of higher moments of potential vorticity reported in [R. V. Abramov, A. J. Majda 2003, PNAS 100 3841–3846].

Exponential Peer Methods
Tamer El-Azab, Rüdiger Weiner

We present a new class of exponential integrators, *Exponential Peer Methods (EPM)*, for the solution of stiff differential systems. The construction of methods of order $p = s - 1$, s the number of stages,with good stability properties are discussed. Numerical tests of EPM and comparison with exponential integrators of the Expint package are given.

Time discretisation of nonlinear evolution problems
Etienne Emmrich

The mathematical formulation of time-dependent problems in science and engineering often leads to the initial-value problem for a nonlinear evolution equation of first or second order. Typical examples are the equations arising in fluid dynamics or elasticity theory.
In this talk, we present new results on the convergence of several standard numerical methods, focussing on the temporal semi-discretisation on uniform as well as non-uniform time grids. Examples are the two-step backward differentiation formula, stiffly accurate Runge–Kutta methods and the discontinuous Galerkin method.
The evolution equation is assumed to be governed by a possibly time-dependent operator that is coercive, monotone, and fulfills a certain growth and continuity condition. Strongly continuous perturbations are also studied.
By employing algebraic relations, which reflect the stability of the numerical method under consideration, and based upon the theory of monotone operators, the convergence of piecewise polynomial prolongations of the time discrete solutions towards a weak solution is shown. The analysis does not require any additional regularity of the exact solution.
The results apply, e.g., to non-Newtonian shear-thickening fluid flow.

Consistent initialization for structured DAEs
Diana Estevez Schwarz

One of the difficulties associated with the numerical integration of DAEs is the computation of consistent initial values. A consistent initial value has to fulfil the explicit constraints as well as the hidden constraints that may result from differentiation.
If some structural assumptions are given, then a consistent initialization can be determined sequentially starting from a value that fulfils the explicit constraints. In a second step, a correction of this value is computed solving successively linear subproblems that involve the hidden constraints. The presentation will provide an overview of this approach for some classes of DAEs.
For the DAEs resulting from circuit simulation, such an approach resulted to be especially suitable and allowed a better understanding of numerical features observed in applications.
For DAEs in Hessenberg form of arbitrary order, the approach is also feasible if certain assumptions regarding the nonlinearity are given. The DAEs resulting from multibody dynamics precisely fulfil these conditions and the method for the consistent initialization coincides with well-understood approaches from multibody dynamics literature.
Finally, it will be discussed how to generalize these results for some DAEs in triangular chain form with Hessenberg subsystems.

Mathematical modelling of fuel-cells with heterogenous parameter distribution

István Faragó, Izsák, Ferenc and Szabó, Tamás

The fuel cells are simple devices that convert chemical energy directly to electricity without spark ignition. With fuel cells, there is no combustion, so nothing but water released into the environment. To increase the efficiency of the fuel cells their properties must be analyzed deeply. To this aim, we construct continuous and discrete mathematical models which describe the physical phenomena.
Under the homogeneous parameter assumption, we arrive at the equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \nu^2 \exp u. \tag{1}$$

We present numerical (computer) results for different scenarios.
We extended the continuous model for the heterogenous parameter's distribution case. Then the new equation is as follows

$$\begin{aligned} & aC_{\text{dl}}\partial_t \eta(t,x) \\ & = \partial_x\left(\frac{\kappa_{\text{eff}}}{\kappa_{\text{eff}}+\sigma_{\text{eff}}}\right)\left(I(t)\frac{\kappa_{\text{eff}}+\sigma_{\text{eff}}}{\kappa_{\text{eff}}}(t,0) - \int_0^x \sigma_{\text{eff}}(t,s)\partial_x\eta(t,s)\,\mathrm{d}s\right) \\ & + \frac{\kappa_{\text{eff}}}{\kappa_{\text{eff}}+\sigma_{\text{eff}}}\partial_x(\sigma_{\text{eff}}\partial_x\eta(t,x)) - ai_0 g\left(\alpha\frac{F}{RT}\eta(t,x)\right). \end{aligned} \tag{2}$$

We analyze this model, also we construct the numerical model and we illustrate the efficiency of this approach by several computer experiments.

An Extension of Albrecht's Approach for Stochastic Differential Equations

Maria Ferro, Evelyn Buckwar

In this talk we consider the numerical approximation of solutions of Itô Stochastic Differential Equations by Stochastic Runge–Kutta methods. We base our convergence analysis issue on the concepts of mean-square consistency, mean-square zero-stability and mean-square convergence. As an alternative to using stochastic coloured rooted trees, we present a stochastic version of the so-called Albrecht's approach to derive order conditions for Stochastic Runge–Kutta methods. The talk is based on joint work with Evelyn Buckwar (Heriot-Watt University).

Theoretical Modeling of a New Membrane Dual -Type Fischer-Tropsch Reactor in GTL Technology

Amir Ahmad Forghani, Rahimpour M. R., Shariati A.

In this study, investigation on a novel reactor configuration with hydrogen-permselective membrane was done for Fischer-Tropsch (F-T) synthesis in GTL technology. This model is used to compare the performance of a membrane dual-type Fischer-Tropsch reactor (MDR) with a conventional fixed bed Fischer-Tropsch reactor. In this new configuration, the synthesis gas is converted to hydrocarbons in two catalytic reactors in which the generated heat in the first reactor is removed with water circulating on the shell side and in the second reactor; the heat of reaction is operated to preheat the synthesis gas fed to the first reactor. A hydrogen selective permeation (palladium-silver) membrane has been used in the tube of gas-cooled reactor, to obtain a major increase in reactor performance by process intensification. This new membrane dual-type reactor (MDR) is used for production of high octane gasoline from synthesis gas on bifunctional Fe-HZSM5 catalyst in F-T synthesis. A comparison between conventional fixed bed single type reactor model

(CR), fixed bed dual type reactor model (FDR) and membrane dual-type reactor model (MDR) is carried out in terms of temperature, gasoline, CO2 and Methane yields, H2 and CO conversion as well as selectivity of productions. The Results show an enhancement in the yield of gasoline production and diminishing in the undesired products (CO2 and Methane) formation, and also favorable temperature profile along the membrane dual-type F-T reactor in the comparison with conventional fixed bed reactor was obtained. The governing equations of this model form a set of differential algebraic equations which is consisted of the equations of mass and energy conservative rules of both solid and fluid phases in first reactor and second reactor, and bed to tube heat transfer equation in second reactor, which have to be coupled with non-linear algebraic equations of the kinetic model. Backward finite difference approximation is applied here to solve this set of equations.

Numerical solution of semilinear systems of Fractional Differential Equations

Roberto Garrappa, Marina Popolizio

In recent years the development of models based on fractional differential equations (FDEs) has gained popularity in the investigation of dynamical systems in several areas, ranging from physics to electrochemistry, biology, economics, probability theory, etc.
In this talk we discuss the numerical solution of semilinear systems of FDEs. Problems of this kind arise for instance after spatial discretization of partial differential equations involving fractional derivatives. The resulting systems are usually of large dimension, according to the number of spatial grid points.
Unlike ordinary differential equations (ODEs), in FDEs there is a persistent memory which causes an increase in computational complexity. Numerical methods are therefore required to solve the problems in an efficient way.
Some numerical methods for efficiently solving semilinear FDEs are developed by generalizing to the fractional case some approaches already studied for ODEs. Results concerning stability and accuracy are discussed together with technical aspects concerning the implementation of the methods. Numerical experiments, with respect to some test problems, are hence presented in order to validate theoretical results and compare performances among different methods.
This is a joint work with Marina Popolizio from the University of Bari (Italy).

Nonhydrostatic atmospheric modeling on icosahedral grids

Almut Gaßmann

Global atmospheric modeling in the field of climate modeling and numerical weather prediction aims at numerical methods that guarantee for energy and mass conservation. Within the Hamiltonian viewpoint those goals may easily be achieved by obeying the antisymmetric structure of the Poisson brackets in the spatial discretisation. The underlying concept here is the product rule for derivatives, which may also be applied to the temporal discretisation, that is not described by the Poisson brackets.
On the base of the described theory, a dynamical nonhydrostatic model core has been built. First results with C-grid staggering on optionally a triangular or a hexagonal/pentagonal grid on the sphere will be presented.
The presented work is part of a joint development effort, called ICON, taken by the Max Planck Insitute for Meteorology (Hamburg) and the Deutscher Wetterdienst (Offenbach) towards a new operational model suite for climate projection and numerical weather prediction.

Iterative Splitting Schemes as time integration methods: Theory and Application

Jürgen Geiser

In this paper we present iterative splitting schemes as a novel approach to time decomposition methods.
We discuss consistency and stability analysis of the iterative splitting scheme, [1] and [2] with respect to a time integration method. Based on the fundamental problems to discretize first in time or first in space, we deal with two different theories: Time integrator problems or L^p problems for PDE's.
For the applications, we take into account decomposition methods to accelerate the solver processes. We present different applications in fluid dynamics and discuss the near- and far-field contexts are based on multi-scales.
The results are discussed with experiments to give valid models and decomposition methods.

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Peer-Methods for Time-Dependent Finite Element Computations

Alf Gerisch, Jens Lang, Helmut Podhaisky, Rüdiger Weiner

The finite element software KARDOS solves time-dependent nonlinear PDEs following the Rothe-Method. In this approach, a linearly-implicit time-integration scheme is applied to the PDE problem leading to one or more linear elliptic problems that must be solved in each time step. The solution of these linear elliptic problems is accomplished using an adaptive finite element scheme. Higher-order one-step time-integration schemes are the typical choice in KARDOS but they may suffer from order-reduction. This phenomenon is avoided if the parameters of the scheme satisfy additional order conditions. However, these conditions lead to an increase in the minimum number of stages required for higher-order methods and consequently increase the computational cost.
PEER methods are a class of general linear methods for which all computed solution approximation have the same order. Linearly-implicit variants of these schemes exist and they do not show order-reduction when applied in the solution of stiff ODE systems. Hence these methods commend themselves as time-integration schemes in KARDOS.
After a brief introduction to the KARDOS framework and PEER methods, we present how both can be combined. The multi-step character of the PEER methods creates particular difficulties for the computation of starting values, in the time-step selection on spatially fixed finite element meshes (temporal error control), and the time-step selection on adaptive finite element meshes (spatio-temporal error control). We will discuss these issues and their resolution and present illustrating numerical tests.

Calculation of vortex patch dynamics in inviscid incompressible fluid
Vasily Govorukhin

The variant of vortex particles-in-cells method is proposed for calculation of plane flows of inviscid incompressible fluid. The governing equations are the 2D Euler equations in terms of stream function and vorticity. The vorticity field is approximated using its values at a set of fluid particles. The stream function is computed using the Galerkin method. We assess and compare the effectiveness of set of integrators for solving the equations of motion of fluid particles. A number of numerical examples with application of symplectic and pseudo-symplectic Runge-Kutta method demonstrats the usefulness of the proposed algorithm. The application of method to flows trough channel problem and multipoles patches dynamics investigation also presented.

Regularization of discontinuous ODEs with application to neutral delay differential equations

Nicola Guglielmi, Giorgio Fusco and Ernst Hairer

In this talk I will consider a general class of delay differential equations of neutral type with delays depending on the solution itself.
For such equations the possible discontinuity in the derivative of the solution at the initial point may propagate along the integration interval giving rise to subsequent points, called breaking points, where the solution derivative is not continuous.
As a consequence, the problem of continue the solution in a right neighbourhood of a breaking point is equivalent to a Cauchy problem for an ODE with a discontinuous right hand side. Therefore a classical solution may either cease to exist or lose uniqueness.
To the aim of recovering a unique solution I will consider some possible regularizations based on singular perturbations.
I will analyze the properties of the solutions of the singularly perturbed problems and discuss their limit as the perturbation parameter goes to zero.
Finally I will discuss some peculiar aspects relevant to the numerical integration.

Parallel iterative time domain decompositions based on deferred correction methods for solving ODE systems

David Guibert, Damien Tromeur-Dervout

The development of large computational resources leads to search for parallel implementation not only based on space decomposition. In this talk we will propose to combine time domain decomposition and the simple deferred correction. The deferred correction [1, 2] builds a perturbated problem which the exact solution is known. The defect difference between the perturbated solution and the solution of the original problem, is computed by a process increasing the time accurary at each iteration.
The iterative correction is computed sequentially on each time steps. To introduce parallelism, we gather the time steps into subdomains distributed among processors. A parallel pipe is then defined as: a processor computes its correction, sends it to the next subdomain and starts its next iteration. Hence a cyclic distribution of the time subdomains is introduced to reduced the startup of the first step of the iterated correction process. Numerical results and parallel efficiency will be presented.

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Exponential Smoothing Splines for Spot Market Price Simulation

Michael Günther

Pricing derivatives in electricity market makes use of spot market models for describing and forecasting the dynamics of the electricity tariff. The price-load curve is in the core of such market models, relating prices to the demand based on measured (historical) data and various assumptions. As these data are rather noisy, stricitly positive but show strong exponential behaviour in

some parts, we propose a combination of smoothing and exponential spline with positivity preserving implementation. We describe the derivation, analysis and implemention of smoothing exponential splines which aim at positivity preserving for approximating the price-load curves within a dynamic spot-market model. Numerical simulation will show the usefulness of this approach.
This work is a joint work with Philipp Werneburg (Wuppertal) and Sven-Olaf Stoll (EnBW Trading GmbH Karlsruhe).

High order splitting methods for semigroups

Eskil Hansen, Alexander Ostermann

Splitting methods constitute an effective class of time integrators and have been widely used for both ODEs and PDEs. The general error analysis of such methods have often been conducted in a fairly classical ODE setting, including Taylor expansions and nonstiff order conditions, which is not directly applicable in a PDE context.
In this talk we survey our recent work [1, 2], where we prove that exponential splitting methods retain their nonstiff order when applied to abstract evolution equations which are evolved by semigroups. As a concrete application we consider parabolic PDEs and their dimension splittings. We also present a systematic derivation of new splitting methods of orders three to fourteen based on complex coefficients. These results resolve the open question whether there exist splitting schemes with convergence rates greater then two in the context of semigroups.
The sharpness of our theoretical results is finally illustrated by numerical experiments.

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High-order time integration in structural finite element analysis based on material non-linearities

Stefan Hartmann, A.-W. Hamkar, K. J. Quint

In engineering applications the finite element method is one of the major tools to predict the behavior of design elements. One aspect of this broad numerical method is related to the account of realistic material behavior for quasi-static problems. In the field of Continuum Mechanics constitutive models for describing the hardening behavior of the material under consideration are mostly described by ordinary differential equations or in some models by differential-algebraic equations. Due to the historical development of finite elements, there was a longer period where the combination of solving the boundary-value problem and evaluating the constitutive models has been done in a more engineering sense. Today, it is known that the application of the vertical method of lines yields after the spatial discretization a system of differential-algebraic equations, where the algebraic part results from the discretized weak formulation (equilibrium conditions) and the differential part stems from the evolution equations for the internal variables (constitutive equations for the hardening behavior of the material) evaluated at all spatial integration points of the boundary-value problem.
In this lecture the entire procedures, which are implemented into a three-dimensional, time-adaptive finite element program, and a comparison of various DAE-solvers (step-size controlled

stiffly accurate, diagonally implicit Runge-Kutta methods and Rosenbrock-type methods) is carried out showing the applicability, the current drawbacks, and some open questions. Moreover, we address some aspects of efficiency due to the large number of unknowns to be solved many times.

An efficient family of strongly A-stable Runge-Kutta collocation methods for stiff systems and DAE's. Convergence results

Domingo Hernández-Abreu, Severiano González-Pinto

In this talk we discuss the convergence properties of $s-$stage $SAFERK(\alpha)$ methods, which have been recently introduced in [1] for the numerical integration of ordinary differential equations. For each $s \geq 3$, $SAFERK(\alpha)$ methods are A-stable collocation Runge-Kutta methods possessing a first internal stage of explicit type and coefficients depending on the free parameter α, which can be selected for optimization purposes. This family of methods includes the well-known family of LobattoIIIA methods, and it is based on the characterization of $s-$point interpolatory quadrature rules of Precision Degree $q = 2s - 4$, having two prefixed nodes $c_1 = 0$ and $c_s = 1$.
In particular, we derive global error estimates on finite intervals for $SAFERK(\alpha)$ methods when applied to several kinds of stiff problems and differential-algebraic systems (DAEs). Moreover, the global orders of convergence of the $s-$stage $SAFERK(\alpha)$ and the $(s-1)$-stage Radau-IIA method are compared, since both methods possess the same number of implicit stages.
Despite $SAFERK(\alpha)$ methods are neither $L-$stable nor algebraically stable, this family of methods proves to be of interest for the numerical integration of stiff systems and DAEs, as it is illustrated by means of some numerical experiments involving the $3-$stage Radau-IIA, the $4-$stage Lobatto-IIIA and some strongly A-stable 4-stage $SAFERK$ methods.

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A Uniform Framework for DAE Integrators in Flexible Multibody Dynamics

Christian Hesch, Peter Betsch

The present talks deals with a uniform approach to the discretization in time of rigid body dynamics, nonlinear structural mechanics and flexible multibody systems. In particular, it is shown that a uniform set of differential-algebraic equations (DAEs) with *constant* mass matrix governs the motion of rigid bodies and semi-discrete formulations of structural components (such as geometrically exact beams and shells) resulting from a finite element discretization in space.

The extension to multibody dynamics can be easily accomplished by appending additional algebraic equations to the DAEs [1]. Similarly, large deformation contact problems can be handled by applying an active set strategy [2].

The simple structure of the DAEs makes possible the design of structure-preserving time integrators. In particular, both energy-momentum schemes popular in nonlinear structural dynamics as well as symplectic-momentum variational integrators shall be investigated [3].

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G-matrices for algebraically stable general linear methods

Adrian Hill

This paper describes a technique from Control whereby the G–matrix for an algebraically stable general linear method may be found in terms of the generalised eigenvectors of a generalised eigenproblem associated with the method.

Time integration meets inverse problems

Marlis Hochbruck, Michael Hönig and Alexander Ostermann

It is well known that the solution of inverse problems requires appropriate regularization techniques. Interestingly, some of the most popular methods can also be interpreted as time integration schemes for the solution of a certain evolution equation.
Given a nonlinear inverse problem $F(u) = y^\delta$, with a perturbed right-hand side y^δ, it has been shown that the solution $u(t)$ of the evolution equation $u'(t) = F'(u(t))^*(y^\delta - F(u(t))$, $u(0) = u_0$ yields a stable approximation to the solution of the inverse problem for *large* t. The regularization properties of this so-called asymptotic regularization (Showalter's method) have been analyzed by Tautenhahn in 1994. In this talk we discuss the numerical realization of asymptotic regularization of inverse problems. Application of standard integration schemes yield well-known regularization methods. For example, the explicit Euler method and the linearly implicit Euler method are equivalent to the Landweber method and the Levenberg-Marquardt regularization, respectively.
Further, we discuss the regularization properties of the Levenberg-Marquardt method and of the exponential Euler method applied to the Showalter equation. In particular, we will present a variable step size analysis which allows to prove that optimal convergence rates are achieved under suitable assumptions on the initial error.
We will also present some numerical examples illustrating the theoretical results.

Exponential fitting and deferred correction for BVPs

Davy Hollevoet, Marnix Van Daele, Guido Vanden Berghe

During this talk, we will look into the combination of deferred correction and exponential fitting, applied to methods for solving boundary value problems.
The idea behind the often used deferred (difference) correction is to promote a low-order method to a higher order by approximating the residual with a second, higher order method. If certain conditions concerning the combination of these methods are satisfied, such a scheme obtains an order of accuracy equal to that of the second method. The well-known code TWPBVP by Cash implements such schemes and is based on mono-implicit Runge-Kutta (MIRK) methods. In the context of this research, the original TWPBVP code was translated from Fortran into Matlab code.

Exponential fitting is a procedure which produces variants of classical methods, aimed to solve problems with oscillating solutions more efficiently. Whenever the solution of a problem falls within the fitting space of such a method, approximations up to machine accuracy can be found. In general however, the free parameter can be tuned to specific frequencies such that one or more orders of accuracy are gained.
In this presentation, we will show how we combined both correction techniques by applying deferred correction schemes to exponentially fitted MIRK methods.

Computational Time Series Analysis of Multidimensional Non-Stationary Data
Illia Horenko

In recent years there has been considerable increase of interest in the mathematical modeling and computational analysis of complex non-stationary and non-equilibrium systems. Such systems can be found, e.g., in weather forecast (transitions between weather conditions), climate research (processes associated with global warming), fluid mechanics (transitions between different flow regimes) and in econometrics (e.g., phases of different market dynamics, crashes, etc.). In all cases the accumulation of sufficiently detailed multidimensional time series has led to the formation of huge databases containing enormous but still undiscovered treasures of information. However, the extraction of essential information out of the data is usually hindered by the multidimensional and non-stationary nature of the signal. The standard filtering approaches have in general unfeasible numerical complexity in high dimensions, other standard methods (like f. e. Kalman-filter,MVAR, ARCH/GARCH etc.) impose some too restrictive assumptions about the type of the underlying dynamics.
A new method for analysis of multidimensional non-stationary time series will be presented (I.Horenko (2008)). The approach is based on optimization of the averaged clustering functional in appropriate function spaces. Considered functional describes the quality of data representation in terms of several optimally localized models and a persistent process switching between the models. Resulting computational framework is based on application of the finite element method (FEM) to the variational minimization of the introduced functional. The computational advantages of the presented method will be discussed in comparison to the standard stochastic approaches (like Hidden Markov Models (HMMs)). The application of the computational framework will be briefly demonstrated in context of subgrid-scale parameterization of Lorenz'96 system and in context of climate trend factor analysis.

Unconditionally stable time integration with operator splitting
Róbert Horváth, M. Botchev, I. Faragó

Standard numerical time integrators for the time-domain Maxwell equations often handle the wave curl terms explicitly and the lossy conductivity terms implicitly. The explicit treatment of the curl terms triggers a stability restriction on the time step size. This restriction can be quite severe, especially when caused by some local phenomena such as material inhomogeneity or local grid refinement. The economical ADI-FDTD (Alternating Direction Implicit – Finite Difference Time Domain) schemes are unconditionally stable and, thus, are free from the time step size restriction but can only be used on Cartesian finite difference grids. On the other hand, the fully implicit time integrators do not always yield to a reduction in total computational costs as compared to the standard schemes.
Motivated by these needs for unconditionally stable, yet relatively cheap, numerical integrators, we consider the operator splitting approach combined where implicit time integration is employed at each split step. A number of unconditionally stable, second order accurate schemes

are obtained. The numerical tests are presented for the full three-dimensional Maxwell equations discretized in space with either finite differences or vector finite elements.

An anisotropic mesh adaptation method for the finite element solution of variational problems

Weizhang Huang, Xianping Li

In this talk we are concerned with anisotropic mesh adaptation for the finite element solution of variational problems. A bound for the first variation of a general functional is derived, which is semi-a posteriori in the sense that it involves the residual and edge jump, both depending on the computed solution, and the Hessian of the exact solution. A formula for the metric tensor M for use in anisotropic mesh adaptation is defined such that the bound is minimized on a mesh that is uniform in the metric specified by M. Interestingly, when restricted to isotropic meshes, a similar but completely a posteriori bound and the corresponding formula for the metric tensor can be obtained. Once M has been defined, an anisotropic adaptive mesh is generated as a uniform mesh in the metric M. Numerical results demonstrate that the new mesh adaptation method is comparable in performance with existing ones based on interpolation error and has the advantage that the resulting mesh also adapts to changes in the variational structure of the underlying problem.

Global Sensitivity Analysis of Ordinary Differential Equations via solution of the associated PDE problem

Wilhelm Huisinga, Andrea Y. Weiße

Ordinary differential equations are ubiquitous in mathematical models of biological problems. When simulation studies are performed for a fixed set of parameters, the question arises as how experimental uncertainty, and equally important, biological variability in input data effect the conclusions drawn from the single parameter study. The propagation of uncertainty & variability through the model dynamics and their effect on the output is studied by sensitivity analysis. Global sensitivity analysis is concerned with variations in the model input that typically span a large domain.

Two major problems that complicate the analysis are the high dimensionality of the model and the reliability of the estimated sensitivity. Current numerical approaches to global sensitivity analysis mainly focus on scalability to high-dimensional models. However, to what extent the estimated sensitivity is an reliable approximation typically remains unclear.

We present a new error-controlled approach to global sensitivity analysis of ordinary differential equations [1]. The approach is based on a reformulation of the problem as a first-order hyperbolic partial differential equation of Liouville type, which describes the evolution of the state uncertainty & variability in terms of a probability density function. The scheme is based on a semidiscretization in time, and a subsequent solution of the resulting stationary problems by a special variant of approximate approximations, a powerful new spatial discretization technique [2]. We prove convergence of the method and investigate the performance of approximate approximations discrein the adaptive scheme. The theoretical results directly indicate how to design an efficient implementation, in particular how to couple temporal and spatial accuracy. Numerical examples illustrate the theoretical results and show that the method yields highly accurate estimates of the true output uncertainty. Extensions to higher dimensions based on sparse-grid techniques and meshless grid approaches will be discussed.

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On the Collocations and Least Squares Method Capabilities

Vadim Isaev, Vasily Shapeev

The collocations and least squares (CLS) method is a projection method for numerical solving of mathematical physics equations. It was successfully used by various researchers for elliptic, hyperbolic and parabolic equations in rectangular and curvilinear domains. We developed new versions of the CLS method for Navier-Stokes equations in the present work. Capabilities of the method were extended here by

1. a good choice of its parameters (we made an investigation of the dependence of method's properties on its parameters and found good domains of their values);
2. use of orthogonal linear algebra algorithms;
3. use of a new method for convergence acceleration of a linear iterative process (it is used in the CLS method for solving of a system of linear algebraic equations);
4. use of adaptive grids.

Improvements of the CLS method proposed here allow us to compute an approximate solution on fine grids (up to 1280×1280) on a single-processor PC (the total number of unknowns of the method on a grid with 1280×1280 cells is about $25 \cdot 10^6$). Abilities and other improvements of the CLS method done here are demonstrated in the present work on 2D lid-driven cavity flow problem. Calculations of this flow were carried out here in a wide range of Reynolds numbers (from 1 to 7500). Recent results obtained by the CLS method agrees with the most accurate results among available now (Botella & Peyret, 1998, Shapeev & Lin, 2009) with the accuracy 10^{-6} for Re = 100 and Re = 1000. Here, a vortex BR4 is visualised in numerical experiments at Re=7500 (according to Ghia's notations). This vortex is found by the CLS method for the first time. A stationary flow regime is not observed at Re>7500 (in particular at Re = 10000) here as well as in papers of other researchers (Garcia S., 2007). These and some other facts indicate that the CLS method has a good potentiality for a simulation of viscous fluid flows.

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Asymptotic numerics of highly oscillatory equations

Arieh Iserles, Marissa Condon, Alfredo Deaño

In this talk I introduce a novel methodology, based on combination of asymptotic and numerical techniques, for the computation of ordinary differential equations with rapidly oscillating forcing terms. I focus on a family of nonlinear second-order equations which generalise the familiar van der Pol oscillator and appear in numerous applications, in particular in electronic engineering. It will be demonstrated that their solution can be expanded asymptotically employing modulated Fourier expansions. The calculation of expansion terms requires solely manipulation of non-oscillatory quantities, therefore is easily affordable and the computational cost is uniform in frequency.

The methodology of this talk can be extended to other families of ordinary and partial differential equations and DAEs with extrinsic high oscillation. Time allowing, I'll discuss these extensions. In particular, I hope to mention asymptotic–numerical expansions for the equation of inverted pendulum forced by high oscillation.

Numerical solutions of differential equations on using Bernoulli polynomials

Md. Shafiqul Islam

In this talk, a numerical method for solving some classes of differential equations by approximating the solution in the Bernoulli polynomial functions is proposed. The basic shapes of the first 10 Bernoulli polynomials are shown graphically. These polynomials can be defined on any interval to form a complete basis over the interval. A rigorous mathematical formulation is provided to describe how these polynomials are used to obtain highly accurate solutions to the BVP. For this, the Galerkin weighted residual method is exploited and the Bernoulli polynomials are treated as trial functions. Here, second order linear differential equations with essential and suppressible boundary conditions, and also nonlinear differential equations are considered. In each case the formulation is demonstrated in details and is also verified through numerical examples. The approximate results with the exact solutions are compared, and the agreement is obtained as nearly by using first 10 Bernoulli polynomials only, which are depicted in figures. It is observed that if we use more polynomials, the approximate solutions converge to the exact solutions monotonically with large significant digits. This technique may be applied to solve also fourth order differential equations with great accuracy.

Continuous two-step peer methods for ODEs

Giuseppe Izzo, Zdzislaw Jackiewicz

We construct a class of peer methods and their continuous extensions of order p=s, where s is the number of stages. The continuity of the output of this class of methods allows us to compute in an easy way the numerical solution and the local error estimate, not only at the grid point, but all over the integration interval. This is a very important feature that can be exploited to develop an efficient technique for step size changing during the integration process. We also describe the construction of highly stable methods, in particular methods which are A-, L- and algebraically stable. We use Schur criterion to search for methods which are A- and L-stable and the criterion based on Nyquist stability function to search for algebraically stable methods. Examples of methods will also be given.

Search for Highly Stable General Linear Methods for Ordinary Differential Equations

Zdzislaw Jackiewicz, R. D'Ambrosio, G. Izzo

In this talk we describe the construction of highly stable general linear methods (GLMs) for the numerical solution of ordinary differential equations (ODEs). We describe the construction of some classes of GLMs which are A-stable and L-stable using the Schur criterion, and algebraically stable methods using criteria proposed recently by Hill, Nonlinear stability of general linear methods, Numer. Math. 103(2006), 611–629, and Hewitt and Hill, Algebraically stable general linear methods and the G-matrix, to appear in BIT. We illustrate the results for the class of two-step Runge-Kutta methods with inherent Runge-Kutta stability for which one of the coefficient matrices is assumed to have a one-point spectrum. We also describe our search for algebraically stable methods in this class without imposing any restrictions on the coefficient matrices.

Effective numerical circuit simulation regarding the variation in parameters

Lennart Jansen, Monica Selva Soto, Caren Tischendorf

Circuit simulation often requires sensivity analysis. A circuit is described by the perticular units and the resulting stress and electricity functions for different measuring points. To every unit there is a set of parameters which characterize that certain unit. When these parameters change, it naturally has an effect on the stress and electricity functions. It's interesting how sensitive these functions are towards this aforementioned change of the parameters. To capture these effects on the stress and electricity functions, you would want to calculate their derivations in respect of all parameters. To realize this numerically, we use the difference method in which the derivation is approximated by the difference quotient. To achieve this you have to know the stress and electricity functions for all sets of parameters which you are interested in. This would mean having to numerically solve a circuit describing network equation for every set of parameters at every point of time. If more than one parameter changes, the amount of sets of parameters will potentially multiply with the amount of parameters which will course a immense rise of costs. It is imperative to lower these efforts massively. The idea for achieving this, results from becoming clear about the fact that each of the network equations only slightly change on each adjoining set of parameters, because the distance between two sets of parameters has to be very small to be able to approximate the derivation later on. According to this you very often solve very similar equations. We will see that you can come by the remaining solutions of the network equations with far less costs, if you have solved a fraction of the network equations conventionally before.

Implicit Peer Methods for the Compressible Euler Equations

Stefan Jebens, Rüdiger Weiner, Oswald Knoth

In atmospheric models the highest-frequency modes are often not the physical modes of interest. On the other hand severe stability constrains for the numerical integrator arise from those meteorologically irrelevant modes. One strategy to avoid this problem is a splitting ansatz where the differential equation is split into two parts where the slow part is integrated with a numerical method and a time step size restricted by the CFL number of the low-frequency modes while for the integration of the high-frequency modes a simpler method is used together with smaller time steps so that these small time step sizes satisfy the CFL condition dictated by the high-frequency modes. This strategy fails when using a cut-cell approach for the representation of orography (which means that the orography is cut out of the Cartesian grid) because very small cells can occur and therefore the maximal time step is restricted by the CFL condition for these small cells. The same problem occurs when computing on the sphere with a latitude-longitude grid because of the pole singularities. Therefore this talk deals about A-stable linear-implicit methods. Because of the A-stability even the smallest cells do not restrict the time step size. Furthermore it is easy to obtain higher-order methods in contrast to split-explicit methods where the order conditions are very complicated. As implicit integrator we will use implicit peer methods which also have been applied successfully to other problem classes.

Taylor expansions for stochastic partial differential equations

Arnulf Jentzen

Taylor expansions are a fundamental and repeatedly used means of approximation in mathematics, in particular in numerical analysis. While local approximations and local expansions of a function yield a better understanding of local properties of such a function from a theoretical point of view, many numerical schemes for various types of differential equations are based on Taylor

expansions of the solution of such an equation. In this talk, we present Taylor expansions of the solution of a stochastic partial differential equation (SPDE) of evolutionary type and their first applications to numerical analysis. The key instruments for deriving such Taylor expansions are the semigroup approach, i.e. to understand the SPDE as a mild integral equation, and an appropriate recursion technique.

Construction of Higher Order Numerical Method

Ram Jiwari, R. C. Mittal

In this paper, a higher order numerical method is proposed to solve time dependent Burger-Huxley equation $u_t - \varepsilon u_{xx} + \alpha u u_x = \beta(1-u)(u-\gamma)u$ with appropriate initial and boundary conditions. The equation describes the interaction between convection, diffusion and reaction. When $\alpha = 0$ and $\varepsilon = 1$ the equation reduces to Huxley equation. This equation describes nerve pulse propagation in nerve fibers and wall motion in liquid crystals. On the other hand, when $\beta = 0$, the equation reduces to the Burgers' equation at high Reynolds number that establishes a balance between time evolutions, nonlinearity and diffusion. So the considered equation has great importance in the theory of shock waves, mathematical modeling of turbulent fluid and in continuous stochastic processes. The presence of the nonlinearity in the problem leads to severe difficulties in the solution approximation. In construction of the numerical scheme, quasilinearization is used to tackle the nonlinearity of the problem which is followed by semi discretization for spatial direction using differential quadrature method (DQM). Semi discretization of the problem leads to a system of first order initial value problem. For total discretization, we discretize the system of first order initial value problem resulting from the space semi-discretization using RK4 scheme with constant step length. The method is analyzed for stability and convergence. Finally, a set of numerical experiment is carried out with small values of ε in support of the developed method and find that the scheme is quite suitable when $\varepsilon \to 0$.

Numerical procedure for solutions of a strongly nonlinear problem

Aleksandr Kolpakov, Sergei Rakin

We analyze the following boundary-value problem in planar domain $Y = [0,1]^2$:

$$div(\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|)\nabla\varphi(\mathbf{x})) = 0 \text{ in } Y; \tag{1}$$
$$\frac{\partial\varphi}{\partial\mathbf{n}}\,|_{x=0} = \frac{\partial\varphi}{\partial\mathbf{n}}\,|_{x=1} = 0; \varphi\,|_{y=0} = -E/2; \quad \varphi\,|_{y=1} = E/2,$$

where

$$\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|) = \begin{cases} 1, \mathbf{x} \in P \subset Y, \\ \dfrac{\varepsilon_0 - \varepsilon_\infty}{1 + k\,|\nabla\varphi|^2} + \varepsilon_\infty, \mathbf{x} \in Y \backslash P, \end{cases} \tag{2}$$

ε_0, ε_∞ are constants. It means that the partial differential equation in (1) is linear in domain $P \subset Y$ and strongly nonlinear in domain $Y \backslash P$. The problem (1), (2) is strongly nonlinear because those coefficient depends on $\nabla\varphi(\mathbf{x})$.

Using specific form of the coefficient (2), we transform the problem (1), (2) to the equivalent minimization problem

$$F(\varphi) = \int\limits_P \frac{1}{2}\,|\nabla\varphi(\mathbf{x})|^2\,d\mathbf{x} + \tag{3}$$
$$+ \int\limits_{Y\backslash P} \left(\frac{\varepsilon_0 - \varepsilon_\infty}{2k} \ln(1 + k\,|\nabla\varphi(\mathbf{x})|^2) + \frac{\varepsilon_\infty}{2}\,|\nabla\varphi(\mathbf{x})|^2 \right) d\mathbf{x} \to \min,$$

considered on the functional set $V = \{\varphi(\mathbf{x}) \in H^1(Y) : \varphi|_{y=0} = -E/2; \varphi|_{y=1} = E/2\}$. Functional (3) is strictly convex and semicontinious from above on V under condition

$$\frac{\varepsilon_0 - \varepsilon_\infty}{2k} \cdot \left(2\varepsilon_\infty - \frac{\varepsilon_0 - \varepsilon_\infty}{2k}\right) > 0.$$

Then the minimization problem (3) has unique solution.
We construct discrete approximation for the functional (3). We construct uniform $N \times N$ net in Y, denote $h = 1/N$ and write the following approximation:

$$|\nabla\varphi|^2 = \frac{(\varphi_{i,j+1} - \varphi_{i,j})^2}{h^2} + \frac{(\varphi_{i+1,j} - \varphi_{i,j})^2}{h^2} \tag{4}$$

where $\varphi_{i,j}$ means value of the function $\varphi(\mathbf{x})$ in the node with coordinates $x = ih, y = jh$, $i, j = 0,\ 1, ..., N$. Substituting (4) into (3), we obtain nonlinear function $\bar{F}(\varphi_{ij})$ of $N^2 - 1$ variables. Function $\bar{F}(\varphi_{ij})$ is strictly convex on R^{N^2-1}. Then it has unique minimum.
The finite-dimensional problem $\bar{F}(\varphi_{ij}) \to \min$ can be solved by using various methods. We developed numerical method and computer program, which use gradient method with variable step.

Strang Splitting for Reaction-diffusion Equations

Felix Kramer, Eskil Hansen, Alexander Ostermann

In this talk, we present results on the applicability of the Strang splitting method to reaction diffusion equations. They extend prior analysis of the Strang splitting done by Lubich, Descombes and Schatzmann, Hansen and Ostermann to name a few. We investigate the Strang splitting applied to parabolic equations with nonlinear inhomogeneity. Essentially, we derive second order for bounded homogeneities; for relatively bounded inhomogeneity, our bound depends on the extent of relative boundedness. With some additional restrictions, we derive an error bound resulting in an order reduction of the same magnitude as the parameter of relative boundedness. In the final chapter, we present some numerical results, derived by application of the Strang Splitting onto the Chafee-Infantee equation.

Preserving accuracy and stability in the numerical integration of dynamic contact problems

Rolf Krause, Mirjam Walloth

The numerical simulation of dynamical contact problems puts high demands on the discretization methods employed in space and time. Particular effort is required in order to treat the non-linear effects at the contact interfaces accurately. This includes the non-penetaration condition, which usually is modelled by means of inequality constraints, as well as highly non-linear effects as friction. Thus, for this problem class the development of energy preserving (or at least dissipative) and stable discretization methods is far from trivial. As it turns out, the interplay of the spatial and the temporal discretization has crucial influence on the structural properties of the resulting space/time discretization.
In this talk, we give an overview on current developments in the area of dynamic contact problems and dicuss different approaches to obtain stable space/time discretization schemes. This will include approaches based on the method of lines as well as approaches based on Rothes method. Structural properties as energy preservation as well as the stability of the contact stresses will be on the focus of our talk. We finally will present a new stabilized time discretization scheme for frictional contact problems in the context of Rothes method. Furthermore, we will comment on the difficulties arising from the theoretical as well as the practical point of view, in case in space an adaptive discretization is employed. Illustrative numerical results in 3D will be presented.

Numerical solution of DAE's using method of continuation with respect to a parameter

Evgenii Kuznetsov, Stanislav Dmitriev

The integral curve (solution) to a system of differential - algebraic equations is constructed using the method of continuation with respect to a continuation parameter. The necessary and sufficient conditions of the transformation of a problem to the best argument are proved. Integro-differential-algebraic equations with delay argument are also considered. It is shown that the best argument provides the best conditionality to the linear system of continuation equations to be solved. We prove further that the best argument is the arc-length of the integral curve. Numerical examples illustrate efficiency of the approach, especially, when one is required a solution passing through limit singular points as well.

B-series analysis of stochastic Taylor methods

Anne Kværnø, Kristian Debrabant

In the modeling of many applications, e.g., in chemical reaction systems and electrical circuits, taking stochastic effects into account often leads to stochastic differential equations (SDEs) of the form

$$X(t) = x_0 + \int_{t_0}^{t} g_0(X(s))ds + \sum_{l=1}^{m} \int_{t_0}^{t} g_l(X(s)) \star dW_l(s)$$

which can be stiff, i. e., explicit approximation methods do not work efficiently, and implicit methods have to be considered. An important class of derivative free approximation methods for solutions of SDEs are stochastic Runge–Kutta (SRK) methods. In the last years, implicit SRK methods have been developed both for strong and weak approximation. For these methods, the stage values are only given implicitly. However, in practice these implicit equations are solved by iterative schemes like simple iteration, modified Newton iteration or full Newton iteration. Using the theory of B-series and rooted trees, it has been proven in [1] that the iteration error can be accurately described in terms of certain growth functions defined on trees, allowing to determine precisely how many iterations are needed to achieve a certain order of convergence. In our talk, this theory will be extended to the case of implicit Taylor methods. In particular, we will develop a B-series theory for implicit Taylor methods which can also be used for the construction of new methods, both for weak and strong convergence.

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Numerical aspects in the dynamic simulation of geometrically exact rods

Holger Lang, Martin Arnold

We present a viscoelastic rod model that is suitable for fast and sufficiently accurate dynamic simulations of large deformations. It is based on Cosserat's and Kirchhoff's geometrically exact theory of rods with an internal dissipation model of Antman and is able to represent extension, shearing bending and torsion.
We use the method of lines with a non-standard finite difference scheme on a staggered grid for the spatial discretisation. All our choices for the discrete Cosserat strain and curvature measures are

frame indifferent by construction. We discuss all of them and some hybrid versions with the Kirchhoff rod model, concerning stability properties, eigenvalue behaviour and numerical costs. We further discuss appropriate index reduction, explicit computation of the inverse mass-constraint matrix (at exactly the same numerical cost as the mass-constraint matrix itself) and stabilisation of the internal spherical constraints for the quaternions, which are used to parametrise the rotatory degrees of freedom.
The resulting model is completely free of higher algebraic (e. g. root) or transcendent (e. g. exponential, logarithmic or trigonometric) functions and is therefore numerically cheap to evaluate. The total task to evaluate the right hand side function f of the dynamical system $\dot{u} = f(t, u)$ for a robust curvature choice of Bobenko type, for non-equidistant discretisation and non-symmetric cross sections amounts to not more than $671N$+255 basic arithmetic operations, where N is the number of rod segments. An evaluation of the sparse Jacobian $\partial f/\partial u$ – with upper and lower bandwidths equal to ten – is about eleven times as expensive.
For the time integration of the system, we use well established solvers like RODAS, RADAU5 or DASPK. We discuss the problem of inherent extensional and shearing stiffness for the Cosserat rod and give pros and cons of choosing a discrete inextensible Kirchhoff rod model as an alternative for pure bending and torsion scenarios in order to circumvent stiffness.
Our model reflects structural mechanics sufficiently correct, as excellent agreement with 1D and 3D finite element solutions shows. As it yields computational times within milliseconds, it is suitable for interactive manipulation in virtual reality, robotics, path planning and multibody system dynamics simulations.

Finite element approximation of the stochastic wave equation
Stig Larsson, M. Kovacs and F. Saedpanah

Semidiscrete finite element approximation of the linear stochastic wave equation with additive noise is studied in a semigroup framework. Optimal error estimates for the deterministic problem are obtained under minimal regularity assumptions. These are used to prove strong convergence estimates for the stochastic problem. The theory presented here applies to multi-dimensional domains and spatially correlated noise. Numerical examples illustrate the theory.

Stochastic-Dynamical Methods for Controlled Variables
Benedict Leimkuhler

The purpose of many large scale dynamical simulations is the recovery of statistical-mechanical averages. For such computations to be useful, the parameters of the model (the "ensemble") must be regulated by auxiliary control laws. Typically these would represent thermal or pressure controls, although there are many other possibilities. In this talk I will describe a rather general approach to controlled variable molecular dynamics based on a family of stochastic-dynamic methods, illustrating the technique with specific examples of ensemble controls and numerical experiments.

Parallel time integration of ODEs by symmetrization of the time interval
Patrice Linel, Damien Tromeur-Dervout

This paper concerns the development of a parallel method to solve ODE or DAE. This kind of systems are involved in most of the modeling as mechanical systems modeling or chemical reactor modeling. These systems are usually stiff with a large number of unknowns and a large computational cost. This is a challenge problem because the usual time integrators are sequential,

the solution at the previous time steps are required in the time advancing scheme. We propose an Aitken-Schwarz method that allows to cut the time integration in time slices. Time integration is performed on each time subdomain updating transmission conditions between time subdomains. The main difficulty is the unknown boundary condition at the final time. Consequently, there is no feed back coming from the end time of integration, and the information is propagated only in the forward direction.
We transform the ODE initial value problem in an boundary values problem. Then the classical Schwarz domain decomposition with transmission conditions between time slices is performed. We demonstrate the pure linear divergence or convergence of this algorithm applied to system of linear ODE. This property allows us to accelerate the convergence of the solution at the time slices boundaries with the Aitken's acceleration technique of the convergence. The methodology can also be applied to systems of non linear ODEs, but the method needs to iterate the acceleration steps.
Another approach is developed using time-reversible integration scheme and a system of conditions satisfied by the subdomains's solution.
Numerical results show the efficiency of the proposed method on linear and non linear problems. Such methods are really interesting, when a large number of processors is available.

A Quadrature Based Method for Evaluating the Exponential-Type Functions for Exponential Methods

María López-Fernández

We consider the evaluation of the exponential-type functions required by exponential methods when they are applied to solve semilinear parabolic equations. We propose to evaluate these operators by means of a quadrature formula that converges like $O(e^{-cK})$, with K the number of quadrature nodes. The algorithm allows also the evaluation of the associated scalar mappings. The approach is based on the numerical inversion of sectorial Laplace transforms. Several numerical illustrations are provided to test the algorithm.

The parameterization method for numerical solution of delay singular differential equations

Igor Lutoshkin

The research talk is devoted to applying the parameterization method (PM) for delay implicit differential equations: $F(\dot{x}(t), x(t), x(t-\tau), t) = 0, t_0 \le t \le T, x(t) = \varphi(t), t_0 - \tau \le t \le t_0$, where $x \in R^n$, $F : R^{3n+1} \to R^n$, and the system is unsolvable (or difficultly solvable) with respect to derivatives $\dot{x}$.
The PM was created for optimal control problems by V.K.Gorbunov in 1979 and proved yourself very effectively for different singular problems [1,2,3]. Here noting $u(t) = \dot{x}(t)$ and introducing discrepancy functional $J(u) = \|F(u(t), x(t), x(t-\tau), t)\|^2$ we get a dynamic optimization problem. The PM is based on the minimization of $J(u)$ and approximation of $u(t)$ via its representation by some generalized spline with moving knots. The parameterized optimization problem becomes a finite-dimensional nonlinear programming of a small dimension in comparison with the finite-difference approximations. To apply the gradient or Newton methods for the problem it is required to get the first and the second derivatives. The derivatives with respect to the control parameters may be effectively calculated with the help of variational techniques and adjoint variables. Besides, the problems of optimization and numerical solution of differential equations are separated.

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Mixed-Mode Oscillations in a Modified Chua's Circuit

Wieslaw Marszalek, Zdzisław W. Trzaska

We consider a singularly perturbed system of differential equations of the form $\epsilon du/dt = g(u, v, \lambda)$, $dv/dt = f(u, v, \lambda)$, where $(u, v) \in R^3$, $0 < \epsilon \ll 1$ and λ is a set of parameters. Such a system describes a modified Chua's circuit with mixed-mode oscillations (MMOs). MMOs consist of a series of small-amplitude oscillations and large-amplitude relaxations. In the paper we use the singularly perturbed model to analyse a modified Chua's circuit with a nonlinear resistor, linear inductors and capacitors, controlled and constant voltage (or current) sources. In particular, we analyze the occurrence of the *Farey sequence* L^s, where L and s are the numbers of large-amplitude relaxations and small-amplitude oscillations, respectively.

"Look-Ahead" Linear Multistep Methods

Taketomo Mitsui

We are concerned with numerical solutions of the initial-value problem of ordinary differential equations (ODEs):

$$\frac{dy}{dx} = f(x, y) \quad (a \le x \le b), \quad y(a) = y_I.$$

We have many existing numerical solutions, among which the discrete variable methods (DVMs), like as the Euler method, the Runge-Kutta methods and the linear multistep methods (LMMs), are most popular because of their flexible capability for the solution. On the other hand, numerical analysis is still pursuing a new method with better performance and higher reliability. From this point of view, we will try to find more for the numerical solution of ODEs.
In the talk, we will propose a new class of LMM which has a potential of wide applications. The basic idea is as follows. Suppose we are now at a certain step-point x and an approximation y_0 to $y(x)$ is available. With the constant stepsize h, usually we try to obtain the approximation y_1 of the next step-point $x + h$. Here, introducing a scheme for y_2 at $x + 2h$ by employing y_0 and y_1, we compute it. The value y_2 stands for a "look-ahead". Then, by another scheme incorporating y_0, y_1 and y_2, we correct the value y_1.
These methods were proposed in the 80ies, but, as a matter of fact, ancestors can be found in the literature before. We will try to study the methods both theoretically and practically.

Higher Order Method for Burger's Equation
Ramesh Chand Mittal

The title of the talk by R. Mittal is "Higher Order Method for Burger's Equation".

Model order reduction for differential algebraic equations using the direct approach.
Kasra Mohaghegh, Roland Pulch, Jan ter Maten

Nowadays electronic circuits comprise about a hundred million components on slightly more than one square centimeter. The model order reduction (MOR) techniques are among the most powerful tools to conquer this complexity and scale although the nonlinear MOR is still an open field of research. On the one hand, the MOR techniques are well developed for linear ordinary differential equations (ODEs). On the other hand, we deal with differential algebraic equations (DAEs), which result from models based on network approaches. There are the direct and the indirect strategy to convert a DAE to an ODE. We apply the direct approach, where an artificial parameter is introduced to the linear system of DAEs. A substitute model of a transmission line yields a test example for the direct approach and is also simulated both in frequency and time domain. We analyze the sensitivity of the solution with respect to the artificial parameter. Uniform convergence of the transfer function of the regularized system towards the transfer function of the system of DAEs is proved in the general linear case.

Monotonicity and boundedness properties of general linear methods.
Anna Mozartova, W. Hundsdorfer, M.N.Spijker

In this work an analysis of monotonicity and boundedness properties is provided for the class of general linear methods which includes Runge-Kutta methods and linear multistep methods. We present a framework for deriving optimal stepsize conditions which guarantee boundedness. General results are presented for linear multistep methods either with starting vectors or with suitable starting procedures. The last allows to include in the theory many popular methods used in practice. Several numerical illustrations will be given to verify the theory.

Numerical Mathematics Aspects of Computational finance
Cornelis W. Oosterlee, Fang Fang, Lech Grzelak

In this presentation we will discuss some topics in Finance that require Mathematics, and, in particular, efficient numerical techniques. We will discuss option pricing, for example, for option contracts based on more than one underlying stock, and contracts with advanced stochastic models for the underlying stock price dynamics. We will focus on a mathematical framework in which we perform this research. One of the aims is to price the options as fast as possible.

Direct Walsh-Hybrid Method for Variational Problems
Yadollah Ordokhani

A direct Ritz method for solving variational problems with fixed and free boundary conditions is demonstrated Walsh-hybrid methods bases are used as the basis functions. It is shown how the form of the operational matrix of integration affects accuracy of the obtained approximate solutions. The properties of the Walsh-hybrid functions with the operational matrix of integration and the cross product of two Walsh-hybrid function vectors are utilized to reduce a variational problem to the solution of algebraic equations. The method is computationally attractive and application are demonstrated through illustrative examples.

Operator splitting methods: analysis and convergence

Alexander Ostermann, Eskil Hansen

Splitting methods constitute an important class of competitive time integration schemes for evolution equations. Despite of the extensive use of splitting methods in pratical applications, their convergence properties for partial differential equations are still far from being fully understood. In this talk, we will present a new framework for analyzing convergence of splitting methods. The framework is based on (analytic) semigroups and their related φ-functions. It can be applied to a large class of splitting schemes, including exponential operator splitting methods as well as the traditional Peaceman–Rachford splitting. In the talk, we will concentrate on linear problems with constant or time-depending coefficients.

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Two-step modified collocation methods with structured coefficient matrices for ordinary differential equations

Beatrice Paternoster, R. D'Ambrosio

In the context of the numerical integration of initial value problems based on ordinary differential equations, it is the purpose of this talk to introduce new continuous methods whose coefficient matrices show a structured shape in order to get an efficient implementation. These methods belong to the class of two step Runge–Kutta methods, introduced by Jackiewicz and Tracogna in [6] and further investigated by many other authors (see [5] and reference therein). The technique we use to provide a continuous approximation to the solution is a modification of multistep collocation, the so-called *almost two-step collocation* technique [1, 2, 3], i.e. the approximation is provided by an algebraic polynomial satisfying some oppurtune interpolation and collocation conditions, in order to create a good balance between high order of convergence and strong stability properties (e.g. A-stability and L-stability). We present the constructive technique, discuss the order of convergence and the stability properties of the resulting methods, provide reliable local error estimates exploiting the continuous approximant and show some numerical results originated by variable stepsize implementations [4].

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A variable time step–size code for advection-diffusion-reaction PDEs

Soledad Perez-Rodriguez, Severiano Gonzalez-Pinto

We present a variable time-stepsize algorithm for the integration of initial value problems (IVPs) in ordinary differential equations (ODEs) of the form

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0, \quad t_0 \leq t \leq t_{end}, \quad y, f \in \mathbb{R}^m,$$

which arise when some spatial discretization of time–dependent partial differential equations (PDEs), especially of Advection Diffusion Reaction type, is made by following standard techniques (Finite Differences, Finite Elements, etc). To cope with the presence of stiffness, the time integration is based on the two-stage Runge-Kutta Radau IIA scheme, which is a *third order, L-stable formula*. The solution of the highly implicit systems involved with the stage values of the Radau scheme is the main drawback to get an efficient implementation in the PDE context. However, in [1] we have coupled an Approximate Matrix Factorization (AMF) technique (inner iterations) to a Single–Newton iteration (SNI) (outer iterations of Newton-type) which reduces the computational effort to a manageable level for 2D-and-3D (spatial) PDEs. It was also shown that the new approach keeps the good stability and convergence properties of the Radau formula for 2D-spatial PDEs. In the case of 3D-spatial PDEs it loses some stability for large values in the imaginary axis, but it still performs quite well on advection dominated problems. This scheme was assessed in [1] only for some PDEs by using a fixed time step-size strategy. In this talk we pursue a variable step-size integration, which is currently much more efficient. For that goal we propose and analyze an embedded second order formula to estimate the local time error and we test the whole scheme on several nonlinear real-life problems and compare it with some standard PDE solvers such as IMEXRKC and VODPK.

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Numerical solution of forest fire initiation problem

Valeriy Perminov

In the present paper a mathematical model for description of heat and mass transfer processes at crown forest fire initiation is developed. It is based on numerical solution of three dimensional Reynolds equations of turbulent flow taking into account diffusion and convection of chemical species and equations of energy conservation for gaseous and condensed phases. It is assumed that the forest can be modeled as a two-temperature multiphase non-deformable porous reactive medium during a forest fire. The boundary value problem was solved numerically using the method of splitting according to physical processes. A discrete analog for the system of equations was obtained by means of the control volume method. The developed numerical model of forest fire initiation and spreading would make it possible to obtain a detailed picture of the variation in the velocity, temperature and chemical species concentration fields with time. It should help to establish the limiting conditions of forest fire initiation.

Proper Orthogonal Decomposition in Decoupling Large Dynamical Systems

Duc Toan Pham, Damien Tromeur-Devout

We investigate the proper orthogonal decomposition (POD) as a useful tool in decoupling large dynamical systems suitable for parallel computing. POD is well known to be applied to model reduction for different applications. It is based on snapshots on iterated solutions and allows to generate a low dimensional system for the approximation of the solution. We will focus on the parallelism potential with decoupling ODE systems by separating the whole system into subsystems and using reduced-order system for the coupled terms.
Our new approach consists in the decoupling of the system through the model reduction method. Indeed, extra-systems solved in reduced form are very computational attractive. When applying model reduction to dynamical systems, the snapshots of previous time steps are used to compute the POD basis to yield an optimal representation of the data in the sense of optimal least squares. Combined with Galerkin projection method, we can generate a lower dimensional model of the system. We extend this notion of model reduction to decouple the system into smaller subsystems. Therefore, we propose in this paper to a new form of error estimates by computing a residual based on the ODE which resulting the error. This residual leads us to a criterion on how well the reduced model is still appropriated, and based on what we can get an idea when to exchange information between sub-systems.
This method has been tested on several examples including stiff problems from PDEs, unsteady flow problem and provides interesting numerical results as well as great computing performance on parallel computers.

General linear methods with inherent Runge-Kutta stability for stiff problems

Helmut Podhaisky, Will Wright and John Butcher

The class of general linear methods was first constructed in 1965, however it has been only recently that subclasses of methods, which are not the traditional Runge–Kutta or linear multistep methods, have been identified as likely practical alternatives to these traditional methods. One such class of practical methods recently developed is known to possess the Inherent Runge–Kutta Stability (IRKS) property.
In this talk we identify practical methods for stiff problems within the class of IRKS methods of low order. We discuss the minimization of error constants and the size of the coefficients of the methods.

Variable step-size fractional step Runge-Kutta methods for time-dependent partial differential equations

Laura Portero, Andres Arraras and Juan Carlos Jorge

Fractional step Runge-Kutta (FSRK) methods are a class of additive Runge-Kutta schemes which provide efficient time integrations of evolutionary partial differential equations. The key point of an FSRK method lies in decomposing both the elliptic operator –involving the spatial derivatives– and the source term in order to get much simpler subproblems to solve. In certain cases, such a decomposition may be done by spatial directions, giving rise to extensions of the well-known family of alternating direction implicit (ADI) methods. By contrast, in some other cases, this decomposition can be related to a suitable partition of the spatial domain into a number of overlapping subdomains, thus obtaining the so-called domain decomposition splitting methods.
Within this framework, this work tackles the design and analysis of variable step-size time integrators of fractional steps type. In particular, we propose embedded pairs of FSRK schemes

which suitably estimate the local error at each time step in order to adapt the step-size efficiently. Such embedded pairs are then combined with standard spatial discretization schemes to provide efficient numerical methods for multidimensional parabolic problems. Finally, some numerical experiments illustrate the behaviour of the proposed algorithms.

Polynomial Chaos for Boundary Value Problems of Dynamical Systems

Roland Pulch

We consider boundary value problems of time-dependent systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs). Typically, physical parameters appear in the systems, which may exhibit some uncertainties. We replace such parameters by random variables and thus the solution of the systems becomes a random process. A Monte-Carlo simulation can be used to resolve the stochastic model. Alternatively, we apply the strategy of the generalised polynomial chaos. An intrusive approach yields a boundary value problem of a larger coupled dynamical system. We focus on a non-intrusive method, where boundary conditions are imposed on unknown functions, although these functions do not satisfy a system of ODEs or DAEs but a projection. This spectral approach demands just the solution of a single large nonlinear system in a numerical method. In contrast, many small nonlinear systems have to be solved in a Monte-Carlo method, where additional algorithms are required to control the convergence of involved Newton iterations efficiently. We present simulation results of a stochastic model using the discussed numerical techniques.

Reduction of CO_2 Emission in FT Synthesis Using a Novel Combination of Fixed and Fluidized Hydrogen-permselective Membrane Reactor-Separator loop

M. R. Rahimpour, E. Darzi

Highly paraffinic products in Fischer-Tropsch synthesis are desirable because they exhibit excellent combustion and lubricating properties. Unfortunately, a disadvantage of the Fischer-Tropsch process is emission of large amounts of CO_2 during the conversion of natural gas assets into saleable products. Accordingly, in view of the above disadvantage of the Fischer-Tropsch and GTL processes, there is a need for a process that is capable of producing desirable Fischer-Tropsch petroleum products while significantly minimizing CO_2 emissions commonly generated during the production of such products. The present work proposes a one-dimensional heterogeneous model to analyze the performance of combination of Fischer-Tropsch Synthesis (FTS) reactors in which a fixed-bed reactor is combined with a membrane assisted fluidized-bed reactor in loop. This model is used to compare the performance of the proposed combined system with a fixed-bed single stage reactor for Fischer-Tropsch synthesis loop. In the new concept, the synthesis gas is converted to FT products in two catalytic reactors. The first reactor is fixed-bed type and is cooled by water circulating on the shell side while the second reactor is fluidized-bed and the generated heat in this stage is transferred to the synthesis gas which is fed to the water cooled reactor. Due to lessen of H_2/CO usage ratio to values far from optimum reactants ratio along the conventional fixed bed reactor, the membrane concept is suggested for second stage to control hydrogen addition. Moreover, a bubbling fluidized bed system has been proposed to solve some observed drawbacks of industrial fixed-bed FT reactors such as high pressure drop, heat transfer problem, internal mass transfer limitations and radial gradient of concentration and temperature. The reactor model is tested against the pilot plant data of Research Institute of Petroleum Industry (RIPI) in Iran. The simulation results show that there is a favorable profile of product and CO2 in the membrane dual-type reactor relative to conventional systems. Therefore, the performance of Fischer-Tropsch reactor systems improves when a membrane is used in a conventional Fischer-Tropsch reactor loop.

Numerical analysis of homogenized tunability of composite material

Sergei Rakin, A. Kolpakov

We consider material with permittivity $\varepsilon(E)$ depending on electric field E applied. The ratio $\frac{\varepsilon(0)-\varepsilon(E)}{\varepsilon(0)}$ is called relatively tunability. For composite material, we can introduce the homogenized permittivity $\hat{\varepsilon}(E)$ [1] and homogenized tunability [2,3] $\hat{t}(E) = \frac{\hat{\varepsilon}(0)-\hat{\varepsilon}(E)}{\hat{\varepsilon}(0)}$.

We consider 2-D model of nonlinear ferroelectric composite of periodic structure and assume that the periodicity cell Y contains symmetric dielectric inclusion P. Because of the symmetry, we arrive at the following problem on the periodicity cell Y:

$$div(\varepsilon(\mathbf{x}), |\nabla\varphi(\mathbf{x}|) = 0 \text{ in } Y; \tag{1}$$
$$\frac{\partial\varphi}{\partial\mathbf{x}} = 0 \text{ if } x = 0, 1; \varphi = -E/2 \text{ if } y = 0, \varphi = E/2 \text{ if } y = 1;$$

E is the overall electric field. For ferroelectric (in domain $Y \setminus P$) approximation $\varepsilon(\mathbf{x}, |\nabla\varphi|) = \frac{\varepsilon_0 - \varepsilon_\infty}{1 + k|\nabla\varphi|^2} + \varepsilon_\infty$ is used, $\varepsilon(\mathbf{x}) = \varepsilon_d$ in dielectric inclusion P. Solution of the cellular problem (1) is equivalent to minimization of functional, which is potential for the operator (1) (if exists). We construct potential for the problem (1) and develop numerical method and computer program for numerical solution of the problem (1).

Tests. (1) Weak fields. In this case the problem (1) can be approximated with the linear problem with local permittivity equal to ε_0 in the domain occupied by ferroelectric. (2) Very strong fields. The problem (1) can be approximated with the linear problem with local permittivity equal to ε_∞ in the domain occupied by ferroelectric.

The problem was solved with our program of and ANSYS. Note that our program solves nonlinear problem in all cases, while ANSYS solves linear problem. The solutions obtained were in good agreement.

Analysis of tunability. For the values of the overall electric field between weak and very strong, we obtained solution of the problem (1) using our program and compute $\hat{\varepsilon}(E)$ and $\hat{t}(E)$. One of the results of our numerical analysis is conclusion that dilution of nonlinearity material with linear inclusions slowly reduce the homogenized tunability even the volume fraction of the dielectric (linear) inclusions is large. This is specific property of nonlinear problem, which has no analog in linear homogenization.

Adaptive time step control for the incompressible Navier-Stokes equations

Joachim Rang

This paper presents numerical studies for the incompressible Navier-Stokes equations in the case of two-dimensional laminar time-dependent flows. The concentration on laminar flows (instead of turbulent ones) avoids the use of a turbulence model. The turbulence model would be an additional factor which influences the computational results. Even for the two-dimensional laminar regime, the question of an optimal discretization approach is not yet answered. The most important requirements for the numerical solution of the Navier-Stokes equations are accuracy and efficiency. It turned out in the last decade that for accurate results temporal discretizations of at least second order and spatial discretizations with at least second order velocity and first order pressure should be used. The use of even higher order discretizations in space leads to severe difficulties in the solution of the arising discrete problems. Thus, the second requirement, a fast solution of the Navier-Stokes equations, will not be met for such discretizations. Also the use of

explicit time stepping schemes, whose length of the time step is restricted by the CFL condition results in general in an inefficient solution process. The discretization in space of the Navier-Stokes equations leads to a differential-algebraic equation (DAE). Solving a stiff ODE or a DAE a good time integration method needs an error estimator for increasing the efficiency. This error estimator suggests a new time step size to reach a given accuracy. If the time step size is too small then a lot of unnecessary computational work has to be done. Otherwise if the time step size is too large, the results become less accurate. A more effective control of time steps can be done with the so-called embedding technique. A lot of one-step methods allow that a second solution can be computed with almost the same coefficients, i.e. there are almost no further computational costs. Examples of such schemes are diagonally implicit Runge-Kutta and Rosenbrock-Wanner methods (linear implicit Runge-Kutta methods) which give accurate results.
In this paper we compare the fractional-step-θ-scheme with other diagonally implicit Runge-Kutta and Rosenbrock-Wanner schemes using automatic timestep length control.

Data assimilation using continuous ensemble Kalman filters

Sebastian Reich, Georg Gottwald, Kay Bergemann

We consider evolution problems for which the initial conditions are not known precisely and some solution components are observed subject to measurement errors. The solution to this problem is provided by the celebrated Kalman filter in case the system is linear and all errors and the initial conditions are normally distributed. Various extensions to nonlinear differential equations have been proposed in the past. One of the currently most popular approaches is provided by the ensemble Kalman filter technique which is now widely being used, for example, in meteorology. However, a number of open questions need to be addressed. Most of these questions relate to small ensemble sizes and poor approximations to the ensemble covariance matrix. In this talk, I will describe regularization techniques, such a ensemble inflation and localization, to overcome artifacts of small ensemble sizes in the context a continuous update formulation of the ensemble deviation matrix.

Discontinuous Galerkin finite element method for shallow two-phase flows

Sander Rhebergen, Onno Bokhove and Jaap van der Vegt

A common approach to model dense liquid-solid flows is to assume that both the liquid and the solid phases are continuous. This assumption results in three dimensional (3D) two-fluid two-phase flow equations. Assuming the flow is shallow, Pitman and Le [4] derived a depth-averaged two-phase flow model for debris flows in a similar manner as that the shallow water equations are derived from the 3D incompressible Navier-Stokes equations. We present a discontinuous Galerkin finite element method (DGFEM) to solve the depth-averaged two-phase flow model which contains nonconservative products. We have developed a general theory within the DGFEM to cope with nonconservative products [1] and the capabilities of our scheme were shown by solving numerous challenging test cases [1,2]. We recently also qualitatively validated our numerical results against laboratory experiments [3]. These experiments consist of liquid-solid flows through a contraction. Supercritical flows result in hydraulic jumps and oblique jump patterns are observed. Numerically, spurious oscillations may occur near these hydraulic jumps and a WENO slope limiter is applied in conjunction with a discontinuity detector to detect the regions where spurious oscillations appear.

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Multi-level Algorithms for Stochastic Heat Equations

Klaus Ritter, Simone Graubner and Thomas Müller-Gronbach

A basic computational problem for stochastic processes X is the evaluation of expectations $E(f(X))$ of functionals f on the path space. In this talk X will be the solution of a stochastic heat equation, driven by space-time or colored noise, and we will employ multi-level Monte Carlo methods to compute $E(f(X))$. We will present error bounds and numerical experiments and also point to optimality results, which are valid for Lipschitz-continuous functionals f.

Multi-level Monte Carlo methods with higher order schemes for the weak approximation of the solution of SDEs

Andreas Rößler, Kristian Debrabant

We consider the problem of weak approximation of solutions of stochastic differential equations (SDEs). Therefore, the multi-level Monte Carlo method is applied together with a second order weak approximation method. While the weak first order Euler-Maruyama scheme is applied for the reduction of variance, we propose to apply some higher order method in order to minimize the bias. Then, the mean-square error of the estimator for the expectation of a functional applied to the solution of the underlying SDE has asymptotically nearly optimal order. As the main novelty, the computational effort can be reduced by a fourth if a second order weak approximation scheme is applied. This will be revealed by some numerical examples.

Analytical averaging, numerical ordinary differential equations and multiscale methods

J. M. Sanz-Serna, M. P. Calvo, Ph. Chartier

The method of averaging, that goes back to Laplace and Gauss, provides a means to find the long-time behaviour of oscillatory dynamical systems without tracking all the details of the short time-scales. The heterogeneous multiscale method introduced by E and Engquist may be viewed as a technique to perform averaging in a purely numerical, efficient way. In the first part of the talk we shall show how the tools of the modern analysis of *numerical* methods for ordinary differential equations (trees, B-series, modified equation, ...) may be advantageously used to implement the *analytical* method of averaging. We shall then formulate new numerical algorithms that may be seen as improved versions of the heterogeneous multiscale method.

Numerical solution of Linear Ordinary Differential Equations in Quantum Chemistry by Spectral Methods

Masoud Saravi, F. Asrafi, S. R. Mirrajei

As we know, most differential equations concerning physical phenomenon could not be solved by analytical method. Even if we use Series Method, some times need an appropriate change of variable, and even when we can, their closed form solution may be so complicated that using it to obtain an image or to examine the structure of the system is impossible. In this paper, after introducing Clenshaw method, which is a kind of Spectral methods and Pseudo-spectral, we try to solve such equations and compare these two methods with some numerical examples.

DG vs Nedelec in the finite element time-domain computations of the second-order Maxwell equations

Domokos Sarmany, J.J.W. van der Vegt, M.A. Botchev, J.G. Verwer

We study the roles of different time- and space-discretisation schemes in the time integration of the second-order three-dimensional Maxwell equation with a possibly non-zero conduction term. The semi-discrete system is obtained through either of two finite element discretisation (FEM) techniques: the discontinuous Galerkin FEM (DG-FEM) and the $H(\mathrm{curl})$-conforming FEM. While DG-FEM suffers from an increased number of degrees of freedom compared with $H(\mathrm{curl})$-conforming FEM, it has the advantage of a purely block-diagonal mass matrix. This means that it is no longer necessary to solve linear systems when an explicit time-integration method is used. In this work, we use a hierarchic construction of $H(\mathrm{curl})$-conforming finite element space [1] for both types of spatial discretisation. The standard approach in high-order DG discretisations in time domain is to use an explicit high-order Runge-Kutta time-integration method to preserve the accuracy of the spatial discretisation. However, a nonzero conduction term may require a rather stringent time-step restriction on the time-integration process [2]. Therefore, alternative methods are necessary that treat the conduction term implicitly. The purpose of this work is twofold. We give a direct comparison of the two spatial discretisations in terms of computational work; and we investigate the stability and accuracy of the fully discrete system when a number of the most popular time-integration methods are used.

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Partitioning strategies for multirate time stepping for DAEs

Valeriu Savcenco

For large systems of differential algebraic equations (DAEs) some components may show a more active behavior than other. We address multirate time integration which aims to approximate the solution of DAEs with efficiently different time steps according to locally highly different dynamics behaviour. Partitioning of the differential and algebraic variables in different classes of activity directly influences the accuracy and the efficiency, and therefore is crucial for multirate methods. In our talk we present an automatic partitioning strategy and show the results for several numerical tests.

Stabilized modular time integration of coupled DAEs

Tom Schierz, Martin Arnold

The modeling of technical systems often leads to differential equations that are coupled by constraints. This results in a set of coupled differential-algebraic equations (DAEs). For efficiency concerns the full system of DAEs is split in several subsystems, which are solved separately by modular time integration methods, while necessary data from other subsystems is approximated per macrostep by extrapolation or interpolation. After each macrostep, at discrete predefined or adaptively defined communication points, the data is updated or synchronized respectively. The approximations of data between these communication points (for the current macrostep) lead to an additional error in the time integration and may even cause instability, which, differently from ODEs, can not be fixed by reducing the stepsize below a small stability bound.
We present a novel stabilization strategy fixing these problems resulting in stable modular time integration of coupled DAEs. The application of this strategy is presented for some benchmark problems.

Convergence of continuous approximations for discontinuous ODEs

Hagen Schiller, Martin Arnold

We consider ordinary differential equations with discontinuous right-hand-side

$$\dot{y}(t) = f(y) = f^{\alpha}(y), \quad \alpha_i = \operatorname{sign}(\psi_i(y)), \tag{1}$$

where the functions f^{α} are continuous and α is a multi-index depending on the signs of the components of the vector-valued switching function ψ. The discontinuities cause considerable difficulties for the numerical treatment of (1). Therefore, in practice, equation (1) is often replaced by a continuous approximation

$$\dot{z}_{\epsilon}(t) = f_{\epsilon}(z_{\epsilon}), \tag{2}$$

which depends on a regularisation parameter ϵ. Previous work on this subject almost exclusively deals with the case of a scalar-valued switching function ψ.
In our talk, we prove that the solutions of (2) converge to a suitably defined solution of the original system (1) whenever ϵ goes to zero. In the case of a scalar-valued switching function, the convergence can be shown to be linear in ϵ under reasonable conditions. We conjecture that linear convergence also holds for the vector-valued case. Numerical evidence is given to substantiate this claim.

Spatial Simulation of Pushbelt CVTs with Timestepping Schemes

Thorsten Schindler, Heinz Ulbrich, Friedrich Pfeiffer, Arie van der Velde, Arjen Brandsma

With a pushbelt Continuously Variable Transmission (CVT) the whole drivetrain including the engine of a passenger car can operate in an optimal state at any time. For further improvements with respect to fuel consumption, dynamic simulations of the system were investigated by Bosch and the Institute of Applied Mechanics of the Technische Universität München in the last years [1, 2].
The underlying mathematical models are characterised by numerous contacts and a large degree of freedom. To avoid high numerical stiffnesses due to springs and to encourage an efficient as well as stable and robust numerical treatment, a nonsmooth contact description is chosen. Timestepping schemes are used to integrate the resulting measure differential inclusions (MDI) [3].

This paper deals with a spatial transient mathematical model of pushbelt CVTs to consider also out-of plane effects, for instance pushbelt misalignment. The equations of motion are derived using methods of multibody theory and nonlinear mechanics. Thereby, the bodies themselves are described using rigid and large deflection elastic mechanical models. In-between the bodies, all possible flexible or rigid contact descriptions, namely frictionless unilateral contacts, bilateral contacts with 2D-friction and even unilateral contacts with 3D-friction occur.
In comparison with the planar case the calculation time increases significantly mainly because of the large degree of freedom and the number of contact possibilities. Stationary initial value problems are solved and parallelisation techniques are applied to reduce the computational effort.

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Numerical Solution of Multiscale Problems in Atmospheric Modeling

Martin Schlegel, Oswald Knoth, Ralf Wolke, Martin Arnold

In atmospherical sciences the evolution of contaminants in the atmosphere is often described by advection-diffusion-reaction equations, using wind fields provided by an online coupled weather forecast model. Special challenges arise in the simulation of realistic scenarios. Due to convection and local grid refinement the characteristic times of horizontal and vertical transport may differ significantly. For the efficient solution of the advection equation in this context we propose an operator split generic multirate (MR) time integration scheme. This scheme is extended to a multirate implicit/explicit (IMEX) scheme allowing for the incorporation of chemistry reactions for aerosol chemistry modeling. The full method is implemented in a multi scale chemistry transport model. Results from real scenario simulations will be presented.

On algebraic stability of general linear methods and peer methods

Bernhard A. Schmitt

Algebraic stability of General Linear Methods (A, U, B, V) is characterized by the existence of a definite symmetric matrix G making a certain 2×2 block matrix positive semidefinite. Under a mild assumption being satisfied by many GLMs from the literature this condition is equivalent to definiteness of a much simpler block matrix containing G in two places. Further transformations lead to a neccesary condition depending on one aggregated coefficient matrix only. For peer two-step methods which use $A = B$ and $U = V$ this latter condition is also sufficient and we relate further formulations to a recent result of Adrian Hill. For peer methods with 2 or 3 stages a G-matrix can be constructed in explicit form and many algebraically stable 3-stage methods have been found.

Numerical Simulation of Relativistic Laser-Plasma Interaction
Julia Schweitzer, Marlis Hochbruck

In laser-plasma physics, many phenomena can be described by a nonlinear wave equation coupled to an equation for the plasma responce. Since the interesting physical problems are huge, fast and efficient numerical solvers are required. In this talk, we present some advances on the solution of these application problems.

Three Dimensional Numerical Simulation of Thin Metal Plates Laser Welding
Vasily Shapeev, Vadim Isaev, Anatoly Cherepanov

A three-dimensional quasi-stationary mathematical model of thin metal plates laser welding is proposed in the present work. The welding is performed by radiation of a CO2 laser with Gaussian intensity distribution. A presence of a steam channel near the laser axis is taken into account. Heat fluxes from the direct and reflected laser beams at the surface of the steam channel are included into boundary conditions. Heat losses through upper and bottom surfaces of the plates are also considered in the model. These losses occur due to blow of the weld area by inertial gas, and the heat radiation into the surrounding space (in parvo). The simulation of heat-and-mass transfer processes is performed with the use of heat conduction equation and Navier-Stokes equations here. Boundary value problems for these equations are numerically solved by known conservative finite-difference scheme and new versions of the collocations and least squares method (CLS) developed in the present work. Computer program created here allows one to find (like in Stefan problem) unknown boundaries in the computational domain between sub domains occupied by different metal phases. The surface of the steam channel is automatically constructed during numerical solution by a new algorithm proposed here. Three-dimensional calculations for steel and aluminum plates were conducted. The simulated widths of weld seam satisfactorily coincide with corresponding experimental data.
The work was supported by RFBR, Project No. 08-08-00249-a and the Integration Project of SB RAS No. 26.

Solving Transient Saddle Point Problems in Computational Mechanics
Bernd Simeon

Systems of partial differential equations with constraints and Lagrange multipliers arise in various application fields. Examples of such saddle point formulations can be found in incompressible fluid flows, biological tissue models, contact mechanics, and in two-field problems with separate interface variables. This talk is aimed at introducing a general framework for the problem class, with particular emphasis on the connection with differential-algebraic equations and with efficient and robust time integrators. Two examples will provide specific insight into some of the key aspects. The first example is a model for skeletal muscle tissue, which is discretized in space by Taylor-Hood finite elements and whose index varies, depending on certain physical parameters, between one and three. The second example, a fluid dynamics simulation with stabilized equal-order finite elements, addresses the issue of adaptivity in space and time.

Numerical solution of the Dirichlet problem for linear parabolic stochastic partial differential equations based on averaging over characteristics
Vasile Stanciulescu, M.V. Tretyakov

Numerical methods for the Dirichlet problem for linear parabolic partial differential equations are constructed. The methods are based on the averaging-over-characteristic formula and the weak-sense numerical integration of ordinary stochastic differential equations in bounded domains. Their orders of convergence in the mean-square sense and in the sense of almost sure convergence are obtained. The Monte Carlo technique is used for practical realization of the methods. Results of some numerical experiments are presented.

Peer methods for the one-dimensional shallow water equations with CWENO space discretization

Gerd Steinebach, Rüdiger Weiner

For many practical problems an efficient solution of the one-dimensional shallow water equations (Saint-Venant equations) is important, especially when large networks of rivers, channels or pipes are considered. In order to test and develop numerical methods four test problems are formulated. These problems include the well known dam break and the hydraulic jump problems and two steady state problems with varying channel bottom, channel width and friction.
The space discretization of the partial differential equations is based on a finite volume approach with central WENO interpolation and local Lax-Friedrich fluxes. For time-integration new linearly-implicit two-step peer methods of orders three and four are developed. These methods are especially adapted to the usage within the method of lines framework. They show a good performance compared to the well established methods like `ode15s`, `radau5` or `rodasp`.

One-parameter family of steady states in the model of population dynamics

Vyacheslav Tsybulin

The dynamics of three populations that share a common areal is modelled by nonlinear parabolic equations. For some choice of parameters and boundary conditions the given system has a cosymmetric family of steady states. By computer experiment based on the finite difference approach we show different scenarios for the evolution of stationary and nonstationary regimes. Influence of the boundary conditions on regime transformations is analyzed. Transitions of the family of equilibria to a limit cycle or/and isolated steady states under perturbation of the Dirichlet boundary conditions are found.

Convergence of space-adaptive algorithms

Andreas Veeser

There has been recent progress in the understanding of the convergence of adaptive algorithms with finite elements. In particular, the plain convergence results are established under quite general or even necessary assumptions.
This talk will overview such plain convergence results for adaptive algorithms. Doing so, the difference to the classical convergence theory will be emphasized and the roles of stability and error estimator will be highlighted.

On the time integration of Maxwell's equations
Jan Verwer

Numerical integration of Maxwell's equations is often based on explicit methods accepting a stability step size restriction, notably Yee's scheme or a related one. In literature it has been pointed out that there is also a need for unconditionally stable methods, as exemplified by the successful alternating direction implicit - finite difference time domain scheme. In this lecture we will assess unconditionally stable integration for a general semi-discrete Maxwell system allowing non-Cartesian space grids as encountered in finite element discretizations. Such grids exclude the alternating direction implicit approach. Particular attention will be given to the second-order trapezoidal rule implemented with preconditioned conjugate gradient iteration and to a second-order exponential integrater using Krylov subspace iteration. A three-space dimensional test problem is used for numerical assessment and comparison with the most economical second-order explicit integrator. Our experience with this test problem, although still limited, indicates that the explicit integrator is hard to beat. The lecture is based on joint work with Mike Botchev, Twente University, published in

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Goal Oriented Space-Time Adaptivity for Simulation and Optimization of Parabolic Systems
Boris Vexler, Dominik Meidner, Michael Schmich

In this talk we discuss a general approach for adaptivity and error estimation for simulation and optimization of problems described by parabolic differential equations. Both temporal and spatial discretizations are based on finite element methods. For this class of discretizations we derive error estimators assessing the discretization error with respect to a given quantity of interest. The presented estimates separates the influence of the temporal and the spatial discretization, which allows for balancing these two types of error. Moreover, the error estimators provide information for separate refinement of the finite element meshes corresponding different time steps. Numerical examples are presented illustrating the efficency of our method.

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Quasistatic approximations for stiff second-order differential equations

Steffen Weber, M. Arnold, M. Valášek

Stiff terms in second-order differential equations may cause long computation time due to high frequencies. Quasistatic approximations eliminate these high frequency solution components by neglecting inertia forces.
Equations of motion are given by

$$M(q)\ddot{q} = f(q, \dot{q}),$$

where M denotes a state-dependent mass-matrix that is symmetric and positive definite. This can be transformed into a semi-explicit differential equation

$$\begin{aligned} \ddot{x} &= f(x, y, \dot{x}, \dot{y}) \\ \varepsilon\ddot{y} &= g(x, y, \dot{x}, \dot{y}), \qquad 0 < \varepsilon \ll 1, \end{aligned}$$

using various methods which shall be analyzed.
Under suitable conditions this equation can be reduced to a less complex equation

$$\begin{aligned} \ddot{x} &= f(x, y, \dot{x}, \dot{y}) \\ 0 &= g(x, y, \dot{x}, \dot{y}) \end{aligned}$$

where the solutions of both equations converge to each other.

Efficient Global Error Estimation and Control in Explicit Parallel Peer Methods

Rüdiger Weiner, Gennady Yu. Kulikov

Recently, Kulikov [1] presented the idea of double quasi-consistency, which facilitates global error estimation and control, considerably. More precisely, a local error control implemented in such methods plays a part of global error control at the same time. However, Kulikov studied only Nordsieck formulas and proved that there exists no doubly quasi-consistent scheme among those methods.
In this paper, we prove that the class of doubly quasi-consistent formulas is not empty and present the first example of such sort. This scheme belongs to the family of superconvergent explicit two-step peer methods constructed by Weiner et al. [2]. We present a sample of s-stage fixed-stepsize doubly quasi-consistent parallel explicit peer methods of order $s-1$ when $s = 3$. The notion of embedded formulas is utilized to evaluate efficiently the local error of the constructed doubly quasi-consistent peer method and, hence, its global error at the same time. Numerical examples confirm clearly that the usual local error control implemented in doubly quasi-consistent numerical integration techniques is capable of producing numerical solutions for user-supplied accuracy conditions in automatic mode.
Then, we discuss variable-stepsize explicit parallel peer methods grounded in the interpolation idea. Approximation, stability and convergence are studied in detail. In particular, we prove that some interpolation-type peer methods are stable on any variable mesh in practice. Double quasi-consistency is utilized to introduce an efficient global error estimation formula in the numerical methods under discussion. The main advantage of these new adaptive schemes is the capacity of producing numerical solutions for user-supplied accuracy conditions in automatic mode and almost at no extra cost. This means that a usual local error control mechanism monitors and regulates the global error at the same time because the true error of any doubly quasi-consistent numerical method is asymptotically equal to its local error. Numerical experiments support theoretical results of this paper and illustrate how the new global error control concept works in practice. We also conduct a comparison with explicit ODE solvers in MatLab.

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Stability of rational approximations to the exponential function with restricted denominator

Daniel Weiß, John Butcher

The stability function of a singly-implicit Runge-Kutta method, that is a method with the property $\sigma(A) = \{\lambda\}$, is a rational approximation to the exponential function with a restricted denominator:

$$R(z) = \frac{N(z)}{(1-\lambda z)^s},$$

where s denotes the number of stages and $\deg(N) \leq s$. All L-stable stability functions are known with order $p = s \leq 15$. There are L-stable methods up to order $p = 8$, except for $p = 7$. The corresponding SIRK methods are suitable for the numerical solution of stiff equations. An undesirable property of methods, with stage order $q = s > 2$, is that some absissae c_i are greater than 1.
In this talk, L-stable methods will be discussed for $p = q = s - 1$ and $p = q = s - 2$. We will derive intervals of possible L-stability by use of order arrows and order stars arguments. In case of $p = s - 1$ there are intervals of L-stable methods up to $p = 10$, except for $p = 9$. Getting more freedom in case of $p = s - 2$ we explore the stability depending on two parameters.
Finally we will show that the abscissae can be chosen freely.

Simulation of an isentropic layer model by particle methods

Jörg Wensch, Sebastian Reich

Particle trajectories in atmospheric motion lie in layers of constant potential temperature under the assumption of adiabatic thermodynamics. This motivates an isentropic layer model where potential temperature serves as a vertical coordinate. The horizontal discretization in each layer is done by a Lagrangian method based on a Hamiltonian principle – the smoothed particle-mesh method. For the hydrostatic case pressure and layer height are computed from the advection of a generalized density. We present numerical results for 2D- and 3D mountain flow.

Ritz Legendre Multiwavelet Method for the Damped Generalized Regularized Long-Wave (DGRLW) Equation

Sohrab Ali Yousefi, Z. Barikbin

A numerical method is proposed to approximate the solution of the nonlinear damped generalized regularized long-wave (DGRLW) equation with a variable coefficient. The DGRLW equation is a partial differential equation that describes the amplitude of the long-wave, which can be written as

$$u_t - (\phi(x,t)u_{xt})_x - \alpha u_{xx} + u_x + u^p u_x = f(x,t), \quad x \in \Omega, \quad 0 < t \leq T$$

with inital condition

$$u(x,0) = f_0(x), \quad x \in \overline{\Omega}$$

and boundary conditions

$$u(0,t) = g_0(t), \quad u(1,t) = g_1(t), \quad 0 \leq t \leq T$$

where $\phi(x,t)$ is a known function, $\alpha > 0$, $p \geq 1$ is an integer and $u(x,t)$ being the amplitude of the long-wave at the position x and at time t.
The method is based upon Ritz Legendre multiwavelet approximations. The properties of Legendre multiwavelet are first presented. These properties together with Galerkin method are then utilized to reduce the nonlinear DGRLW equation to the solution of algebraic equations. Illustrative examples are included to demonstrate the validity and applicability of the technique.
Keywords: Legendre Multiwavelet, DGRLW equation, Ritz method, Galerkin method.

Numerical modeling of kinetics of radiation defect clusters nucleation and radiation-induced swelling in graphite

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Reactor materials under influence of high-energy neutron irradiation undergo size and physical properties changes. These changes are defined dominantly by temperature, neutron fluence and sample microstructure. As a result of high-energy neutron irra-diation of materials, occurs the generation of point radiation defect excess: inter-stitials and vacancies. In the process of diffusive motion they recombinate with each other, form clusters of radiation defects and absorb on such sinks as grain bounda-ries and dislocation loops. All these processes lead to such effect as swelling that reduces the radiation stability of materials. In the present report the general physical mechanisms of radiation swelling of gra-phite materials are investigated based on the numerical modeling radiation defect cluster nucleation and growth. The theoretical model is based on the solution of kinetic equation system for point radiation defects and defect clusters in irradiated material. Original presence and following generation of point admixtures is implied to describe the set of complex processes that occurs in graphite under irradiation more completely and precisely. Generally problem of swelling rate simulation accounting the process of admixtures generation is solved. Interesting effect of local swelling minimum formation (shrin-kage) is simulated and showed graphically. The analysis of defects concentration influence upon characteristic form of time dependence shape for irradiation-induced swelling is realized.

Analysis and Computation of Non-monotonous Travelling Waves in a Non-equilibrium Richard's Equation

Paul Zegeling

Space-time evolution described by nonlinear PDE models involves patterns and qualitative changes induced by parameters. In this talk we will emphasize the importance of both the analysis and computation in relation to a bifurcation problem in a non-equilibrium Richard's model from hydrology. The extension of the Richard's equation to take into account additional dynamic memory effects was suggested by Hassanizadeh and Gray in the 90's. This gives rise to an extra third-order mixed space-time-derivative term in the PDE. It is possible, by using a travelling wave formulation, to analyse the related dynamical system in the phase plane. It is derived, that for special choices of the dynamic capillary pressure parameter, we can expect different solution behaviour, varying from smooth waves to solutions with a plateau value, but also oscillatory waves. The analysis is supported by numerical solutions of the full PDE model through an adaptive grid method with a sophisticated monitor function. It is shown that, in this framework, theory from applied analysis, accurate numerical PDE solutions and also the experimental observations can be nicely fitted.

On the Numerical Solution of the Fokker-Planck Equation on Geodesic Grids
Evgeniy Zharovsky, Bernd Simeon

The addition of rigid-rod like particles is able to reduce the drag loss in pipe flows. From a mathematical point of view, this leads to a coupled system for the fluid flow and the particle dynamics. More specifically, to predict drag reduction caused by such elongated particles (fibers), it is important to approximate the orientation distribution function (ODF) of the fibers in the domain. This leads to a special Fokker-Planck equation on a unit sphere, where each point on the surface of the sphere represents a particular orientation. The classical approach to solve this problem numerically is a Galerkin projection usually onto spherical harmonics. However, in case of large drag reduction, which is very important in applications, the ODF density is approaching a delta distribution, leading to the problem that a high number of modes is needed to represent the solution properly. The computationally expensive classical approach becomes prohibitive in such a situation.
We want to present a new approach based on a geodesic icosahedral type grid. We study different time integration schemes for some test cases on a quasi uniform grid and give an outlook for adaptive techniques.

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