The seminar NUMDIFF–13 is jointly organised 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)

- Helmut Podhaisky (Halle)

- Rüdiger Weiner (Halle)

- Jason Frank (Amsterdam)

- Willem Hundsdorfer (Amsterdam)

Conference office

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

Acknowledgements

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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. Parking spaces are available.
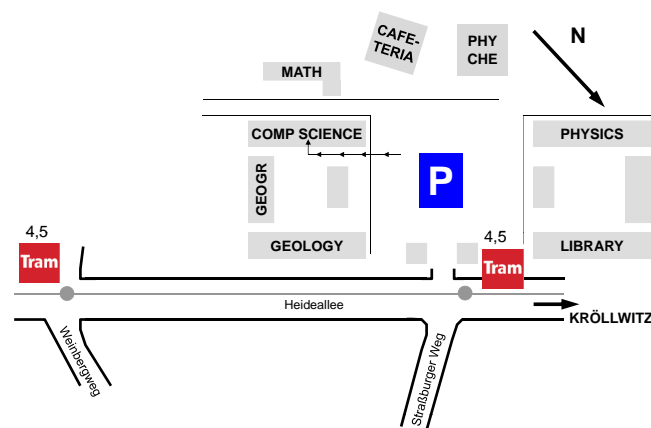
   The conference will begin at 9:00 on Monday, 10 September 2012, and will finish around 12:15 on Friday, 14 September 2012. From Tuesday to Friday, the lectures will start at 8:30. To reach the conference site from the Best Western Hotel you can use the tram lines 2,9,10 and 11 first, leaving in front of the hotel from stop "Zentrum Neustadt" towards "Beesen" or "Hauptbahnhof", then get off at the third stop "Rennbahnkreuz" and change to tram line 4 or 5, direction "Kröllwitz", leaving from the track perpendicular to the arriving track (100 meter walk), and finally get off at the third stop "Straßburger Weg".

2. **Conference Office and Registration**
   The conference office will be open on Sunday, 9 September 2012, from 17:00 to 20:00 in the lobby of the Best Western Hotel Halle-Neustadt (+49 345 69310). On the other days the conference office will be situated at the conference site in room 1.03. It will be open on Monday, Tuesday and Thursday from 8:00 to 16:00, and on Wednesday and Friday from 8:00 to 12:00. You can reach the conference office by phone +49 345 5524799 and by fax +49 345 5527004. These lines will be active from Monday, 10 September 2012.

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

3. **Lecture Rooms and Audio-Visual Requirements**
   The opening of the seminar as well as all plenary lectures will take place in lecture room 3.28.

All lecture rooms will be equipped with laptop and data projector. Speakers should load their talk onto the conference laptop of their lecture room before the beginning of their session.

4. **Time of Lectures and Discussion**
   Please note that the lecture times as given in the programme already include five minutes for discussion. Session chairs will make sure that speakers do not exceed their allocated time.

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

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

6. **Computer and Internet Access**
   At the conference site you can access the internet. We have reserved room 1.30 for discussions and there you can also use your own computer.

7. **Conference Dinner**
   The conference dinner will be held in the Best Western Hotel Halle-Neustadt on Thursday, 13 September at 19:00. One dinner ticket is included in the conference fee.

8. **Tour to "Gartenreich Wörlitz" on Wednesday afternoon**
   The Wörlitz Park is part of the Garden Kingdom of Dessau-Wörlitz, which was added to the UNESCO World Heritage List in November 2000. The whole Garden Kingdom is situated in the midst of the Biosphere Reserve of the Middle Elbe River. If you are interested then please register for the excursion at the conference office. Busses will leave from the conference site at 13:00 and will return to Halle at around 19:30.

9. **Conference Proceedings**
   The proceedings of NUMDIFF-13 will be published as a special issue of the *Journal of Computational and Applied Mathematics*. Guest editors are M. Arnold, J. Frank, W. Hundsdorfer, H. Podhaisky and R. Weiner.

   Every speaker of NUMDIFF-13 can submit a manuscript for consideration of publication in this special issue. Submitted manuscripts must deal with original work not published elsewhere and will be refereed according to the standard journal procedure.

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

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

   Authors are encouraged to use the journal style files. The paper length is restricted to 20 style file pages. The deadline for manuscript submission is 15 December 2012.

   The manuscripts should be submitted through `http://ees.elsevier.com/cam/`. Please indicate that your article is for this special issue by selecting article type *"NUMDIFF13"*. Please also send a copy directly to `willem.hundsdorfer@cwi.nl`.

1 Programme Overview

Monday, September 10, 2012

	R 3.28	R 1.23	R 1.26	R 1.27
9:00	–Opening–			
9:20	Hairer			
10:10	–Break–			
10:40	Betsch			
11:30	Blanes			
12:20	–Lunch–			
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14:25	Becker	Kelly	Schmitt	Heubes
14:50	Vu	Guias	Kulikov	Niemeyer
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16:10	Jansen	Lang	Mushtaq	Burger
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17:00	Horváth	
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2 Scientific Programme

Monday, September 10, 2012

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11:30 **Blanes**, Sergio
Symplectic methods for the time integration of the Schrödinger equation

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14:00 **Arnold**, Martin
Spurious oscillations in an index-3 DAE solver for constrained mechanical systems

14:25 **Becker**, Urs
On Rosenbrock methods for singular singularly perturbed problems and their application to nearly incompressible materials

14:50 **Vu**, Linh
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15:15 **Valášek**, Michael
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14:25 **Kelly**, Conall
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14:50 **Guias**, Flavius
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15:15 **Rezaeian**, Ramezan
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14:00 **Mitsui**, Taketomo
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14:25 **Schmitt**, Bernhard A.
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14:50 **Kulikov**, Gennady
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15:15 **Schröder**, Dirk
Adjoint Consistent Implicit Peer Methods

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14:25 **Heubes**, Daniel
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14:50 **Niemeyer**, Julia
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15:15 **Rouhparvar**, Hamid
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16:35 **Schierz**, Tom
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16:35 **Steinebach**, Gerd
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17:00 **Wensch**, Jörg
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17:25 **Naumann**, Andreas
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16:10 **Mushtaq**, Asif
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16:35 **Bader**, Philipp
Splitting methods with complex coefficients for the Schrödinger equation in imaginary time

17:00   **Einkemmer**, Lukas
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17:25   **Dörsek**, Philipp
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16:35   **Ha**, Phi
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17:00   **Kulikova**, Maria
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17:25   **Saravi**, Masoud
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9:20 **Tischendorf**, Caren
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11:05 **Braś**, Michał
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11:30 **Jamil**, Noreen
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11:05 **Ghovatmand Jazei**, Mehdi
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11:30 **Chistyakova**, Elena
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11:55 **Pandit**, Sapna
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11:30   **Zakharov**, Alexander
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        Dynamic Response of Highway Bridges to Heavy Vehicle Loads

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14:30   **Reich**, Sebastian
        Impact of model errors on data assimilation algorithms

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        Convergence of the implicit-explicit Euler scheme applied to perturbed dissipative
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        Semi-Lagrangian schemes for Hamilton-Jacobi-Bellman equations

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Exponential integrators for parabolic PDEs

16:30   **Hernández-Abreu**, Domingo
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17:00   **González Pinto**, Severiano
Simplifying AMF-schemes for Inexact Jacobians in large Stiff ODEs

17:30   **Beck**, Steffen
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Goal-adaptivity for fluid-structure interaction

9:20   **Butcher**, John
Symmetry of general linear methods and the underlying one-step method

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10:20   **Hill**, Adrian
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10:45   **Norton**, Terence
G-symplectic General Linear Methods

11:10   **Imran**, Gulshad
Order conditions for G-Symplectic methods

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10:20   **Wandelt**, Michele
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10:45   **Shcherbakov**, Dmitry
Structure-Preserving Projection Methods for Hamiltonian Systems

11:10   **Müller**, Andreas
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10:20   **Leitenberger**, Frank
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10:45   **Fiedler**, Robert
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11:10   **Mohaghegh**, Kasra
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10:45   **Zegeling**, Paul Andries
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11:10   **Marszałek**, Wiesław
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9:20   **Kværnø**, Anne
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11:05   **Bartel**, Andreas
On the convergence rate of dynamic iteration for coupled problems with multiple subsystems

11:30   **Gauckler**, Ludwig
Stability of plane waves in nonlinear Schrödinger equations: mathematical and numerical analysis

11:55   **Geiser**, Jürgen
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11:30   **Kuhn**, Karen
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11:55   **Koskela**, Antti
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10:40   **Weber**, Steffen
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11:05   **Schiller**, Hagen
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11:30   **Scholz**, Lena
Self-conjugate differential and difference operators in the optimal control of descriptor systems

11:55   **Lamour**, René
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11:30 **Perminov**, Valeriy
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11:55 **Khashin**, Sergei
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14:30 **Johnson**, Evan
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15:00 **Rossmanith**, James
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15:30 –Break–

16:00 **Baum**, Ann-Kristin
Positivity preserving simulation of Differential-Algebraic Equations

16:30 **Higueras**, Inmaculada
Positivity preservation of time-stepping methods

17:00 **Horváth**, Zoltán
Discrete positive invariance of sets

17:30 **Ketcheson**, David
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14:00 **Brumm**, Bernd
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14:30 **Weiß**, Daniel
Integrating Highly-Oscillatory Mechanical Systems with Solution-Dependent Frequencies

15:00   **Legoll**, Frederic
       A micro/macro parareal algorithm for a class of multiscale-in-time systems

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16:00   **Leboucher**, Guillaume
       Stroboscopic method for wave equation

16:30   **Kettmann**, Markus
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       using the heterogeneous multiscale method

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9:20   **Dieci**, Luca
       Filippov sliding motion on a co-dimension 2 discontinuity surface

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10:30   **Montijano**, Juan Ignacio
       Runge-Kutta projection methods for conservative and non conservative problems

11:20   **Mehrmann**, Volker
       Modelling, simulation and control of differential-algebraic systems

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3 Abstracts

The implementation of general linear methods
Saghir Ahmad, John C. Butcher, *Tue 11:30 R 3.28*

Numerical integrators for solving stiff and non-stiff problems are usually based on either multi-stage methods or multistep methods and each of these has its own advantages and disadvantages. In this project, we will use general linear methods (GLMs) which have the potential to provide the best features from each of the traditional classes. A special design choice amongst GLMs will be presented in this talk, whose main features are the IRKS- and F-properties. Also, there are some difficult design issues in the implementation of classical methods. These include error estimation and step size and order control. There is still considerable theory to investigate and analyse, but we believe that GLMs are likely to provide good solutions. Although the main aim of our project is to construct an algorithm for both stiff and non-stiff systems, here the implementation of some low order explicit methods of the design proposed will be presented in the form of a preliminary algorithm.

Operator Index Reduction in Elastodynamics
Robert Altmann, *Tue 10:40 R 1.26*

In flexible multibody dynamics, boundary conditions of the involved bodies play a crucial rule. Therefore, we analyse the equations of elastodynamics with weakly enforced Dirichlet constraints. The use of Lagrange multipliers leads to a problem of saddle point structure,

$$
\begin{aligned}
(\rho \ddot{u}, v)_{L^2(\Omega)} + a(u, v) + b(v, \lambda) &= \langle f, v \rangle && \text{for all } v \in [H^1(\Omega)]^2, \\
b(u, \mu) &= \langle g, \mu \rangle && \text{for all } \mu \in [H^{-1/2}(\partial\Omega)]^2.
\end{aligned}
$$

A standard semi-discretization in space by finite elements leads to a differential algebraic equation of index 3. Performing the time-integration by Newmark's method, we achieve second order convergence for the deformation variable but no convergence for the Lagrange multiplier. In the context of coupled systems, the Lagrange multiplier equals the stress in normal direction at the boundary. Thus, an index reduction such as minimal extension is advisable. This technique provides an extended index-1 formulation which guarantees the boundary constraints, i.e., we avoid a drift at the boundary.

In this talk, we present an index reduction technique at operator level. This procedure acts on the partial differential equation, i.e., on the continuous model. The result is an extended operator DAE with the property that a semi-discretization in space leads directly to an index-1 formulation. Furthermore, we show that the index reduction and semi-discretization steps commute.

Spurious oscillations in an index-3 DAE solver for constrained mechanical systems
Martin Arnold, *Mon 14:00 R 3.28*

Generalized-α time integration methods are quite popular in structural dynamics and may be extended straightforwardly to constrained mechanical systems that are desribed by 2nd order index-3 DAEs. From the pure numerical viewpoint, the methods should be combined with some kind of index reduction to avoid the well known problems of higher index DAE time integration. On the other hand, the direct application to the original index-3 formulation of the equations

of motion allows a more direct implementation of generalized-α methods in existing industrial simulation tools.

We will show that these methods suffer from order reduction and spurious oscillations in the initial phase of time integration. Order reduction may be avoided by perturbed starting values or by a modified first time step that guarantees second order convergence for reasonable values of algorithmic parameters.

Splitting methods with complex coefficients for the Schrödinger equation in imaginary time
Philipp Bader, *Mon 16:35 R 1.26*

An efficient method to compute the ground states of the Schrödinger equation is the propagation in imaginary time. In this work, we propose new splitting methods with complex coefficients in order to obtain higher order methods that cannot be achieved with classical splittings because of a problem that is analogous to integrating the heat equation backward in time - numerical instabilities occur for the computation of $\exp(hA)$, where A is the Laplacian and $h > 0$ for methods of order greater than two. Complex coefficients allow us to overcome this limitation. The study is complemented with numerical results.

On the convergence rate of dynamic iteration for coupled problems with multiple subsystems
Andreas Bartel, Markus Brunk, Sebastian Schöps, *Thu 11:05 R 3.28*

Simulator coupling is a standard technique for the transient simulation of coupled multiphysics problems. At synchronization times data between simulators is exchanged. Each simulator computes the solution for its domain only. Iteration ensures the consistency of the overall solution. In applications, this is referred to as cosimulation. In mathematics it is usually branded as dynamic iteration, since a fixed-point iteration is required to obtain convergence.

Time integration of spatially discretized partial differential equations results typically in coupled differential algebraic equations (DAEs). Whereas the convergence of cosimulation of ordinary differential equations (ODEs) is guaranteed, this does not hold for DAEs unless a contraction condition is met. In either case the convergence is linear with a rate strongly dependening on the coupling structure.

In this paper, we discuss the rate of convergence, i.e., the error reduction per iteration, for coupled problems that consist of multiple subsystems. Furthermore, we discuss several factors which influence the rate of convergence.

Positivity preserving simulation of Differential-Algebraic Equations
Ann-Kristin Baum, Volker Mehrmann, *Thu 16:00 R 3.28*

Positive dynamical systems arise in every application in which the considered variables represent a material quantity that does not take negative values, like e.g. the concentration of chemical and biological species or the amount of goods and individuals in economic and social sciences. Beside positivity, the dynamics are often subject to constraints resulting from limitation of resources, conservation or balance laws, which extend the differential system by additional algebraic equations. In order to obtain a physically meaningful simulation of such processes, both properties, the positivity and the constraints, should be reflected in the numerical solution. In this talk, we discuss these issues for linear time-varying systems, as they arise for example in the linearization of non-linear systems in chemical reaction kinetics or process engineering.

As for linear time-invariant systems [1], we pursue a projection approach based on generalized inverses that admits to separate the differential and algebraic components without changing coordinates.

We first consider index-1 problems, in which the differential and algebraic equations are explicitly given and explain under which conditions we can expect a positive numerical approximation that meets the algebraic constraints.

We then extend these results to higher index problems, i.e., problems in which some of the algebraic equations are hidden in the system, using derivative arrays and the index reduction developed by Kunkel and Mehrmann [2].

References

[1] Numerical Integration of Positive Linear Differential-Algebraic Systems. A.K. Baum and V. Mehrmann, Preprint TU Berlin, 2012. `http://www3.math.tu-berlin.de/multiphysics/Publications/Articles/BauM12_ppt.pdf`

[2] Differential-Algebraic Equations. Analysis and Numerical Solution, P. Kunkel and V. Mehrmann, EMS Publishing House, Zürich, CH, 2006.

Implicit Peer-methods using AMF and Krylov-techniques for large stiff ODE systems
Steffen Beck, Rüdiger Weiner, *Tue 17:30 R 1.23*

We discuss the application of implicit two-step Peer methods [1] of the form

$$Y_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{i} g_{ij} F_{m,j}, \quad i = 1, 2, \ldots, s$$

for 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 linear systems in the Newton iteration are solved with the Krylov method FOM or by using approximate matrix factorization (AMF).

We developed a Matlab-code of two-step Peer methods of order three with Krylov method and AMF for the solution of the linear systems. The performance of our code is compared with other solvers in the current literature, such as the AMF-version of the two-stage Radau IIA method [3], ROWMAP [4] and EXP4 [2], on three problems of parabolic type.

References

[1] S. Beck, R. Weiner, H. Podhaisky and B.A. Schmitt *Implicit peer methods for large stiff ODE systems*, J. Appl. Math. Comput. 38 (2012), 389-406.

[2] M. Hochbruck, Ch. Lubich, and H. Selhofer, *Exponential integrators for large systems of differential equations*, SIAM J. Sci. Comput. 19 (1998), 1552–1574.

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On Rosenbrock methods for singular singularly perturbed problems and their application to nearly incompressible materials
Urs Becker, Bernd Simeon, *Mon 14:25 R 3.28*

In structural mechanics, the modeling of nearly incompressible materials makes use of a constraint that measures the change of volume and that becomes part of a mixed problem formulation as transient saddle point problem. Studying the mathematical structure of the finite element discretization, the system turns out to be a differential-algebraic equation (DAE) that can be interpreted as singular singularly perturbed problem (SSP) with respect to the bulk modulus as perturbation parameter. Though this problem is for physically meaningful parameter values of index 1, it is close to an index 3 limiting system and may become hard to solve numerically. A simple example of the problem class can be stated as follows: For some given function $\phi(t)$ we want to solve

$$\ddot{q} = \ddot{\phi} - \lambda$$
$$\epsilon^2 \lambda = q - \phi.$$

This model equation in the fashion of the classical Prothero Robinson equation captures already some of the relevant phenomena and is of index 1 for $\epsilon > 0$ and of index 3 for $\epsilon = 0$.

In the nonlinear case, the numerical integration of SSPs using implicit Runge-Kutta methods suffers from step size restrictions and bad convergence of Newtons-method, in combination with order reduction phenomena [1, 2]. Rosenbrock type methods avoid the use of a Newton iteration by linearization of the nonlinear equations and thus may avoid some of the mentioned convergence problems. In the talk, we are giving an overview on different Rosenbrock methods and analyze their performance and order behavior when applied to SSPs and the special class of nearly incompressible structural dynamic systems.

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Data and Range-Bounded Polynomials and their Derivatives in ENO Methods
Martin Berzins, *Thu 14:00 R 3.28*

Essentially Non-Oscillatory (ENO) methods and Weighted Essentially Non-Oscillatory (WENO) methods are of fundamental importance in the numerical solution of hyperbolic equations. A key property of such equations is that the solution must remain positive or lie between bounds. A modification of the polynomials used in ENO methods to ensure that the modified polynomials are either bounded by adjacent values (data-bounded) or lie within a specified range (range-bounded) is considered. It is shown that this approach helps both in the range boundedness in the preservation of extrema in the ENO polynomial solution. An additional consideration with ENO methods is that to ensure boundedness of the pde solution it is important to bound the derivative of the reconstruction function. We derive a new limiter for the reconstruction function that bounds its derivative between values at mesh points and compare this approach with the new limiter of Zhang and Shu.

Structure-preserving numerical integrators for flexible multibody dynamics
Peter Betsch, *Mon 10:40 R 3.28*

Starting with the nineties, structure-preserving schemes have been developed in the context of nonlinear elastodynamics and structural dynamics. In this field of application a lot of effort has been put into the design of energy-momentum schemes. Energy-momentum consistent integrators satisfy discrete versions of important balance laws for mechanical systems, namely balance of energy and angular momentum. Energy-momentum integrators are known to possess enhanced numerical stability and robustness properties. These advantageous features are of special importance when large deformation analysis are pursued that require time integrations over relatively long time intervals.

Originally the development of energy-momentum schemes has been confined to mechanical systems that belong to the class of Hamiltonian systems with symmetry. Recent developments aim at the extension of their range of applicability to more elaborate problems including large deformation contact, thermo-mechanically coupled systems and flexible multibody dynamics. These developments will be addressed in the talk.

Symplectic methods for the time integration of the Schrödinger equation
Sergio Blanes, Fernando Casas, Joseba Makazaga and Ander Murua, *Mon 11:30 R 3.28*

When investigating the dynamical behavior of quantum systems of low to moderate dimension, very often it is necessary to solve numerically the time dependent Schrödinger equation. After a spatial discretisation, one has to solve a linear differential equation

$$i\frac{d}{dt}u(t) = Hu(t), \qquad u(0) = u_0 \in \mathbb{C}^N, \tag{1}$$

where $u(t)$ represents a discretized version of the wave function at the space grid points. H is an Hermitian matrix associated to the Hamiltonian, and then the problem can be seen as a system of N coupled harmonic oscillators with "unknown" frequencies, $\lambda_1, \ldots, \lambda_N$. However, in general, one can know upper and lower bounds to the extreme eigenvalues of H, say E_{min} and E_{max}, such that $E_{min} \leq \lambda_i \leq E_{max}, \quad \forall i$.

We look for approximate solutions, $\tilde{u}$, to $u(t_f) = e^{-it_f H} u_0$ which only uses products of vectors with the matrix H, i.e. polynomial approximations. Given a tolerance, *tol*, the goal is to look for an efficient scheme which provides $\tilde{u}$ such that $\|\tilde{u} - u(t_f)\| < tol$ with the smaller amount of vector-matrix multiplications and storage requirements.

Among the most employed numerical schemes in the literature within this class are the Chebyshev methods, being in general about twice faster than Taylor methods. However, the analysis of the simple scalar harmonic oscillator (from the perspective of the analysis, optimization, algebra and geometric structure) allows us to build new symplectic methods with better geometric properties which at the same time provide the desired solution between 50% faster and twice faster.

The algorithm contains a subroutine with a set of symplectic methods, each one optimized for different problems which can be used as a black box for the user.

Construction of general linear methods of order p and stage order $q = p - 1$ or $q = p$ for ordinary differential equations
Michał Braś, *Tue 11:05 R 3.28*

This is a sequel to the talk by Z. Jackiewicz: "Efficient general linear methods for ordinary differential equations". In this talk we present examples of highly stable general linear methods with s internal stages and $r = s + 1$ internal stages of order $p = s + 1$ and stage order $q = s$ or $q = s + 1$ for $p = 2, 3$, and 4. We will also discuss local error estimation for these methods.

Heterogeneous Multiscale Methods for Highly-Oscillatory Mechanical Systems with Solution-Dependent Frequencies
Bernd Brumm, Daniel Weiss, *Thu 14:00 R 1.23*

The framework of Heterogeneous Multiscale Methods (HMM) was originally proposed for the efficient computation of multiple time-scale problems. Briefly, HMM deals with systems of differential equations whose exact dynamics can be viewed as a superposition of an underlying averaged macroscale dynamics, which it approximates, and a fast microscale dynamics driving the actual motion. HMM does so without full explicit knowledge of the macroscale forces and provides the missing data via a micro-simulation in each step.

The talk examines an application of HMM to mechanical systems with solution-dependent high frequencies. It is shown that a correct initialization of the micro-simulation depends crucially on the adiabatic invariance of the actions. This almost-invariance property also guarantees the existence of an underlying effective system, which is derived. Using the example of a stiff spring double pendulum, an HMM including RATTLE as a macro-integrator is formulated. The analysis is done using canonical transformations proposed by K. Lorenz and Ch. Lubich.

Optimal Control of Delay-Differential Algebraic Equations
Michael Burger, *Mon 16:10 R 1.27*

Optimal control problems arise in many application fields, especially in the area of mechanical engineering, e.g., for the derivation of test-rig loads, in trajectory planning for robots or in flight path optimization. The dynamical systems considered in these areas are often rigid or flexible multibody systems, possibly extended by models of other mechatronical devices. The mathematical description of these models is typically in terms of differential-algebraic equations (DAEs), whence, one is faced with optimal control problems involving DAEs.
In addition, due to modelling effects, *delay terms* may appear in the DAE description. That is, the state and control variables have to be evaluated not only at the current time, but also at delayed (also retarded) instances of time. Accordingly, optimal control problems for delay-DAEs have to be considered. In this talk, we present a corresponding optimal control formulation. We derive necessary optimality conditions for optimal control problems with index-2 delay-DAEs. To this end, a solution-operator is introduced that maps control functions to the corresponding delay-DAE solution. Continuity and Fréchet-differentiability of the solution operator are proved.
We illustrate our results with an academic example from vehicle engineering.

From cells to tissue: coping with heterogeneity when modelling the electrophysiology of the human heart
Kevin Burrage, *Tue 8:30 R 3.28*

In biology, as in many sciences, stochasticity manifests itself at many temporal and spatial scales. How do modellers capture this inherent variability? How does a biological system use it productively? When is it filtered? How do modellers validate models in the presence of this variability? This talk makes some attempts to address these deep issues in the context of modelling and simulating the electrophysiology of the heart. The main focus will be on the study of ion channel dynamics in a cardiac cell through the stochastic Langevin equation and the modelling of the propagation of an electrical wave in cardiac tissue through the use of

non-local space-fractional reaction-diffusion equations.

This is joint work with Blanca Rodriguez, Annamaria Carusi, David Kay, Alfonso Bueno-Orovio, Ciara Dangerfield, John Walmsley (all Oxford) and Esther Pueyo (Zaragoza).

Runge-Kutta methods for stochastic Hamiltonian problems with additive noise
Pamela Burrage, Kevin Burrage, *Mon 14:00 R 1.23*

In this talk, we extend the ideas of Brugnano, Iavernaro and Trigiante in their development of HBVM(s,r) methods for deterministic Hamiltonian problems to the case of nonlinear, additive noise, stochastic Hamiltonian problems. In particular, by simulating independent Wiener process at each stage of a Runge-Kutta method (rather than just simulating a single Weiner process per step) we can better match the moments of the underlying stochastic problem. We present numerical results demonstrating this improvement, using the modified midpoint rule with two Wiener processes per step.

Symmetry of general linear methods and the underlying one-step method
John Butcher, Adrian Hill, *Wed 9:20 R 3.28*

Let $\mathcal{M}_h : \mathbb{R}^r \to \mathbb{R}^r$ denote the map defined by

$$
\begin{aligned}
Y &= hAF + Uy, \\
F_i &= f(Y_i), \qquad i = 1, 2, \ldots, s, \\
\mathcal{M}_h y &= hBF + Vy.
\end{aligned}
$$

A method is "symmetric" if there exists an involution $L : \mathbb{R}^r \to \mathbb{R}^r$, $L^2 = I$, such that $\mathcal{M}_{-h} = L\mathcal{M}_h L$. Let Φ_h denote the underlying one-step method and $\mathcal{S}_h$ the corresponding starting method, so that $\mathcal{M}_h \mathcal{S}_h = \mathcal{S}_h \Phi_h$. This talk will include an analysis of the order of the method and related properties of $\mathcal{S}_h$ and Φ_h.

Application of the DAE theory in investigation of quasi-stationary hydraulic circuits
Elena Chistyakova, *Tue 11:30 R 1.26*

We consider a quasi-stationary model of a hydraulic circuit written in the form of the differential algebraic equation

$$
\begin{pmatrix} R & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{D}(t) \\ \dot{P}(t) \end{pmatrix} + \begin{pmatrix} S_0 & A^\top \\ A & 0 \end{pmatrix} \begin{pmatrix} D(t) \\ P(t) \end{pmatrix} + \begin{pmatrix} S|D(t)|D(t) \\ 0 \end{pmatrix} =
$$

$$
= \begin{pmatrix} H(t) + A_1^\top P_*(t) \\ Q(t) \end{pmatrix}^\top, \quad t \in [0, \infty) \tag{1}
$$

where $\begin{pmatrix} A^\top & A_1^\top \end{pmatrix} = \overline{A}$ is the incidence matrix of the graph of the hydraulic circuit under consideration;
$D(t) = (d_1(t) \quad d_2(t) \quad \ldots \quad d_r(t))^\top$ is the vector-function of flow rates;
$P(t) = (p_1(t) \quad p_2(t) \quad \ldots \quad p_\mu(t))^\top$ is the vector-function of the pressure at the nodes;

$P_*(t) = (p_{1,*}(t) \quad p_{2,*}(t) \quad \ldots \quad p_{\mu(t),*})^\top$ is the vector-function of the known pressure;

$R = \mathrm{diag}\{\rho_1, \rho_2, \ldots, \rho_r\}$ represents the momentum parameters;

$S = \mathrm{diag}\{s_1, s_2, \ldots, s_r\}$ and $S_0 = \mathrm{diag}\{s_{1,0}, s_{2,0}, \ldots, s_{r,0}\}$ are the resistance parameters of the branches of the hydraulic circuit;

$|D(t)|D(t) = \Big((|d_1(t)|d_1(t) \quad |d_2(t)|d_2(t) \quad \ldots \quad |d_r(t)|d_r(t))\Big)^\top$;

$H(t) = \Big((h_1(t) \quad h_2(t) \quad \ldots \quad h_r(t))\Big)^\top$ and $Q(t) = (q_1(t) \quad q_2(t) \quad \ldots \quad q_r(t))^\top$ represent inflows and outflows correspondingly. The system is index two.

In the talk we discuss local and global existence conditions for system (1) and propose a numerical algorithm based on the reduction of the system to the index one system.

A Bayesian Approach to Shape Registration
Simon Cotter, Colin Cotter and François-Xavier Vialard, *Tue 14:00 R 3.28*

With the advent of more advanced prenatal scanning technologies, there is a need for diagnostic tools for certain congenital conditions. This problem amounts to finding the distance in shape space between a noisily observed scan of a particular organ, be it brain or heart etc., and a library of shapes of organs from babies that had particular conditions.

We frame the problem as a Bayesian inverse problem on function space, where the functions of interest relate to the geodesic flow fields that deform one shape into the other. This is analogous to finding the velocity field in a Lagrangian data assimilation problem. Using regularity results regarding the forward problem, we identify minimal-regularity priors in order to make the inverse problem well-posed. We then present some numerics for simple 2D examples on closed curves, which show how the posterior distributions on function space can be sampled using MCMC methods.

Efficient integrators for shallow water equations
Petra Csomós, Alexander Ostermann, *Mon 14:00 R 1.27*

In this talk we present our preliminary results obtained when applying efficient time integrators for the shallow water equations considered on a rotating plane. The talk is based on a joint work with A. Ostermann (Innsbruck).

Highly stable General Linear Methods for second order Ordinary Differential Equations
Raffaele D'Ambrosio, Beatrice Paternoster, *Tue 11:55 R 3.28*

In this talk we consider the family of General Linear Methods (GLMs) for second order ordinary differential equations (ODEs). Such methods have been introduced in [2] with the aim to provide an unifying approach for the analysis of the properties of convergence, consistency and zero-stability, by extending the results obtained in the literature for GLMs solving first order ODEs [1, 3]. Our investigation is addressed to providing the building blocks useful to analyze the linear stability properties of GLMs for second order ODEs: thus, we present the extension of the classical notions of stability matrix, stability polynomial, stability and periodicity interval, A-stability and P-stability to the family of GLMs. Special attention will be focused on the practical derivation of highly stable methods, by investigating GLMs inheriting the same stability properties of highly stable numerical methods existing in literature, e.g.

Runge-Kutta-Nyström methods based on indirect collocation on Gauss-Legendre points, which are known to be P-stable: this property, in analogy to a similar feature introduced for GLMs solving first order ODEs (compare [1, 3]), is called *Runge-Kutta-Nyström stability.* The stability properties of GLMs with Runge-Kutta-Nyström stability depend on a quadratic polynomial, which results to be the same stability polynomial of the best Runge-Kutta-Nyström assumed as reference. We finally provide and discuss examples of P-stable irreducible GLMs with Runge-Kutta-Nyström stability.

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Semi-Lagrangian schemes for Hamilton-Jacobi-Bellman equations
Kristian Debrabant, Espen R. Jakobsen, *Tue 15:00 R 1.23*

In this talk we consider the numerical solution of diffusion equations of Hamilton-Jacobi-Bellman type

$$u_t - \inf_{\alpha \in \mathcal{A}} \left\{ L^\alpha[u](t,x) + c^\alpha(t,x)u + f^\alpha(t,x) \right\} = 0 \qquad \text{in} \quad (0,T] \times \mathbb{R}^N,$$

$$u(0,x) = g(x) \qquad \text{in} \quad \mathbb{R}^N,$$

where

$$L^\alpha[u](t,x) = \text{tr}[a^\alpha(t,x)D^2 u(t,x)] + b^\alpha(t,x)Du(t,x).$$

The solution of such problems can be interpreted as value function of a stochastic control problem. We introduce a class of monotone approximation schemes relying on monotone interpolation. Besides providing a unifying framework for several known first order accurate schemes, the presented class of schemes includes new methods that are second order accurate in space and converge for essentially monotone solutions. Some stability and convergence results are given and the method is applied to a super-replication problem from finance.

Filippov sliding motion on a co-dimension 2 discontinuity surface
Luca Dieci, *Fri 9:20 R 3.28*

In this talk we consider sliding motion, in the sense of Filippov, on a discontinuity surface Σ of co-dimension 2. In particular, we consider a certain Filippov sliding vector field f_F recently adopted by Dieci and Lopez and show that it enjoys several important properties.
First, restricting to the case of *nodally attractive* Σ, we show that this Filippov vector field is the limiting vector field for a natural regularization of the original problem.
Then, we characterize, and restrict to, the general case of Σ being *attractive through sliding*, and show that f_F exists and is unique. We also propose a characterization of *first order exit conditions*, clarify its relation to generic co-dimension 1 bifurcations phenomena (losses of attractivity) for Σ, and examine what happens to the dynamics on Σ for the vector field f_F.

The talk is based on the works:

(1) "A Filippov sliding vector field on an attracting co-dimension 2 discontinuity surface, and a limited bifurcation analysis", by L. Dieci, C. Elia, L. Lopez.

(2) "Regularizing piecewise smooth differential systems: co-dimension 2 discontinuity surface", by L. Dieci, N. Guglielmi.

High order splitting schemes with complex timesteps and their application in mathematical finance
Philipp Dörsek, Eskil Hansen, *Mon 17:25 R 1.26*

We consider the approximation of the solution of linear evolution equations by high order splitting methods. It turns out that if the generator of the problem is of the sum-of-squares type, which is typical for problems from mathematical finance, the functional analytic setting developed by Dörsek and Teichmann [1] allows us to prove the necessary analyticity of the generated semigroups easily. Full discretisations are obtained using Krylov methods for the approximation of the matrix exponential of the second order part and streamline diffusion finite elements for the first order part, whence robust error estimates for drift-dominated problems are possible. Numerical experiments illustrating the theoretical results are provided.

References
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Convergence analysis of Strang splitting for Vlasov–type equations
Lukas Einkemmer, Alexander Ostermann, *Mon 17:00 R 1.26*

A rigorous convergence analysis of the Strang splitting algorithm for Vlasov–type equations in the setting of abstract evolution equations is provided. It is shown that under suitable assumptions the convergence is of second order in the time step h. As an example, it is shown that the Vlasov–Poisson equation in 1+1 dimensions fits into the framework of this analysis. Also, a number of numerical experiments for the latter case are presented.

Generalized Picard Iterations with Improved Linear Convergence Properties
Boris Faleichik, Ivan V. Bondar, *Tue 11:05 R 1.27*

This talk is about recent advances in development of generalized Picard iterations [1] which are aimed at cheap solution of nonlinear equations systems arising during implementation of implicit Runge–Kutta (IRK) methods. Our main result is the following: the proposed iterative processes converge for all IRK methods with arbitrary stepsize $h > 0$ and all linear ODE systems $y' = Jy$ which satisfy the existence and uniqueness conditions as stated in Lemma 5.2.5 from [2]. Therewith these iterations are applicable in general nonlinear case, they are "matrix-free" (but require the estimate of Jacobi matrix spectral radius), and need $O(ns)$ memory storage for implementation, where n is ODE dimension and s is the number of IRK stages. So the natural purpose of generalized Picard iterations is the solution of big stiff systems with complex spectrum, where explicit Chebyshev-like methods are inapplicable and classical Newton-like iterations are too expensive.
Further properties, such as the interesting relationship between convergence rate and ODE stiffness, and numerical results will be discussed during the talk.

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Fast weak-KAM integrators for solving Hamilton-Jacobi equations
Erwan Faou, Anne Bouillard, Vincent Calvez and Maxime Zavidovique, *Fri 8:30 R 3.28*

We consider numerical schemes for Hamilton-Jacobi equations based on a direct discretization of the Lax-Oleinik semi-group which represents the solution as a minimizer of the action over continuous curves. We prove that this method is convergent with respect to the time and space stepsizes provided the solution is Lipschitz. Moreover, we prove that the numerical scheme is a *geometric integrator* satisfying a discrete weak-KAM theorem which allows to control its long time behavior. Taking advantage of a fast algorithm for computing min-plus convolutions based on the decomposition of the function into concave and convex parts, we show that the numerical scheme can be implemented in a very efficient way.

Coupled differential algebraic equations in the simulation of flexible multibody systems with hydrodynamic force elements
Robert Fiedler, Martin Arnold, *Wed 10:45 R 1.26*

The mathematical modelling of elastohydrodynamic fluid film bearings in combustion engines results in a coupled system of DAEs representing a flexible multibody system model of engine and bearing and the Reynolds equation that describes the nonlinear hydrodynamic effects in the fluid film. The hydrodynamic forces depend strongly on the position and elastic displacement of crankshaft and bearing shell.
In the present paper, we discuss the influence of space discretization on result accuracy and numerical effort. Since fine space discretization would slow down the numerical solution substantially, we propose an asymptotic analysis using methods from singular perturbation theory to speed-up time integration.
Numerical tests for a simplified benchmark problem will illustrate the benefits of this approach.

Numerical approximation of the Mittag–Leffler function and applications in fractional calculus
Roberto Garrappa, *Wed 10:20 R 1.27*

The Mittag–Leffler (ML) function, introduced at the beginning of the last century by the Swedish mathematician Magnus Gösta Mittag–Leffler, is nowadays receiving renewed interest because of its applications in fractional calculus; indeed, the ML function plays for fractional differential equations (FDEs) the same key role as the exponential function does for ordinary differential equations (ODEs) of integer order.
In the last years some efforts have been dedicated in extending exponential integrators to the numerical treatment of linear and semi–linear FDEs. This approach, successfully applied to ODEs, essentially consists in solving exactly the linear (and usually stiff) term by evaluating some exponential–type function and hence applying an explicit scheme to the nonlinear (and usually non–stiff) term.

The generalization of exponential integrators to FDEs involves the evaluation of some generalized ML functions in the form

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(-t^\alpha\lambda), \quad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)},$$

where t is an independent variable, λ is a scalar or a matrix and α and β are fixed parameters. The numerical computation of ML functions, possibly with matrix arguments, is a challenging task. The classical definition in terms of the series is not useful for practical computation because of its slow convergence. Thus, efficient and reliable methods need to be devised.

In this talk we present and discuss some methods based on the integral representation of $e_{\alpha,\beta}(t;\lambda)$ and different approaches are compared. For some methods we present a robust error analysis allowing to select the main parameters of the method with the aim of achieving any prescribed accuracy. Some applications in the solution of FDEs are also shown.

Stability of plane waves in nonlinear Schrödinger equations: mathematical and numerical analysis
Ludwig Gauckler, Erwan Faou, Christian Lubich, *Thu 11:30 R 3.28*

The cubic nonlinear Schrödinger equation

$$i\partial_t u = -\Delta u + \lambda|u|^2 u, \qquad u = u(x,t), \tag{1}$$

with periodic boundary conditions in space $(x \in \mathbb{R}^d/(2\pi\mathbb{Z})^d)$ has solutions that are plane waves:

$$u(x,t) = \rho e^{i(m\cdot x - \omega t)}$$

solves (1) for arbitrary $m \in \mathbb{Z}^d$ and $\omega = |m|^2 + \lambda\rho^2$.

In the first part of the talk the stability of these plane wave solutions under perturbations of the initial data is discussed. We show their (orbital) stability under generic perturbations that are small in a high Sobolev norm. This stability result holds over long times that extend to arbitrary negative powers of the smallness parameter. The perturbation stays small in the same Sobolev norm over such long times.

In the second part of the talk we turn to a standard numerical discretization of the cubic nonlinear Schrödinger equation, the split-step Fourier method, where a spectral collocation method in space is combined with a splitting integrator in time. Does the stability result for the exact solution extend to the fully discrete solution?

Multi-product expansion of solving Hamiltonian equations: Theory and Application in Levitron Problems
Jürgen Geiser, *Thu 11:55 R 3.28*

This talk is about our recent research to develop time-integrators for symmetric rigid bodies. The ideas are to apply second order Poisson integrators and generalize to higher order schemes via multi-product expansion. First we present the underlying model-problems based on a magnetic top in an axisymmetric magnetic fields (Levitron problem). Next we discuss the time-integrator based on the Poisson integrators with the time-stepping operator $\exp h(A + B)$ and its products of $\exp hA$ and $\exp hB$. In the context of solving Hamiltonian dynamics, see [1], we discuss an alternative approach to higher order schemes based on Suzuki's forward-time derivative. Structure preserving ideas are given with respect to momentum preserving of the underlying Poisson integrator and its extensions. We discuss the convergence analysis and a generalization of the extrapolation method, see [2]. Numerical experiments are given with test and benchmark algorithms and real-life stability discussions for a Levitron problem, see [3].

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On the positivity in nonlocal PDE models of cell adhesion
Alf Gerisch, *Tue 10:40 R 1.23*

This talk is about a nonlocal PDE model of cell adhesion. Cell adhesion is a fundamental process in many developmental processes and has also been implicated in tumour progression and metastasis. It can be shown that solutions of this model, representing cell density, are nonnegative for nonnegative initial data and suitable boundary conditions. This qualitative property, termed positivity, of the solution should be preserved by the numerical scheme employed for the model simulation.

We consider a method of lines approach with a finite volumes spatial discretisation for the numerical solution of the model equations. Positivity is essential in the following aspects of the overall scheme

- nonnegative reconstruction of the solution from nonnegative finite volume cell averages;
- sign-preserving quadrature formulas;
- positivity preserving spatial discretisation;
- positivity preserving temporal discretisation.

We will describe options in each of these areas, discuss their relations and also the impact on an efficient numerical solution.

Related to positivity is the issue of boundedness of the solution, which we will touch upon briefly.

Solving of Fuzzy Differential-Algebraic Equations
Mehdi Ghovatmand Jazei, S. Aliabadian, *Tue 11:05 R 1.26*

In this work, we try to solve system of fuzzy differential-algebraic equations. Solving of this system is done in two parts. The first part, index reduction technique is implemented for fuzzy differential-algebraic equations. Then, He's variational iteration method is used to solve the reduced fuzzy differential-algebraic equations. It is well known fuzzy differential-algebraic equations can be difficult to solve when they have an index greater than 1. So the proposed index reduction technique for differential-algebraic equations is generalized for fuzzy differential-algebraic equations, then one try to solve the system. Hence, He's variational iteration method is generalized for solving fuzzy differential-algebraic equations. The proposed method by He is effectively and easily used to solve other such as delay differential-equations, Laplace equations and ordinary differential system.

Simplifying AMF-schemes for Inexact Jacobians in large Stiff ODEs

Severiano González Pinto, Domingo Hernández Abreu, Soledad Pérez Rodríguez,
Tue 17:00 R 1.23

Splitting schemes of AMF (Approximate Matrix Factorization)-type for the implementation of Rosenbrock methods in the time integration of Advection Diffusion Reaction PDE systems semi-discretized in space by means of Finite Differences or Finite Volume, are considered.

The main point in the proposed Modified AMF schemes is that allows the use of inexact Jacobian matrices in the splitting without losing in the convergence order of the underlying Rosenbrock method, which is of great interest for non-linear problems. Besides the new Modified AMF schemes allow to deal in a explicit way with some part of the derivative function, such as the advection terms, without restricting the CFL number for pure advection problems, in a significant way.

Particular attention will be paid to the one stage Rosenbrock method (ROS1) of order two, which for autonomous ODEs is given by

$$(I - \frac{\Delta t}{2} J_n)(y_{n+1} - y_n) = \Delta t F(y_n), \quad J_n := \frac{\partial F}{\partial y}(y_n).$$

A stability analysis for different splitting of the Jacobian and several Modified AMF approaches will be presented and some connections with existing schemes will be shown.

A 2D-Radiation-Diffusion model of very practical interest in Physics [3, 1, 2] (of parabolic type) consisting of two strongly coupled non-linear PDEs having a stiff reaction part, will be integrated with ROS1 in the different versions of the proposed AMF-schemes and with other classical methods currently used in the literature. It will be shown that the Modified AMF-iteration implemented in ROS1 supposes a noticeable improvement regarding the standard AMF implementation and also is an attractive alternative to existing integrators.

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Applications of the stochastic direct simulation method at systems of evolution partial differential equations with strongly nonlinear diffusion part

Flavius Guias, *Mon 14:50 R 1.23*

We illustrate the applicability of a stochastic scheme based on path simulations of Markov jump processes at systems of nonlinear partial differential equations in two space dimensions, which usually require computationally demanding, specifically adapted, deterministic algorithms. The general principle of the method of lines reduces evolution partial differential equations to semi-discrete approximations consisting of systems of ordinary differential equations. Our approach is to use for this resulting system a stochastic scheme which is essentially a direct simulation of the corresponding infinitesimal dynamics. We consider as test problem the time-dependent

radiation-diffusion equation and show that, in the framework of an appropriate implementation, the stochastic scheme can be a real alternative to deterministic solvers, having the advantage of a simple mathematical core. We discuss also the improvement of the convergence order by exploiting further the full path simulation and performing periodically Picard iterations and/or Runge-Kutta steps based on the computed trajectories. This very general basic scheme can be applied at various problems, while the efficiency of the method depends mainly on the implementation part: data structures and sampling algorithms.

Solvability analysis of delay differential-algebraic equations
Phi Ha, Volker Mehrmann and Andreas Steinbrecher, *Mon 16:35 R 1.27*

Delay differential equations (DDEs) arise in a variety of applications, including biological systems and electronic networks. If the states of the physical system are constrained, e.g., by conservation laws or interface conditions, then algebraic equations have to be included and one has to analyze delay differential-algebraic equations (DDAEs).
In this talk, we study the solvability analysis of linear time invariant delay differential-algebraic equations. We propose algorithms that explicitly read off underlying delay differential equations, and also all hidden constraints. The constructed condensed forms are used to address structural properties of the system like solvability, regularity, consistency and smoothness requirements.

Symmetric multistep methods for constrained Hamiltonian systems
Ernst Hairer, Christian Lubich, Paola Console, *Mon 9:20 R 3.28*

This talk considers the numerical solution of constrained Hamiltonian systems. These are differential-algebraic equations of index 3, for which the flow on the constrained manifold is a symplectic transformation. A method of choice for the long-time integration of such problems is the Rattle algorithm. It is symmetric, symplectic, and nearly preserves the Hamiltonian (justified by a backward error analysis), but it is only of order two and thus not efficient for high accuracy requirements.
We present symmetric linear multistep methods of arbitrarily high order, and show how they can be applied to constrained Hamiltonian systems. Their implementation and computational cost is comparable to that of the Rattle algorithm. Although the method is not symplectic, we prove that it nearly conserves over long times the Hamiltonian and quadratic first integrals such as the angular momentum in N-body problems. The proof is based on techniques related to backward error analysis. The essential ingredient is the construction of adiabatic invariants, which permits to prove that the parasitic solution components remain bounded and small over long times.

Numerical Modelling of Reaction and Diffusion Systems in a Biological Cell Including Surface Reactions by Homogenization
Michael Hanke, Qasim Ali Chaudhry, Kristian Dreij, Ralf Morgenstern, *Tue 11:05 R 1.23*

A human cell consists schematically of an outer cellular membrane, a cytoplasm containing a large number of organelles (mitochondria, endoplasmatic reticulum etc.), a nuclear membrane and finally the cellular nucleus containing DNA. The organelle membranes create a complex and dense system of membranes or subdomains throughout the cytoplasm. The mathematical description leads to a system of reaction-diffusion equations in a complex geometrical domain, dominated by thin membraneous structures with similar physical and chemical properties. In

a previous model, we considered only spatially distributed reaction and diffusion processes. However, from experiments it is known that membrane bound proteins play an important role in the metabolism of certain substances. In the talk we will present a new homogenization approach including homogenization of surface reactions and diffusion.

Convergence of the implicit-explicit Euler scheme applied to perturbed dissipative evolution equations
Eskil Hansen, Tony Stillfjord, *Tue 14:30 R 1.23*

We present a convergence analysis for the implicit-explicit (IMEX) Euler discretization of non-linear evolution equations. The governing vector field of such an equation is assumed to be the sum of an unbounded dissipative operator and a Lipschitz continuous perturbation. By employing the theory of dissipative operators on Banach spaces, we prove that the IMEX Euler and the implicit Euler schemes have the same convergence order, i.e., between one half and one depending on the initial values and the vector fields. Concrete applications include the discretization of diffusion-reaction systems, with fully nonlinear and degenerate diffusion terms. The convergence and efficiency of the IMEX Euler scheme are also illustrated by a set of numerical experiments.

Convergence of AMF-Radau-type methods for the time integration of advection diffusion reaction PDEs
Domingo Hernández-Abreu, Severiano González Pinto, *Tue 16:30 R 1.23*

A family of methods for the time integration of evolutionary Partial Differential Equations (PDEs) of Advection Diffusion Reaction type semi-discretized in space by Finite Differences is presented. These methods consider up to three inexact Newton Iterations of Approximate Matrix Factorization type (AMF) applied to the two-stage Radau IIA method along with a very simple predictor. The overall process reduces the algebraic costs involved in the numerical solution of the multidimensional linear systems to the $1D-$level.

Some specific AMF-Radau methods are selected after studying the expression for the local error in semi-linear equations, and their linear stability properties are described. The wedge of stability of the methods depends on the number of splittings used for the Jacobian matrix of the spatial semidiscretized ODEs, $J_h = \sum_{j=1}^{d} J_{h,d}$, where h stands for the spatial grid resolution. A-stability is obtained for the cases $d = 1, 2$, and $A(0)$-stability for any $d \geq 1$.

Numerical experiments on a semi-linear test problem with Dirichlet boundary conditions reveal that the AMF-Radau methods can attain order two (resp. three) in time just by giving one iteration (resp. two iterations) per integration step. A theory supporting the uniform convergence of order two and three on time, independently of the spatial resolution h, is presented. Uniform bounds for the global time-space errors when simultaneously the time step-size $\tau \to 0^+$ and the spatial grid resolution $h \to 0^+$ are obtained when the multidimensional PDEs are semi-linear with time-independent Dirichlet Boundary Conditions. For the case of time-dependent Boundary Conditions, a Boundary Correction Technique is proposed in order to avoid the order reduction phenomenon.

Characteristic Boundary Conditions in LBM for Fluid and Gas Dynamics
Daniel Heubes, Matthias Ehrhardt, Andreas Bartel, *Mon 14:25 R 1.27*

In this work we focus on characteristic boundary conditions in a computational fluid dynamics (CFD) simulation and its application with the lattice Boltzmann method (LBM).
Frequently, the equations of interest in a CFD simulation are the Euler equations extended by a viscous term
$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\,\mathbf{v} + \frac{1}{\rho_0}\nabla p = \nu \Delta \mathbf{v}, \qquad \nabla \cdot \mathbf{v} = 0.$$
The lattice Boltzmann method is a relatively new approach in CFD which is based on a microscopical description of the fluid by the Boltzmann equation.
For a numerical simulation, independent of the method, it might happen that not all boundaries of the numerical domain coincide with physical ones.
Unlike physical boundaries where for instance an inlet or outlet condition holds, the task for these artificial boundaries is to find a procedure which does not induce unphysical effects to the fluid. This is achieved by transparent or characteristic boundary conditions.
Here, we present different approaches of characteristic boundary conditions and derive Dirichlet conditions at these artificial boundaries. These Dirichlet conditions from a PDE formulation are then transferred to the LBM framework. Among all these different approaches, we will propose new characteristic boundary conditions for LBM, which are stated in 2D. We compare the unphysical reflections of the different approaches in a numerical simulation for a simple benchmark problem.

Positivity preservation of time-stepping methods
Inmaculada Higueras, *Thu 16:30 R 3.28*

Spacial discretization of some partial differential problems (PDEs) give rise to ordinary differential equations (ODEs). Sometimes, the solutions to these PDEs have qualitative properties, e.g., positivity, which are relevant in the context of the problem. In these cases, it is convenient to preserve these properties both in the spatial discretization of the PDE and in the time stepping process of the resulting ODE.
A common class of methods widely used in the literature are Runge-Kutta methods. For these schemes, positivity can be ensured under certain stepsize restrictions given in terms of the radius of absolute monotonicity. However, for some problems, several schemes with trivial radius of absolute monotonicity also provide positive solutions.
In this talk we will explain how, under additional conditions on the problem, positivity can be obtained for some methods with trivial radius of absolute monotonicity.

Characterisations of symmetric general linear methods and G-symplecticity
Adrian Hill, John Butcher, *Wed 10:20 R 3.28*

This is the second of two talks on the design of general linear methods (A, U, B, V) suitable for the integration of Hamiltonian or time–reversible problems. The ultimate goal is to achieve the broad range of applicability of symplectic Runge–Kutta methods, but with less implicitness in the stage matrix A.
In this talk, we discuss how zero–stability, parasitism, time–reversal symmetry and G–symplecticity may all be analysed in terms of the linear stability function,
$$M(Z) := V + BZ(I - AZ)^{-1}U, \qquad Z = \mathrm{diag}(z_1, \ldots, z_s) \in C^{s \times s}.$$

We also characterise time–reversal symmetry and G–symplecticity in terms of the Nyquist or transfer function,

$$N(\zeta) := A + U(\zeta I - V)^{-1}U, \qquad \zeta \in C \setminus \sigma(V),$$

and show how this leads to identifying methods with both properties.

Discrete positive invariance of sets
Zoltán Horváth, *Thu 17:00 R 3.28*

As a generalization of positivity, we consider positive invariance of closed, convex sets for differential equations and their discretizations with Runge-Kutta methods. The aim is to find a step size for invariance, i.e. the time step size for the discretization method that guarantees preservation of the positive invariance of the set under consideration. In addition to the usual sufficient assumption with the Explicit Euler condition, we shall conclude step sizes for invariance from more relaxed conditions as well.

Moreover, we shall investigate the positive invariance of certain convex and some non-convex sets as well, with examples arising from dicretization of inertial manifolds. We shall see that in this case the step size for invariance is much larger than that resulting from the Explicit Euler condition (if the latter applies).

Finally, we demonstrate our findings with examples from different diffusion-reaction systems.

Order conditions for G-Symplectic methods
Gulshad Imran, John Butcher, *Wed 11:10 R 3.28*

General linear methods for the solution of ordinary differential equations are both multivalue and multistage. Although they cannot be symplectic, they can satisfy the related condition of being G-symplectic, and this makes them attractive options for many mechanical and other physical problems. A B-series approach will be used to find methods in this family of increasingly high orders.

Efficient general linear methods for ordinary differential equations
Zdzisław Jackiewicz, M. Braś, *Tue 10:40 R 3.28*

In this talk we discuss general linear methods characterized by abscissa vector c and coefficient matrices A, U, B, and V, with s internal stages and $r = s+1$ internal stages of order $p = s+1$ and stage order $q = s$ or $q = s + 1$. These methods are more efficient the class of DIMSIMs and the class of general linear methods with inherent Runge-Kutta stability. We review the derivation of order and stage order conditions and present representation formulas for the coefficient matrices U and V. We also derive a relationship between coefficient matrices B and V and abscissa vector c which facilitate the construction of efficient methods. Examples of such methods which are A-stable will be presented in a talk by M. Braś: "Construction of general linear methods of order p and stage order $q = p-1$ or $q = p$ for ordinary differential equations".

Constraint Solvers For Graphical User Interface Layout
Noreen Jamil, Christof Lutteroth, Gerald Weber, *Tue 11:30 R 1.23*

Many computer programs have graphical user interfaces (GUIs). To use the screen real estate efficiently, developers need to layout the widgets of the GUI. Constraints have been influential in the construction of GUIs for a long time. In GUIs the main usage of constraints is to define the layout of the widgets. Various algorithms are widely used for solving linear constraints problems in a number of different scientific areas. The most important class of algorithms for sparse problems, as they appear for GUI layout, is that of indirect methods. These algorithms have some limitations, for example they work only with square matrices. We extend iterative methods to solve also non-square matrices and handle soft constraints. Pivot selection is a major issue in this regard. We present two pivot selection strategies, one random and one deterministic strategy. Furthermore, we propose two strategies for handling soft constraints efficiently. These strategies are implemented differently but the solution for both strategies is the same. We also show that iterative techniques have a smaller memory footprint and are faster than a previous approach for solving GUI layout problems. Some computational results which demonstrate the effectiveness of the solvers are presented. It is demonstrated that iterative methods can be designed to converge even in the case of non-square problems.

An Explicit Sparse Formulation of the Maxwell Equations
Lennart Jansen, *Mon 16:10 R 3.28*

The need of combining circuit simulation directly with complex device models to refine critical circuit parts becomes more and more urgent, since the classical circuit simulation can no longer supply sufficiently accurate results. The simulation of such coupled problems leads to large systems and therefore to high computing times. We consider a set of differential-algebraic equations, which arise from an electric circuit modeled by the modified nodal analysis coupled with electromagnetic devices. While the normal circuit elements are 0d-elements, the electromagnetic devices are given by a three dimensional model. Therefore the number of variables can easily go beyond millions, if we refine the spatial discretization. Since we are confronted by a system of DAEs we cannot make use of explicit methods in general. So we are forced to solve very large implicit systems. We analyze the structure of the discretized coupled system and present a way to transform it into a semi-explicit system of differential-algebraic equations. In the process we make use of a new decoupling method for DAEs which results from a mix of the strangeness index and the tractability index. After this remodeling the electromagnetic part of the equation will be a system of ordinary differential equations with sparse matrices only.

A numerical method for the solutions of two dimensional quasilinear hyperbolic equations
Ram Jiwari, *Thu 10:40 R 1.27*

In this article, we have proposed a numerical technique based on polynomial differential quadrature method (PDQM) to find the numerical solutions of two-space-dimensional quasilinear hyperbolic partial differential equations subject to appropriate Dirichlet and Neumann boundary conditions. The second-order hyperbolic partial differential equations have great importance in fluid dynamics and aerodynamics, theory of elasticity, optics, electromagnetic etc. The PDQM reduced the equations into a system of second order linear differential equation. The obtained system is solved by RK4 method by converting into a system of first ordinary differential equations. The accuracy of the proposed method is demonstrated by several test examples. The numerical results are found to be in good agreement with the exact solutions. The proposed technique can be applied easily for multidimensional problems.

Outflow positivity limiting for hyperbolic systems
Evan Johnson, James A. Rossmanith, *Thu 14:30 R 3.28*

Physical solutions to hyperbolic systems of conservation laws typically stay in a region of states designated as positive. Examples include the shallow water equations, which maintain positivity of the depth, and the Euler gas dynamics equations, which maintain positivity of the density and pressure. Numerical solutions that wander outside the domain of positivity are likely to become unstable due to lack of hyperbolicity for non-positive data. Finite volume methods (such as WENO or DG) are designed to exactly satisfy a discrete conservation law, but it is challenging to maintain positivity of cell average quantities while retaining high-order accuracy in space. For given solution data and numerical fluxes, one can directly calculate the largest stable time step that maintains positivity of cell averages, but this time step can become arbitrarily small, halting the simulation. The challenge is therefore to design numerical fluxes that, while preserving high order accuracy, limit the potential rate of outflow from each cell relative to the cell average, thereby guaranteeing a minimum positivity-preserving time step.

Zhang and Shu have shown how to ensure a positivity-preserving time step by linearly damping the deviation from the cell average of the high-order representation of the solution just enough to enforce positivity at a set of positivity points. We reinterpret their framework in terms of limiting outflow from each cell and thereby show how to simplify and extend their framework to work for mesh cells of arbitrary geometry while guaranteeing the same positivity-preserving time step as if the linear damping were sufficient to enforce positivity at every point in the mesh cell. High-order finite volume methods can be outfitted with outflow positivity limiters without loss of order of accuracy and with marginal additional computational expense.

Non-normal drift structures and linear stability analysis of numerical methods for systems of stochastic differential equations
Conall Kelly, Evelyn Buckwar, *Mon 14:25 R 1.23*

We investigate mean-square asymptotic stability of equilibria of linear systems of stochastic differential equations with non-normal drift coeffcients, with particular emphasis on the role of interactions between the drift and diffusion structures that act along, orthogonally to, and laterally to the flow. Hence we construct test systems with non-normal drift coeffcients and characteristic diffusion structures for the purposes of a linear stability analysis of the θ-Maruyama method.

Once the test systems have been identified, we can discretise them and examine the mean-square asymptotic stability of equilibria of the resulting systems of stochastic difference equations. Finally we give an example that shows how this approach may help to shed light on certain numerical discretisations of stochastic partial differential equations with multiplicative space-time perturbations.

Positivity preserving schemes for hyperbolic conservation laws via downwind-biased discretizations
David Ketcheson, Sigal Gottlieb, *Thu 17:30 R 3.28*

Strong stability preserving (SSP) integrators for initial value ODEs preserve temporal monotonicity solution properties in arbitrary norms. All existing SSP methods, including implicit methods, either require small step sizes or achieve only first order accuracy. It is possible to achieve more relaxed step size restrictions in the discretization of hyperbolic PDEs through the use of both upwind- and downwind-biased semi-discretizations. I will review recent results on

the maximum achievable strongly stable step size for implicit Runge-Kutta methods combining upwind- and downwind-biased spatial discretizations, including second order methods with arbitrarily large step size restrictions and higher order methods that allow reasonably large step sizes.

Numerical solution of penalty formulations for constrained mechanical systems using the heterogeneous multiscale method
Markus Kettmann, Martin Arnold, *Thu 16:30 R 1.23*

The heterogeneous multiscale method (HMM) extends the rather analytical methods of averaging to a purely numerical approach for the solution of problems involving multiple scales. Especially for highly oscillatory ordinary differential equations HMM was recently seen to be competitive with usual time integration schemes. We study this hypothesis in the special case of penalty formulations for index-three differential-algebraic equations arising in multibody dynamics which have the particular property of solution-dependent oscillations with nonconstant frequencies.

In a first part of the talk we motivate some additional assumptions on the structure of the proposed problems and give error estimates extending the results of Engquist et al. Nevertheless numerical test problems of small and moderate size give rise to doubts on the applicability to realistic problems at least in the case of several or even multiple constraints.

To circumvent this lack in efficiency in the second part of the talk we propose a combination of HMM and co-simulation techniques and apply the resulting multiscale schemes to coupled PDE-DAE problems. Numerical tests including problems in nonlinear elasticity and fluid-structure interaction are presented and demonstrate the potential of this approach.

Butcher Algebras
Sergei Khashin, *Thu 11:55 R 1.27*

Runge-Kutta methods of orders up to 7 are well known. However, there are problems that require very high accuracy, and, therefore, they require Runge-Kutta methods of higher orders. We suggest an idea how we can structure Butcher equations from the point of view of Abstract Algebra. As the result the system can be significantly simplified, and some new Runge-Kutta methods of orders 9 have been obtained.

IMEX Rosenbrock methods for solving the compressible Euler equations
Oswald Knoth, Daniel Puschmann, *Thu 10:40 R 3.28*

Nowadays numerical weather prediction are performed by solving the compressible Euler equations. Due to the appearance of sound waves and isotropic grids the equations contain solution parts of different time scales. Implicit explicit (IMEX) time integration methods are a common choice to handle these different time scales in an efficient way. To avoid the solution of nonlinear systems the implicit integrator can be chosen as a linear implicit integration method. Different type of Rosenbrock IMEX methods are presented for this application. Order conditions up to order three are derived. The stability of the methods is tailored with respect to the linearized shallow water equation in the low Mach regime. To find optimal methods the stability restrictions and order conditions are recast into a sparse nonlinear optimization problem. The order of the methods is confirmed by numerical results. Comparison with fully implicit methods and split explicit methods are presented for a gravity wave generator and different type of warm and cold bubbles.

On the generalization of the Bolley-Crouzeix theorems
Tihamer Albert Kocsis, Zoltán Horváth, Adrián Németh, *Tue 11:55 R 1.23*

The classical result of Bolley and Crouzeix gives an order barrier on the unconditionally positivity preserving numerical methods for IVPs. In this talk we present a generalization of this theorem and show its application for a class of splitting methods. We also present examples for unconditionally positive methods that are beyond the scope of this theorem.

Numerical analysis of homogenized tunability of composite material
Aleksandr Kolpakov, A.A. Kolpakov, S.I. Rakin , *Thu 11:05 R 1.27*

If the permittivity $\epsilon(E)$ of ferroelectric depends on electric field E applied, the ratio $t(E) = (\epsilon(0) - \epsilon(E))/\epsilon(0)$ is called relatively tunability. For composite ferroelectric-dielectric material, one can introduce the homogenized permittivity $\hat{\epsilon}(E)$ [1] and the homogenized tunability $\hat{t}(E) = (\hat{\epsilon}(0) - \hat{\epsilon}(E))/\hat{\epsilon}(0)$ [2,3].

We present results of numerical analysis of the homogenized tunability in the case of strong electric field (for weak electric field the problem was analyzed in [2,3]). We consider 2-D model of nonlinear ferroelectric composite of periodic structure and assume that the periodicity cell $Y = [0,1]^2$ contains symmetric dielectric inclusion P. Because of the symmetry, we arrive at the problem on the periodicity cell:

$$div(\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|)\nabla\varphi(\mathbf{x})) = 0 \text{ in } Y; \tag{1}$$

$$\frac{\partial\varphi}{\partial\mathbf{n}}\,|_{x=0} = \frac{\partial\varphi}{\partial\mathbf{n}}\,|_{x=1} = 0; \varphi\,|_{y=0} = -E/2; \quad \varphi\,|_{y=1} = E/2,$$

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_∞, $k > 0$ are constants. It means that the partial differential equation in (1) is linear in domain $P \subset Y$ and strongly nonlinear in domain $Y\backslash P$.

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

$$F(\varphi) = \int_P \frac{1}{2}\,|\nabla\varphi(\mathbf{x})|^2\,d\mathbf{x} + \tag{3}$$

$$+ \int_{Y\backslash P} \left(\frac{\varepsilon_0 - \varepsilon_\infty}{2k}\ln(1 + k\,|\nabla\varphi(\mathbf{x})|^2) + \frac{\varepsilon_\infty}{2}\,|\nabla\varphi(\mathbf{x})|^2\right)d\mathbf{x} \to \min,$$

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 $(\varepsilon_0 - \varepsilon_\infty)(2\varepsilon_\infty - (\varepsilon_0 - \varepsilon_\infty)/2k) > 0$. Then the minimization problem (3) has unique solution.

We construct discrete approximation for the functional (3). We use finite differences approximation for derivatives and arrive at the problem of minimization of nonlinear function $\bar{F}(\varphi_{ij})$ of N variables ($\varphi_{i,j}$ means value of the function $\varphi(\mathbf{x})$ in the node with the coordinates $x = ih, y = jh$, $i, j = 0, 1, ..., N$). Function $\bar{F}(\varphi_{ij})$ is strictly convex on R^N. Then it has unique minimum. We computer program for solution of the problem, which use gradient method with variable step.

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A moment-matching Arnoldi method for phi-functions
Antti Koskela, Alexander Ostermann, *Thu 11:55 R 1.23*

We consider a new Krylov subspace algorithm for computing expressions of the form

$$\sum_{k=0}^{p} h^k \varphi_k(hA) w_k,$$

where $A \in \mathbb{R}^{n \times n}$, $w_k \in \mathbb{R}^n$, and φ_k are matrix functions related to the exponential function. Computational problems of this form appear when applying exponential integrators to large dimensional ODEs in semilinear form $u'(t) = Au(t) + g(u(t))$. Using Cauchy's integral formula we give a representation for the error of the approximation and derive a priori error bounds which describe well the convergence behaviour of the algorithm. In addition an efficient a posteriori estimate is derived. Numerical experiments in MATLAB illustrating the convergence behaviour are given.

Asymptotic stability analysis for recursive multirate Rosenbrock- and Peer-methods
Karen Kuhn, Jens Lang, *Thu 11:30 R 1.23*

Many physical phenomena contain different time scales. One way to solve the descriptive PDE is to discretize first in space and then apply a normal singlerate time integrator to the resulting ODE system. For problems with different time scales this might end up in very small time steps which have to be applied also to components with much less activity. That is why the application of multirate methods is reasonable (see e.g. [1]). Different time step sizes are used for different components, depending on their individual activity. Since the stability character of a singlerate method usually is not carried over to the corresponding multirate method, we study the asymptotic stability for several multirate Rosenbrock- and Peer-methods [2, 3].

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Adaptive Nested Implicit Runge-Kutta Methods with Global Error Control and Their Application in Fluid Mechanics
Gennady Kulikov, P. M. Lima, M. L. Morgado, *Mon 14:50 R 1.26*

This paper deals with a special family of implicit Runge-Kutta formulas of order 4. These methods are of Gauss type; i.e., they are based on the Gauss quadrature formula of orders 4. However, the methods under discussion have only explicit internal stages that lead to cheap practical implementation. Some of the stage values calculated in a step of the numerical integration are of sufficiently high accuracy that allows for dense output of the same order as the Runge-Kutta formula used. On the other hand, the designed methods are *A*-stable, stiffly accurate and symmetric. Moreover, they are conjugate to a symplectic method up to order 6 at least (see [1] for more details).

All of these make the new methods attractive for solving nonstiff and stiff ordinary differential equations, including Hamiltonian and reversible problems. For adaptivity, different strategies of error estimation are discussed and examined numerically, including a cheap global error estimation based on simple summation of local error estimates that are available in any embedded Runge-Kutta pair. An automatic global error control mechanism is also presented (see [2] for more details).

Then, we solve numerically a generalization of the Cahn-Hilliard continuum model for multiphase fluids (see [3]) where the classical Laplacian has been replaced by a degenerate one (i.e., so-called p-Laplacian). This differential problem is treated successfully by a complex technique based on a triple shooting method and the above-mentioned symmetric Runge-Kutta scheme with global error control implemented in MATLAB. Results of this numerical simulation are discussed and compared with earlier computed data.

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A general approach to application of reliable array square-root Kalman filtering methods in dynamic system identification
Maria Kulikova, *Mon 17:00 R 1.27*

This paper addresses the class of array square-root Kalman filtering (KF) algorithms with a J-orthogonal transformation. Such methods are currently preferable for practical implementation of H^2, H^∞ filters and include two main families: square-root array algorithms, which are typically numerically more stable than the conventional one, and fast array algorithms which, when system is time-invariant, typically offer an order of magnitude reduction in the computational cost.

Using this important class of numerically stable KF schemes, we extend its functionality and develop an elegant and simple method of computation of sensitivities of the system state to unknown parameters required in a variety of applications. For example, applications include system identification, optimal input design and so on. This new result generalizes the approach proposed by Bierman et al. in [1]. Our method replaces the standard approach based on

the conventional Kalman filter (and its derivatives) with its inherent numerical instabilities and, hence, improves the robustness of computations against roundoff errors. To illustrate the proposed approach, the method of maximum likelihood is used for parameter estimation in linear discrete-time stochastic systems.

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Stochastic B–series with some applications
Anne Kværnø, Kristian Debrabant, *Thu 9:20 R 3.28*

B–series, series expansions in which each term is expressed in terms of rooted trees, is well known to be an indispensable tool for constructing and analyzing numerical schemes for time-dependent differential equations. But they have also attracted quite some interest by their own terms.

In this talk, we will present a unified approach to the construction of B-series with application to stochastic differential equations (SDEs). The rather obvious use of such series, the construction of order conditions of numerical schemes, is well known. It is less known that by comparing stochastic B–series with the more familiar Wagner-Platen expansions, certain relations between different stochastic integrals are revealed. The use of B–series and growth functions to express iteration errors in implicit methods is another less conventional use of the series.

A few such aspects of stochastic B–series will be discussed in this talk.

Integration of DAEs with the Taylor Series Method using Automatic Differentiation
René Lamour, Diana Estévez Schwarz, *Thu 11:55 R 1.26*

Automatic (or Algorithmic) Differentiation (AD) opens new possibilities to analyze and solve DAEs by projector based methods. In particular, the projector sequence resulting from the tractability index concept can be computed and used for splitting techniques. This approach provides a description of the inherent ODE that makes possible an application of the "classical" Taylor Series Method for integration of initial value problems.

So far, AD applications for solving DAEs were based either on the differentiation or on the structural index concept. In this talk, we investigate the advantages of the application of the tractability index concept in this context. In a first approach, general nonlinear index-1 DAEs are examined and solved numerically. For higher-index DAEs different possibilities are considered and compared.

Adaptive Two-Step Peer Methods in Computational Fluid Dynamics
Jens Lang, Bettina Peth, *Mon 16:10 R 1.23*

In this talk, I will summarize our recent activities in constructing higher order variable timestep integrators for computational fluid dynamics [1,2]. I will mainly focus on two-step peer methods which were first developed for ODEs and subsequently applied to parabolic PDEs. Their main advantage over one-step methods lies in the fact that even in the application to PDEs no order reduction is observed. Our aim is to investigate whether the higher order of convergence of the

two-step peer methods equipped with variable timesteps pays off in practically relevant CFD computations.

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How Does 3DVAR Work: The Navier-Stokes Equation
Kody Law, Andrew Stuart, Dirk Bloemker, Kostas Zygalakis, *Tue 16:30 R 3.28*

In the perfect model scenario two ideas drive accurate filtering: (i) observe enough low frequency information, and (ii) model variance inflation: trust the observations. In this talk I will illustrate this for 3DVAR applied to the Navier-Stokes equations, in the low and high frequency observation limits.

Stroboscopic method for wave equation
Guillaume Leboucher, P. Chartier, F. Méhats, *Thu 16:00 R 1.23*

I am interested by long time numerical integration of highly oscillatory equations. Classical theory says that in order to make a good numerical approximation of the solution, the integration step must be significantly less than one period. This leads to two problems: The time of computation and the performance of computer to integrate this type of equation over millions of periods.

In the periodic case, a strategy is introduced in [1], [2] by M.P. Calvo, P. Chartier, A. Murua and J.M. Sanz-Serna and called stroboscopic method. The idea of this method is to follow the solution along another equation called averaged equation which has two interesting properties. It doesn't oscillate and coincides with the exact solution at the stroboscopic times, i.e., every multiple of the period.

Existence of this averaged equation in the ODE case has been rigorously proved for instance by L.M. Perko in [3]. The observations of P. Chartier & al. lead to a numerical method solving highly oscillatory ODEs over long time with a numerical cost independent of the ratio between the period and the final time of observation.

Perko's proof for ODE can be adapted to partial differential equation like the wave equation or the Schrödinger equation. I will explain how to adapt this proof to the semi-linear wave equation case and show some numerical results to illustrate the benefits of this method.

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A micro/macro parareal algorithm for a class of multiscale-in-time systems
Frederic Legoll, T. Lelievre, G. Samaey, *Thu 15:00 R 1.23*

We introduce and analyze a micro/macro parareal algorithm for the time-parallel integration of singularly perturbed ordinary differential equations. The system we consider includes some fast and some slow variables, the limiting dynamics of which (in the limit of infinite time scale separation) is known.

The algorithm first computes a cheap but inaccurate macroscopic solution using a coarse propagator (by only evolving the slow variables according to their limiting dynamics). This solution is iteratively corrected by using a fine-scale propagator (simulating the full microscopic dynamics on both slow and fast variables), in the parareal algorithm spirit.

The efficiency of the approach is demonstrated on the basis of numerical analysis arguments and representative numerical experiments.

Joint work with T. Lelievre and G. Samaey.

Elastohydrodynamics of a crankshaft in a journal bearing
Frank Leitenberger, *Wed 10:20 R 1.26*

We describe the motion of an elastic cylinder rotating in a journal bearing under hydrodynamic forces of an oil film and cavitation. We obtain a coupled system of 6 ordinary differential equations for the rigid body motion, a vectorial partial diffential equation for elastic waves and a variational inequality for the pressure in the oil film. Semidiscretizing the problem we obtain a nonlinear system of the form

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

whereupon every timestep requires the solution of a discrete cavitation problem. We discuss various aspects of this system.

Data-constrained uncertainty estimation in air quality simulation
Vivien Mallet, Damien Garaud, *Tue 17:00 R 3.28*

Air quality models are 3D chemistry-transport models that rely on complex physical and chemical formulations and on large amounts of data. The physical and chemical formulations are important sources of errors. Most of the input data is provided with high uncertainties in their time evolution and spatial distribution. The numerical approximations can be another important source of errors. The numerical model's state, which contains one to ten million components, is only partially observed by a few hundreds monitoring stations.

In order to better estimate the large uncertainties in models' outputs, modern methods rely on ensembles of simulations. The simulations of the ensembles are based on different physical models (multimodel ensemble) and perturbed input data (Monte Carlo approach). Large ensembles (e.g., with 100 members) can be automatically generated, but these may not properly sample

the uncertainties. The ensemble performance for uncertainty estimation can be evaluated by comparison with observations. Note that this comparison evaluates the ensemble as the whole, not the individual models.

Using the evaluation scores for ensembles, it is possible to devise algorithms for the calibration of ensembles. One strategy is to extract a sub-ensemble (from a given large ensemble) that minimizes a performance criterion over the set of available sub-ensembles. The criterion may the variance of a rank histogram, or a Brier score in case of probabilistic forecasts.

The generation and calibration of ensembles will be illustrated for 2D ozone concentration fields over Europe.

Mixed mode and chaotic oscillations in Newtonian jerk circuits
Wiesław Marszałek, Zdzislaw Trzaska, *Wed 11:10 R 1.27*

Mixed-mode and chaotic behavior are important features of many nonlinear systems not only in physics, biology and chemistry but also in nonlinear processes in economics, dusty plasma, arrhythmias of human hearts and synchronization of massive population of neurons in human brains leading to the epileptic brain cell diseases [1].

Based on a singularly perturbed system of three ODEs with a cubic nonlinear term, we propose two *jerk* circuits that can generate mixed-mode oscillations of various sequences. The circuits are realized using operational amplifiers, passive R and C elements and one voltage-controlled voltage source. The circuits' responses comprise both the large (L) and small (s) amplitude oscillations which result in a periodic L^s sequence. The L^s patterns follow the Farey arithmetic of coprime integers when the circuits' parameters bifurcate in certain intervals [2]. One of the two *jerk* circuits has a Newtonian form as its mathematical model can be derived from the second Newton's law $x'' = F/m$, with $x'' = d^2x/dt^2$ being an "acceleration" variable. This allows for a mechanical interpretation of the electrical variables of the circuits as position, velocity and acceleration. The second *jerk* circuit obtained from the same set of singularly perturbed ODE system is not Newtonian. The third variable in the ODE system does not yield any *jerk* circuit. Several PSPICE and Matlab simulation results are included.

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Modelling, simulation and control of differential-algebraic systems
Volker Mehrmann, *Fri 11:20 R 3.28*

In this talk we will present a framework for modelling, simulation and control of systems governed by automatically generated differential-algebraic systems. In this framework the system is first regularized to a strangeness-free behavior system, including index reduction, construction of consistent initial conditions, so that simulation and control can be performed without many limitations. We will present several examples from applications in multi-physics systems and optimal control.

Performance of "Look-Ahead" Linear Multistep Methods
Taketomo Mitsui, Dauda Gulibur Yakubu, *Mon 14:00 R 1.26*

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

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

We recently proposed "look-ahead" linear multistep methods (LALMM) as a new class of discrete variable solution of the problem. An LALMM scheme involves the "look-ahead" approximation together with the look-for one and corrects the look-for approximation by a predictor-corrector pair. Our anticipation is a good performance of LALMM from both viewpoints of accuracy and stability. We will discuss its actual performance mainly based on "look-ahead" linear two-step schemes.

Passivity Preserving Model Order Reduction Technique
Kasra Mohaghegh, Timo Reis, *Wed 11:10 R 1.26*

Increasing complexity of mathematical models demands techniques of model order reduction (MOR) that enable an efficient numerical simulation. MOR shall achieve accurate statements on a behavior of the dynamical system within an affordable amount of computational time. MOR methods are well developed for linear systems of ordinary differential equations (ODEs), whereas the nonlinear case represents still an open field of research [1]. In this work we present the algorithm which is designed for passivity preserving model reduction of linear time invariant systems. The method is based upon a combination of spectral zero interpolation [2] with positive real balance truncation [3]. It turns out that this method does not require the solution of Lur'e equations. Important properties of these methods are that, respectively, passivity and contractivity are preserved in the reduced-order models and that there exist approximation error bounds. Numerical examples are given.

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Runge-Kutta projection methods for conservative and non conservative problems
Juan Ignacio Montijano, M. Calvo, M.P. Laburta, L. Rández, *Fri 10:30 R 3.28*

Geometric structures (first integrals, orthogonality, Lyapunov functions, symplecticity, etc.) play an important role both in qualitative and quantitative studies of the flow of differential equations. In particular, preservation of invariants of differential systems by numerical integrators is a requirement that can be very important if the qualitative properties of the solution are to be properly reproduced. Some numerical integrators based on Runge-Kutta methods combined with projection techniques can be a simple and good option to preserve invariants.

In addition to orthogonal projection, other directional projections have been proposed that lead to Runge-Kutta methods, which preserve all linear first integrals and are affine invariant. However, the selection of the best direction is an open question. In the first part of this talk the search of a proper projection direction is analysed, attempting to minimize the leading error term of the projected solution. Special attention is paid to oscillatory problems, maximizing the dispersion order. In the second part of the talk, some applications of projection techniques are presented, showing how these techniques can be useful in the numerical integration of problems possessing Lyapunov functions and even for non conservative problems. Numerical experiments showing the performance of the proposed projection methods are presented.

Higher order splitting methods for a class of Hamiltonian equations
Asif Mushtaq, Anne Kværnø, Kåre Olaussen, *Mon 16:10 R 1.26*

A systematic procedure for increasing the accuracy of numerical solutions of a rather general class of Hamilton equations of the form

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}\mathbf{p}^T M \mathbf{p} + V(\mathbf{q}),$$

has been discussed in [1] (and references therein). The schemes introduced here preserve the symplectic structure. The Störmer-Verlet method is of 2nd order. By the use of generating functions it can be increased from 2nd to 8th order. We have tested various orders of the method on a simple anharmonic oscillator, with regard to the very long time behaviour. In this talk, I will give equivalent graphical representations of the schemes, and test them on a wider class of problems. The procedure is conveniently described in terms of rooted trees and B-series. In general, the basic idea is to correct the Hamiltonian used in the splitting scheme with terms of increasing orders. I will show how can we construct the improved Hamiltonian up to higher order. I will also present results of numerical simulations of selected systems.

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On the choice of configuration space for numerical Lie group integration of constrained rigid body systems
Andreas Müller, Zdravko Terze, *Wed 11:10 R 1.23*

When a rigid body moves it performs a translation together with a rotation. Moreover a general rigid body motion is a screw motion, i.e. rotation and translations are not independent. Even though standard integration schemes for multibody systems (MBS) neglect the geometry of Euclidean motion in the sense that, within the integration schemes, the position and orientation updates are performed independently. This problem can only be overcome if the Lie group property of rigid body motions is respected. To this end Lie group integration method have been recently applied to MBS that are further subject to additional constraints. In these approaches the direct product Lie group $SO(3) \times \mathbb{R}^3$ is used as rigid body configuration space. However, three-dimensional Euclidian motions, and thus the motion of a rigid body, are represented by the semidirect product Lie group $SE(3) = SO(3) \ltimes \mathbb{R}^3$. Strictly speaking, the direct product $SO(3) \times \mathbb{R}^3$ can represent the configuration of rigid body but not its motion. The crucial

question is whether or not this observation can be carried over to the application of Lie group integration schemes.

In this paper the implications of using the two representations on the performance of Munthe-Kaas integration schemes are investigated. It is pointed out that, although $SE(3)$ is the only proper representation of rigid body motions, the actual form of the motion equations (using left- or right-invariant, hybrid velocities) also decide about the numerical performance. It is shown that in many cases the $SE(3)$ representation yields optimal numerical performance for unconstrained as well as for holonomically constrained MBS. The analytic discussion is confirmed by several simple numerical examples.

Semi-Lagrangian discretization of the upper-convective derivative in Non-Newtonian fluid flow
Andreas Naumann, J. Wensch, *Mon 17:25 R 1.23*

The simulation of non-Newtonian fluids is a challenging task in computational rheology. The dynamics of the fluid are described by the Navier-Stokes equations. Whereas Newtonian fluids have constant viscosity, in non-Newtonian fluids a variety of models for the viscous terms are available. Viscosity may depend on the shear rate or even on the deformation history. The latter leads to models for the stress-strain rate relation analogous to viscous solids. The Non-Newtonian stresses evolve along particle paths according to an evolution equation. The temporal derivative in this case is the upper convected derivative. We describe a semi-Lagrangian discretization of the upper convected derivative. Numerical results for the flow through a contraction are given.

Numerical Aspects of Ensemble Square-root Kalman filters
Lars Nerger, Wolfgang Hiller, Jens Schröter, *Tue 16:00 R 3.28*

Ensemble square-root Kalman filters are currently the most widely used algorithms for sequential data assimilation. Over the recent years, a number of different algorithms have been introduced. These filters differ in the formulation of the analysis step, which combines the ensemble information from a numerical model with observational data. The relation of different filter algorithms will be discussed with a focus on numerical aspects. The discussion also motivates the new Error Subspace Transform Kalman Filter (ESTKF) that we have recently introduced.

On Finite Element Method - Flux Corrected Transport Schemes for Partial Differential Algebraic Equations
Julia Niemeyer, Bernd Simeon, *Mon 14:50 R 1.27*

Time-dependent advection-dominated flows appear in many computational fluid dynamics problems that involve the transport of scalar quantities, e.g., density or temperature. Since the classical finite element Galerkin discretization is known to produce unphysical oscillations for this type of problems, it is necessary to introduce a stabilized finite element formulation.

The idea of most stabilization techniques, such as the SUPG, SOLD, and LPS schemes, is to modify the bilinear form defining the finite element method. In contrast, the stabilization technique we are interested in, the finite element method - flux corrected transport schemes (FEM-FCT), works by modifying the system matrix and the right hand side vector at the algebraic level. It is a nonlinear high-resolution scheme which switches between high- and low order time discretizations due to the local smoothness of the solution [1].

In this work we apply the FEM-FCT in the context of partial differential-algebraic equations. As a model problem we choose the time-dependent advection-diffusion equation formulated as a differential-algebraic system by appending the boundary conditions by means of Lagrange multipliers. The combination of different time integrators (linear-implicit/implicit or implicit/implicit) and the handling of the additional entries in the system matrix due to the Lagrange multipliers are the main focus of our analysis.

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Exponential integrators for parabolic PDEs
Jitse Niesen, *Tue 16:00 R 1.23*

Exponential integrators are methods for the solution of ordinary differential equations which use the matrix exponential in some form. As the solution to linear equations is given by the exponential, these methods are well suited for stiff ordinary differential equations where the stiffness is concentrated in the linear part. Such equations arise when semi-discretizing semi-linear differential equations. The biggest challenge for exponential integrators is that we need to compute the exponential of a matrix. If a spectral discretization is used, then the matrix can be diagonalized cheaply. In other cases, the computation of the matrix exponential is more tricky and an iterative method needs to be used. This talk will survey the various possibilities that have been proposed.

G-symplectic General Linear Methods
Terence Norton, *Wed 10:45 R 3.28*

G-symplectic general linear methods have similar properties to symplectic Runge-Kutta methods. G-symplectic GLMs have an advantage over symplectic RKMs in that they can achieve high order with a minimally implicit stage matrix. We will discuss the construction of several G-symplectic methods of orders up to and including four, and demonstrate their application to classical separable and non-separable Hamiltonian problems.

A numerical scheme based on Haar wavelets transform for solutions of integral equations
Sapna Pandit, Manoj Kumar, *Tue 11:55 R 1.26*

In this paper, we have proposed a new numerical technique based on Haar wavelet transform for solving Volterra and Fredholm integral equations. Such type of equations occurs widely in the diverse area of the applied mechanics and physics. In the development of numerical technique, first, we convert the integral equations into initial and boundary value problems and then solve it by Haar wavelets based numerical technique. More accurate solution is obtained by wavelet decomposition in the form of a multiresolution analysis of the function which represents solution of initial and boundary value problems. Through this analysis, solution is found on the coarse grid points and refined towards higher accuracy by increasing the level of the Haar wavelets. The accuracy of the proposed method is demonstrated by some test problems. The numerical results are found in good agreement with exact solutions. Finally, the error analysis of the proposed method has been discussed.

Mathematical modeling of crown forest fires spread through firebreaks
Valeriy Perminov, *Thu 11:30 R 1.27*

Mathematical model of forest fire was based on an analysis of known experimental data and using concept and methods from reactive media mechanics. Because of the horizontal sizes of forest massif more than height of forest h, system of equations of general mathematical model of forest fire was integrated between the limits from height of the roughness level - 0 to h. It is assumed that heat and mass exchange of fire front and boundary layer of atmosphere are governed by Newton law. The boundary-value problem is solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions was calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting was then integrated. A discrete analog was obtained by means of the control volume method using the SIMPLE like algorithm In this paper the assignment and theoretical investigations of the problems of crown forest fire spread in windy condition were carried out. In this context, a study - mathematical modeling - of the conditions of forest fire spreading that would make it possible to obtain a detailed picture of the change in the temperature and component concentration fields with time, and determine as well as the limiting condition of fire propagation in forest with firebreaks.

Numerical simulation of differential algebraic equations with random parameters
Roland Pulch, *Mon 17:25 R 3.28*

We consider mathematical models of dynamical systems given by differential algebraic equations (DAEs). Some of the involved physical parameters often exhibit uncertainties due to measurement errors or imperfections of a manufacture process, for example. A stochastic modelling enables an uncertainty quantification, where the corresponding parameters are replaced by random variables. Consequently, the time-dependent solution of the DAEs represents a random process now. The moments of the random process can be resolved by sampling techniques like quasi-Monte-Carlo methods, for example. Alternatively, we focus on numerical techniques using the expansions of the polynomial chaos, where unknown coefficient functions have to be determined approximately. The index of a system of DAEs characterises its analytical and numerical properties. We investigate the index of the DAEs, which appear in the numerical methods for solving the stochastic model. The occurrence of a different index for varying parameters deserves closer attention and implies corresponding modifications of the numerical methods. Finally, we present numerical simulations of test examples from mathematical models of electric circuits.

An analysis of the Prothero–Robinson example for constructing new DIRK and ROW methods
Joachim Rang, *Thu 11:05 R 1.23*

In this talk the order reduction phenomenon of diagonally implicit Runge-Kutta methods (DIRK–methods) and Rosenbrock–Wanner methods (ROW–methods) applied on the Prothero-Robinson example is analysed. New order conditions to avoid order reduction are derived and new DIRK and ROW–method are created.
The new schemes are applied on the Prothero–Robinson example and on the semi-discretised incompressible Navier–Stokes equations. Numerical examples show that the new methods converge with second order for velocity and pressure.

Impact of model errors on data assimilation algorithms
Sebastian Reich, *Tue 14:30 R 3.28*

Most common data assimilation algorithms make the assumption that model errors are random and unbiased. In practice this assumption is often violated. In my talk I will propose a simple setting for studying the impact of systematic model biases on data assimilation algorithms. Results will be presented for particle filter as well as ensemble transform filter algorithms in the context of the Lorenz-63 model.

Stochastic differential equation of wave-drift damping motion
Ramezan Rezaeian, M. Saravi, *Mon 15:15 R 1.23*

The stochastic differential equations play an important role for considering a modeling. In this paper, we described a new method for analytical solution of the second-order stochastic differential equation of wave-drift damping motion model.

Positivity limiting and moment realizability for a class of quadrature-based moment closure methods
James Rossmanith, Yongtao Cheng, *Thu 15:00 R 3.28*

Kinetic models in plasma physics describe the evolution of the plasma in terms of a probability density function (PDF) in phase space. These models generally produce high-fidelity results, but are expensive to solve due to the high-dimensionality of the phase space. Fluid models reduce the complexity of kinetic models by evolving only a small number of moments of the distribution function, but require some model assumptions in order to arrive at a closed system – these assumptions are referred to as the *moment closure*. Developing accurate and robust moment closures is difficult in general and still very much a topic of ongoing research. In this work we study a class of moment closures known as *quadrature-based moment closures*. In particular, we consider the problems of hyperbolicity and moment realizability. We develop a class of numerical methods with *positivity-preserving limiters* that have the ability to approximately evolve a small number of moments of the PDF in a such way that a physically valid PDF can be reconstructed from the moments. The resulting numerical methods are tested on a variety of test problems. In this work we focus on the one-dimensional case, while extensions to higher dimensions are part of ongoing research.
This is joint work with Yongtao Cheng (University of Wisconsin - Madison).

Travelling wave solution of the Nagumo equation by the first integral method
Hamid Rouhparvar, *Mon 15:15 R 1.27*

In this paper, the first integral method is proposed to solve the Nagumo equation. This method is used to construct new travelling wave solutions of the Nagumo equation. The first integral method is easier and quicker than other traditional techniques. The first integral method was first proposed by Feng [1] in solving Burgers-KdV equation. Recently, this useful method is widely used by many for partial differential equations, such as, the modified Benjamin-Bona-Mahony equation [2], the two-dimensional Burgers-KdV equation [3], and by the reference therein [4].
Quasilinear parabolic equations, or nonlinear reaction-diffusion systems arise in the modelling of phenomena in physics, chemistry, biology and other applied sciences. Nagumo equation [5, 6, 7]

$$u_t = u_{xx} + u(a - u)(1 - u), \tag{1}$$

where the parameter $0 \leq a \leq 1$ acts as the ambient, is obtained in modelling a nerve axon as an active pulse transmission line. This equation is also arises in other biological phenomena and circuit theory.

Keywords: Nagumo equation, First integral method, Travelling wave solutions.

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Two Procedures for Solving Second Order Linear Ordinary Differential Equations
Masoud Saravi, *Mon 17:25 R 1.27*

This paper deals with second order linear Ordinary Differential Equations (ODEs), and gives some ideas on solving them. First we deal with method of reduction of order and give a generalization to this method. Then, by introducing the concept of pseudo-exact, we try to solve some specific second order linear ODEs

Runge-Kutta starting procedures for monotonicity of explicit linear multistep methods
Igor Savostianov, *Tue 10:40 R 1.27*

In this talk an analysis of monotonicity properties for linear multistep methods is presented. Following the approach of [1] we will give sufficient and necessary conditions for monotonicity (strong stability preservation) of linear multistep methods with Runge-Kutta starting procedures. The results apply to many popular methods that are used in practice. Several numerical experiments will illustrate the theory.

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Error estimation and communication step size control in modular time integration
Tom Schierz, Martin Arnold, *Mon 16:35 R 3.28*

Co-simulation is a rather general approach for the simulation of coupled technical systems and coupled physical phenomena in engineering with focus on instationary (time-dependent) problems. From the mathematical viewpoint, co-simulation results in a class of time integration methods for coupled systems which are described by time dependent ordinary differential equations (ODE) or differential algebraic equations (DAE) and are typically composed of subsystems. In time integration the data exchange between subsystems is limited to discrete communication points. In a communication step between two communication points the time integration is done separately in the different subsystems (*modular* time integration).

The communication step size has a strong influence on efficiency and accuracy of modular time integration. Reliable and efficient algorithms for the automatic selection of appropriate communication step sizes in co-simulation (communication step size control) may improve the simulation results. The selection of optimal communication step sizes is based on suitable estimates for the local error in one communication step. In this talk we discuss different methods for the estimation of this error and demonstrate the successful application of the communication step size control algorithm for a rather simple practical benchmark problem.

Convergence of an impulse based scheme for rigid multibody models
Hagen Schiller, *Thu 11:05 R 1.26*

We follow an approach that was pioneered by Hahn [1] and expanded upon by Mirtich [2]. The idea of impulse-based dynamic simulation is to treat all contact between bodies by a series of collisions that are modelled as accurately as reasonably possible. Unsurprisingly, this paradigm works very well for systems which exhibit rapid high frequency collisions e.g. a lottery machine or a part feeder. However, even for continuous contact the paradigm still allows for fast and efficient computation [2].

We shall prove that for any sequence of numerical solutions (q_ϵ, v_ϵ) depending on the numerical non-interpenetration threshhold ϵ there exists a subsequence that converges to an appropriately defined generalised solution of the equations of motion.

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Implicit peer methods with embedded sensitivities for parameter-dependent ODEs
Bernhard A. Schmitt, *Mon 14:25 R 1.26*

By design all stages of peer two-step methods possess the full order of the scheme. This property allows for the embedding of additional stages to approximate an arbitrary number of solution derivatives with respect to parameters of the ODE. In fact, one additional satellite stage is sufficient for each ODE parameter. With respect to the time stepsize the satellite stages have the full order of the original scheme, while the accuracy of computed parameter derivatives is of lower order only. Still, there is an improvement for implicit methods compared to explicit

methods discussed previously. This embedding may be cheaper than the standard approach of solving neighbouring problems with the same basic numerical scheme. Numerical tests show that these derivatives are sufficiently accurate for Newton-type iterations in boundary value problems and parameter identification.

Self-conjugate differential and difference operators in the optimal control of descriptor systems

Lena Scholz, Volker Mehrmann, *Thu 11:30 R 1.26*

We analyze the structure of the differential and difference operators associated with the necessary optimality conditions of optimal control problems for descriptor systems in continuous and discrete time.

In the continuous-time case, the *linear quadratic optimal control problem* with constraints given by *differential-algebraic equations (DAEs)* is of the form

$$\text{min.} \quad \frac{1}{2}x(\bar{t})^T M_e x(\bar{t}) + \frac{1}{2}\int_{\underline{t}}^{\bar{t}} \left(x^T W x + x^T S u + u^T S^T x + u^T R u\right)\, dt$$

$$\text{s. t.} \quad E(t)\dot{x} = A(t)x + B(t)u + f(t), \quad x(\underline{t}) = \underline{x} \in \mathbb{R}^n.$$

This problem has recently been discussed in several publications [1, 3, 4, 6] and it has been shown in [4] that the operator associated with the necessary optimality boundary value problem is self-conjugate. If we denote the differential-algebraic equation associated with this boundary value problem by

$$\mathcal{E}\dot{z} = \mathcal{A}z + \tilde{f},$$

then the pair $(\mathcal{E}, \mathcal{A})$ has the property that $\mathcal{E}^T = -\mathcal{E}$ and $\mathcal{A}^T = \mathcal{A} + \dot{\mathcal{E}}$.

On the other hand, we consider the *discrete-time linear-quadratic optimal control problem* given by

$$\text{min.} \quad \frac{1}{2}x_N^T M_e x_N + \frac{1}{2}\sum_{j=0}^{N}(x_j^T W_j x_j + x_j^T S_j u_j + u_j^T S_j^T x_j + u_j^T R_j u_j), \tag{1}$$

$$\text{s. t.} \quad E_{k+1}x_{k+1} = A_k x_k + B_k u_k + f_k, \quad x_0 = \underline{x} \in \mathbb{R}^n.$$

The necessary optimality condition for $((x_k), (u_k))$ to be an optimal solution is the existence of a sequence of Lagrange multipliers (λ_k) such that $((x_k), (u_k), (\lambda_k))$ satisfy the discrete-time optimality system

$$\begin{bmatrix} 0 & E_{k+1} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \lambda_{k+1} \\ x_{k+1} \\ u_{k+1} \end{bmatrix} + \begin{bmatrix} 0 & -A_k & -B_k \\ -A_k^T & W_k & S_k \\ -B_k^T & S_k^T & R_k \end{bmatrix}\begin{bmatrix} \lambda_k \\ x_k \\ u_k \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ E_k^T & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \lambda_{k-1} \\ x_{k-1} \\ u_{k-1} \end{bmatrix} = \begin{bmatrix} f_k \\ 0 \\ 0 \end{bmatrix},$$

together with appropriate boundary conditions, see [5]. We will show that the special structure of the sequences of coefficient matrices corresponds to self-conjugacy of the corresponding difference operator. The relationship between these structures is well understood in the constant coefficient case, see [2, 7]. Here, we will study the relationship between the structures in the discrete- and continuous-time case with variable coefficients and show that self-adjointness of matrix tuples (in continuous- as well as in discrete-time) is an appropriate generalization for even/palindromic, and Hamiltonian/symplectic structures in the constant coefficient case.

Discrete-time optimal control problems of the form (1) arise in the *first-discretize-then-optimize* approach for solving a linear-quadratic optimal control problem (in contrast to the approach

of *first-optimize-then-discretize*). This immediately leads to the question of how to discretize the necessary optimality system in the continuous-time case so that the resulting discrete-time system has the self-adjoint structure that would have been obtained when discretizing the constraint first and then deriving the discrete-time optimality systems. In this way it can be guaranteed that the approaches first-discretize-then-optimize and first-optimize-then-discretize lead to the same structural properties of the optimality system, i.e., discretization and optimization commute, such that we can use the advantages from both approaches.

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Adjoint Consistent Implicit Peer Methods
Dirk Schröder, Jens Lang, Rüdiger Weiner, *Mon 15:15 R 1.26*

This talk is about the adjoint consistency of implicit two-step peer methods. In optimal control of differential equations there are essentially two approaches to generate an optimality system. The first-optimize-then-discretize approach means that the continuous optimality system is discretized, whereas the first-discretize-then-optimize approach solves the optimality system generated from the discretized optimal control problem. It is advantageous in optimal control, if these two approaches are interchangeable. Hence it is important that the discrete adjoint of a time discretization is consistent with the continuous adjoint equation.

While there are promising results for Runge-Kutta methods [Hager(2000)] and W-methods [Lang and Verwer(2011)], multistep methods are in general not adjoint consistent [Sandu(2008)]. In the talk first results for implicit peer methods are discussed. Consistency conditions and stability properties are presented for peer methods in the context of optimal control. Numerical experiments are given for some test problems.

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Structure-Preserving Projection Methods for Hamiltonian Systems
Dmitry Shcherbakov, Matthias Ehrhardt, Michael Günther, Michael Striebel,
Wed 10:45 R 1.23

In this work we consider the numerical solution of Hamiltonian systems via symmetric, symplectic integrators, which preserve simultaneously the energy of the Hamiltonian system. Starting from Hairer's pioneering idea of the symmetric projection methods we design a new structure-preserving numerical scheme.
The proposed methods can be used for solving a wide range of problems, where it is necessary for the integrator to possess structure-preserving properties, e.g in quantum chromodynamics (QCD) calculations.
Finally, we present the numerical results for a hierarchy of Hamiltonian systems ranging from the simple harmonic oscillator to non-separable Hamiltonians to illustrate and give numerical evidence for which setting our approach is already working.

Observation Impact in a Localized Ensemble Transform Kalman Filter
Matthias Sommer, *Tue 15:00 R 3.28*

The impact of observations on forecast quality is in many aspects an interesting quantity: It not only indicates, which observation types could be given more weight in the assimilation algorithm but also helps in tuning observation operators and in the planning of further investments in the observation system. However, the direct computation of observation impact in a assimilation and forecasting system is computationally expensive and therefore not feasible in an operational environment. To address this issue, different approximations have been suggested recently. This talk discusses the mathematical challenges of estimating observation impact and shows first results of assessing it in the localized ensemble transform Kalman filter for the regional weather forecasting model (COSMO-DE) of German Weather Service.

On new spectral methods for hyperbolic conservation laws
Thomas Sonar, Martina Wirz, Philipp Öffner, Andreas Meister, Sigrung Ortlieb,
Thu 8:30 R 3.28

In applications mainly in fluid dynamics nowadays robust but accurate solvers are needed. While good accuracy meant order of 2 some years ago it is now codes of orders of approximations of 4 and higher engineers want to deal with. There is, however, a subtle balance between robustness and order of accuracy and methods of very high order tend generally to be less robust. In a joint project with colleagues from Kassel we have developed two new spectral methods on triangular meshes which should give us stability as well as robustness. Main ingredients of our methods are a powerful nodal/modal filtering as well as the use of different families of polynomials being orthogonal on simplices. We have developed a new shock detection technique with which we can derive Fourier modes of the numerical solution directly from the orthogonal polynomials. I will present some of the recent results and an outlook towards future research.

Modeling and computation of combined free surface and pressure water flow in networks by local Lax-Friedrich and related upwind techniques
Gerd Steinebach, *Mon 16:35 R 1.23*

For the simulation of water flow in large networks a combined modeling approach for free surface and pressure flow is considered. The numerical solution is based on a finite volume discretization in space and a standard method for time integration. Beside the local Lax-Friedrich ansatz some other related decomposition techniques are developed for a suitable upwinding. The focus is on well-balanced schemes which preserve stationary solutions. The methods are tested on a set of eight problems including the different types of flow.

Adaptive space and time discretisations for Gross–Pitaevskii equations
Mechthild Thalhammer, *Tue 14:00 R 1.23*

As a basic principle, benefits of adaptive discretisations are an improved balance between required accuracy and efficiency as well as an enhancement of the reliability of numerical computations. In this talk, the capacity of locally adaptive space and time discretisations for the numerical solution of low-dimensional nonlinear Schrödinger equations is investigated. The considered model equation is related to the time-dependent Gross–Pitaevskii equation arising in the description of Bose–Einstein condensates in dilute gases. The performance of the Fourier-pseudo spectral method constrained to uniform meshes versus the locally adaptive finite element method and of higher-order exponential operator splitting methods with variable time stepsizes is studied. Numerical experiments confirm that a local time stepsize control based on a posteriori local error estimators or embedded splitting pairs, respectively, is effective in different situations with an enhancement either in efficiency or reliability. As expected, adaptive time-splitting schemes combined with fast Fourier transform techniques are favourable regarding accuracy and efficiency when applied to Gross–Pitaevskii equations with a defocusing nonlinearity and a mildly varying regular solution. However, the numerical solution of nonlinear Schrödinger equations in the semi-classical regime becomes a demanding task. Due to the highly oscillatory and nonlinear nature of the problem, the spatial mesh size and the time increments need to be of the size of the decisive (small) parameter, especially when it is desired to capture correctly the quantitative behaviour of the wave function itself. The required high resolution in space constricts the feasibility of numerical computations for both, the Fourier pseudo-spectral and the finite element method. Nevertheless, for smaller parameter values adaptive time discretisations facilitate to determine the time stepsizes sufficiently small in order that the numerical approximation captures correctly the behaviour of the analytical solution. Further illustrations for Gross–Pitaevskii equations with a focusing nonlinearity or a sharp Gaussian as initial condition, respectively, complement the numerical study.

Multiphysical Modeling and Numerical Simulation of Flow Networks
Caren Tischendorf, Sascha Baumanns, Lennart Jansen, *Tue 9:20 R 3.28*

We discuss a multiphysical modeling of electric networks, gas networks, and water distribution networks. Depending on the network topology and the modeling level, we obtain a system of differential equations, differential-algebraic equations, partial differential equations or couplings thereof. We present qualitative and structural properties of these systems and their effects onto the numerical simulation. In particular, we will show that the numerical results do not only depend on the type of the differential equation system and the choice of the numerical method but also significantly on the model formulation. Finally, we address problems to be solved for a successful and robust simulation of such systems concerning linear solvers, nonlinear solvers, numerical methods and the automatic generation of the model equations.

Newton-waveform method for simulation of constrained multibody systems
Paweł Tomulik, Janusz Fraczek, *Mon 17:00 R 3.28*

The Newton-waveform method provides means for distributed integration of differential equations next to other known methods such as multi-rate integration or waveform relaxation. In our work we use Newton-waveform to co-simulate multibody systems coupled by kinematic constraints. Two such algorithms are presented – the one which converts nonlinear equations of motion into series of linear DAEs with time-varying coefficients and the other which solves coupling constraint equations over prescribed time interval while the subsystem equations are integrated by subsystem simulators. Both algorithms are outlined and their basic properties are illustrated with numerical examples.

Dynamic Response of Highway Bridges to Heavy Vehicle Loads
Mustapha Usman, F.A.Hammed, *Tue 11:55 R 1.27*

This paper investigates the analysis of dynamic interaction between heavy vehicles and highway bridges. The partial differential equation is transformed to ordinary differential equation. The governing partial equation is solved using finite difference method. It is observed that as the foundation modulus K increases, the deflection of t the beam increases. An example of simply supported beam is given.

Necessity of formulation of two dynamic models for HMM application to multibody systems
Michael Valášek, L. Mraz, *Mon 15:15 R 3.28*

It is investigated the solution of multibody systems described by differential algebraic equations by reformulation into highly oscillatory ordinary differential equations. It is considered the solution by the application of heterogeneous multiscale methods (HMM). On this example it is demonstrated the necessity to use formulation of two level dynamical models for successful application of HMM. These models must differ by their eigenvalues. It is not necessary to formulate both models explicitly but it is necessary to extract from these two models the suitable choice of two different sets of variables. Several further necessary modifications for successful application of HMM are also described (determination of initial conditions, proper choice of solution time lengths on different scales, etc.).

Goal-adaptivity for fluid-structure interaction
Harald van Brummelen, K.G. van der Zee, P.W. Fick, V.V. Garg, S. Prudhomme, *Wed 8:30 R 3.28*

The numerical solution of fluid-structure-interaction problems poses a paradox in that most of the computational resources are consumed by the subsystem that is of least practical interest, viz., the fluid. Goal-adaptive discretization methods provide a paradigm to bypass this paradox. Based on the solution of a dual problem, the contribution of local errors to the error in a specific goal functional is estimated, and only the regions that yield a dominant contribution are refined. In this presentation, I will discuss recent progress in the development of goal-adaptive approximation methods for fluid-structure interaction and, more generally, boundary-coupled problems and free-boundary problems. In general, two fundamental complications must be addressed to apply goal-adaptive methods to fluid-structure interaction. Firstly, the formulation (interpretation) of the interface coupling conditions has non-trivial consequences for the dual

problem [1-3]. Secondly, the domain dependence engendered by the free-boundary character results in complicated shape derivatives in the linearized dual problem [3-5]. The presentation addresses both these complications. Numerical results are presented to illustrate the differences in the various formulations, and to exhibit the potential of goal-adaptive methods for fluid-structure-interaction problems.

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Efficient integration of matrix-valued non-stiff DAEs by half-explicit methods
Linh Vu, Vu Hoang Linh and Volker Mehrmann, *Mon 14:50 R 3.28*

This talk is concerned with numerical solutions of nonlinear differential-algebraic equations (DAEs) in strangeness-free form. In particular, we focus on efficient methods for solving a special class of semi-linear matrix-valued DAEs which arise in the numerical computation of spectral intervals for DAEs. Half-explicit methods based on popular explicit methods like one-leg methods, linear multi-step methods, and Runge-Kutta methods are proposed and analysed. Compared with well-known implicit methods for DAEs, these half-explicit methods demonstrate their efficiency, particularly for the above mentioned semi-linear matrix-valued DAEs. The theoretical convergence results are confirmed by numerical experiments.

Stiff order conditions for high-order exponential integrators
Luan Vu Thai, Alexander Ostermann, *Thu 10:40 R 1.23*

In recent years, exponential integrators have shown to be very competitive for the numerical solution of large systems of stiff differential equations. The construction of high-order methods relies on the knowledge of the (stiff) order conditions, which are available in the literature up to order four. In this talk, we present a new and simple approach to derive these conditions for exponential Runge–Kutta and exponential Rosenbrock-type methods. Exemplarily, we work out our approach for order five which enables us to construct fifth-order methods. Our setting is adapted to stiff problems and allows us to prove convergence results for variable step size implementations, independently of the stiffness of the problem. Numerical results show that the new integrators are highly competitive.

Symmetric and symplectic projection methods for differential equations on manifolds: the non-Abelian case

Michele Wandelt, Michael Günther, Michael Striebel, *Wed 10:20 R 1.23*

This work is concerned with symmetric and symplectic projection methods. The idea is based on symmetric projection schemes introduced by Hairer for ODE systems in the Abelian case R^n living on a manifold, which combine a symmetric scheme with a projection on the manifold, resulting in an overall symmetric scheme which preserves the constraint defined by the manifold. We have generalized this scheme to projection schemes, which combine a symmetric, time-reversible and symplectic scheme (Leapfrog, for example) with a projection on the manifold described by the Hamiltonian, resulting in a scheme with the aforementioned properties which preserves the Hamiltonian exactly.

In a further step, we adapted the method to the non-Abelian case of matrix Lie groups. In this case, the projection method can be used in quantum field theories as, for example, in Lattice QCD. In these theories, expectation values of some operators have to be computed. This has to be done numerically with high computational cost, and the symmetric and symplectic projection method is promising to reduce this effort.

Semi-analytical methods for singularly perturbed multibody system models
Steffen Weber, Martin Arnold, *Thu 10:40 R 1.26*

Multibody system models with either small masses or large stiffness terms will be considered. Both problems are known to cause high computation time due to high frequency oscillations. A method to integrate such problems is motivated by results from singular perturbation theory which relate the solution of the ODE

$$\dot{u} = f(u, v), \qquad \varepsilon\dot{v} = g(u, v)$$

with a small parameter $\varepsilon > 0$ to the solution of the DAE

$$\dot{u}_0 = f(u_0, v_0), \qquad 0 = g(u_0, v_0).$$

But most theorems in the literature are restricted to unconstrained problems with diagonal mass matrices and bounded stiffness terms. We extend this approach to non-diagonal matrices and investigate scaling for large stiffness terms in flexible multibody systems taking into account the structure of second order equations. Furthermore, the extension to problems with constraints is presented. The computational saving is illustrated by examples.

Integrating Highly-Oscillatory Mechanical Systems with Solution-Dependent Frequencies
Daniel Weiß, *Thu 14:30 R 1.23*

This talk is about the application of several integrators to highly-oscillatory mechanical systems with solution-dependent frequencies. As an example we use the stiff spring double pendulum: two mass points are attached serially by stiff springs to one another. The numerical behaviour of several integrators such as Flavor, the impulse method, the mollified impulse method, and a integrator based on the framework of Heterogeneous Multiscale Methods is studied. It is explained that a correct approximation of the actual motion relies on an almost-invariance property of the actions in the system. Whereas consistent initializations lying on the manifold given by the effective system are sometimes treated properly, one has to take into account the actions in case of inconsistent initial values.

TVD-based split-explicit methods for compressible flow
Jörg Wensch, Oswald Knoth, *Mon 17:00 R 1.23*

The simulation of atmospheric dynamics relies on the numerical solution of the Euler equations. These equations exhibit phenomena on different temporal scales. In the lower troposphere sound waves propagate approximately ten times faster than the advective waves. An approach to overcome the CFL restriction caused by sound waves are split-explicit methods. By multirate techniques the terms relevant for sound waves are integrated by small time steps with a cheap time integration procedure, whereas the slow processes are solved by an underlying Runge-Kutta method using a larger macro step size. We construct such methods based on TVD-RK schemes and discuss order and stability properties.

NOx formations in methane-air combustion under condition of joint processes of chemical kinetics and molecular diffusion
Alexander Zakharov, M. Bochkov, S. Khvisevich, *Tue 11:30 R 1.27*

The problem of NOx emission in combustion of the temperature jump boundary is numerically solved. This formulation serves for studying processes occurring on the front of laminar diffusion flame motion against the cold background. For the consideration of combustion process a scheme of chemical reaction is developed specially for the analysis of NOx emission. The scheme contains 196 chemical reactions for 32 mixture components. The numerical solution of such problem is a rather complicated task because there is a great deal of equations and it is an extremely stiff problem. For the integration we used LSODES code package (from the ODEPACK code collection) designed for problems with the Jacobi matrices with the arbitrary sparse structures (the system contains more than 3000 ODE's). Temperature, pressure and initial mixture of the components were the varied parameters of this problem. The results obtained are used in development of an ecologically safe method of natural gas combustion in gas-burning boilers.

A doubling-splitting approach for the fractional heat equation
Paul Andries Zegeling, *Wed 10:45 R 1.27*

Fractional order differential equations, as generalizations of classical order differential equations, are increasingly used in model problems in fluid flow, in finance and other areas of application, such as advection-dispersion models from hydrology. In this presentation I discuss the space-fractional heat equation:

$$u_t = D_C^\alpha u, \ 1 < \alpha \leq 2, \tag{1}$$

in which the fractional derivative D_C^α is defined 'in the sense of Caputo'. Several numerical approaches are available for the numerical approximation of such equations, yielding systems with (half-) full matrices. An alternative is to use a doubling-splitting approach to the operators in the PDE. Firstly, the operators are doubled to get a higher-order PDE, and then this PDE is split again into a system of lower-order PDEs, now giving a band-matrix structure. The method-of-lines procedure for approximating solutions of this new PDE system will be explained in more detail and illustrated with a series of numerical experiments. Analysis of the spectrum of the final system reveals that a special treatment of the time-integration is necessary to avoid numerical instabilities.

Minimax state estimation for linear differential algebraic equations
Sergiy Zhuk, *Tue 17:30 R 3.28*

This talk presents a generalization of the minimax state estimation approach for singular linear Differential-Algebraic Equations (DAE) with uncertain but bounded input and observation's noise. We apply generalized Kalman Duality principle to DAE in order to represent the minimax estimate as a solution of a dual control problem for adjoint DAE. The latter is then solved converting the adjoint DAE into ODE by means of a projection algorithm. Finally, we represent the minimax estimate in the form of a linear recursive filter.

4 List of Participants

Aceto, Lidia	University of Pisa `l.aceto@dma.unipi.it`	Italy
Ahmad, Saghir	NZ Institute for Advanced Studies, Massey University `s.ahmad@massey.ac.nz`	New Zealand
AL Jammaz, Ammar	University of Marburg `aljammaz@mathematik.uni-marburg.de`	Germany
Altmann, Robert	TU Berlin `raltmann@math.tu-berlin.de`	Germany
Arnold, Martin	Martin Luther University Halle-Wittenberg `martin.arnold@mathematik.uni-halle.de`	Germany
Bader, Philipp	Universidad Politécnica de Valencia `phiba@upv.es`	Spain
Bartel, Andreas	Angewandte Mathematik, BU Wuppertal `bartel@math.uni-wuppertal.de`	Germany
Baum, Ann-Kristin	TU Berlin `baum@math.tu-berlin.de`	Germany
Beck, Steffen	Martin-Luther-Universität Halle-Wittenberg `steffen.beck@mathematik.uni-halle.de`	Germany
Becker, Urs	Fraunhofer ITWM `urs.becker@itwm.fraunhofer.de`	Germany
Berzins, Martin	University of Utah `mb@sci.utah.edu`	USA
Betsch, Peter	University of Siegen `peter.betsch@uni-siegen.de`	Germany
Blanes, Sergio	Universitat Politècnica de València `serblaza@imm.upv.es`	Spain
Boltze, Lothar	Martin Luther University Halle-Wittenberg `lothar.boltze@mathematik.uni-halle.de`	Germany
Braś, Michał	AGH University of Science and Technology, Krakow `bras@agh.edu.pl`	Poland
Bruder, Jürgen	Martin Luther University Halle-Wittenberg `juergen.bruder@mathematik.uni-halle.de`	Germany
Brumm, Bernd	Universität Tübingen `brumm@na.uni-tuebingen.de`	Germany
Burger, Michael	Fraunhofer ITWM `michael.burger@itwm.fraunhofer.de`	Germany

Burgermeister, Bernhard	SIMPACK AG `bernhard.burgermeister@simpack.de`	Germany
Burrage, Kevin	University of Oxford and QUT `kevin.burrage@gmail.com`	UK and Australia
Burrage, Pamela	Queensland University of Technology `pamela.burrage@qut.edu.au`	Australia
Butcher, John	University of Auckland `butcher@math.auckland.ac.nz`	New Zealand
Calvo, Marí Paz	Universidad de Valladolid `maripaz@mac.uva.es`	Spain
Chistyakova, Elena	Institute for System Dynamics and Control Theory SB RAS `elena.chistyakova@icc.ru`	Russia
Cotter, Simon	Oxford University `cotter@maths.ox.ac.uk`	UK
Csomós, Petra	University of Innsbruck `petra.csomos@uibk.ac.at`	Austria
D'Ambrosio, Raffaele	University of Salerno `rdambrosio@unisa.it`	Italy
Debrabant, Kristian	University of Southern Denmark, Department of Mathematics and Computer Science `debrabant@imada.sdu.dk`	Denmark
Dieci, Luca	School of Mathematics, Georgia Tech `dieci@math.gatech.edu`	USA
Dörsek, Philipp	ETH Zurich `philipp.doersek@math.ethz.ch`	Switzerland
Einkemmer, Lukas	University of Innsbruck `lukas.einkemmer@uibk.ac.at`	Austria
Eirola, Timo	Aalto University `timo.eirola@aalto.fi`	Finland
Emamzadeh, Abolghasem	Petroleum University `emamzadeha@gmail.com`	Iran
Estévez Schwarz, Diana	Beuth Hochschule `estevez@beuth-hochschule.de`	Germany
Faleichik, Boris	Belarusian State University `faleichik@gmail.com`	Belarus
Faou, Erwan	INRIA `Erwan.Faou@inria.fr`	France

Fiedler, Robert	Martin Luther University Halle-Wittenberg `robert.fiedler@mathematik.uni-halle.de`	Germany
Frank, Jason	CWI `jason@cwi.nl`	The Netherlands
Garrappa, Roberto	University of Bari `garrappa@dm.uniba.it`	Italy
Gauckler, Ludwig	TU Berlin `gauckler@math.tu-berlin.de`	Germany
Geiser, Jürgen	Department of Physics, University of Greifswald `juergen.geiser@uni-greifswald.de`	Germany
Gerisch, Alf	TU Darmstadt `gerisch@mathematik.tu-darmstadt.de`	Germany
Ghovatmand Jazei, Mehdi	Shahrood University of Technology `mghovat@shahroodut.ac.ir`	Iran
González Pinto, Severiano	University of La Laguna `spinto@ull.es`	Spain
Guias, Flavius	Dortmund University of Applied Sciences `flavius.guias@fh-dortmund.de`	Germany
Günther, Michael	Bergische Universität Wuppertal `guenther@math.uni-wuppertal.de`	Deutschland
Ha, Phi	Technical University Berlin `ha@math.tu-berlin.de`	Germany
Hairer, Ernst	University of Geneva `Ernst.Hairer@unige.ch`	Switzerland
Hanke, Michael	KTH Royal Institute of Technology `hanke@nada.kth.se`	Sweden
Hansen, Eskil	Lund University `eskil@maths.lth.se`	Sweden
Hernández-Abreu, Domingo	University of La Laguna `dhabreu@ull.es`	Spain
Herter, Rainer	Martin Luther University Halle-Wittenberg `herter@mathematik.uni-halle.de`	Germany
Heubes, Daniel	Bergische Universität Wuppertal `heubes@math.uni-wuppertal.de`	Germany
Higueras, Inmaculada	Universidad Publica de Navarra `higueras@unavarra.es`	Spain
Hill, Adrian	University of Bath `masath@bath.ac.uk`	UK

Horváth, Zoltán	Széchenyi István University `horvathz@sze.hu`	Hungary
Hundsdorfer, Willem	CWI `willem.hundsdorfer@cwi.nl`	The Netherlands
Imran, Gulshad	University of Auckland `ggul005@aucklanduni.ac.nz`	New Zealand
Jackiewicz, Zdzisław	Arizona State University `jackiewicz@asu.edu`	USA
Jamil, Noreen	The University of Auckland `njam031@aucklanduni.ac.nz`	New Zealand
Jansen, Lennart	Humboldt University of Berlin `lejansen.math@gmail.com`	Germany
Jiwari, Ram	Thapar University `ram1maths@gmail.com`	India
Johnson, Evan	University of Wisconsin–Madison `e.alec.johnson@gmail.com`	USA
Kelly, Conall	University of the West Indies `conall.kelly@uwimona.edu.jm`	Jamaica
Ketcheson, David	King Abdullah University of Science and Technology `david.ketcheson@kaust.edu.sa`	Saudi Arabia
Kettmann, Markus	Martin Luther University Halle-Wittenberg `markus.kettmann@mathematik.uni-halle.de`	Germany
Khashin, Sergei	Ivanovo State University `khash2@gmail.com`	Russia
Knoth, Oswald	Leibniz-Institut für Troposphärenforschung `knoth@tropos.de`	Germany
Kocsis, Tihamer Albert	Szechenyi Istvan University `katihi@sze.hu`	Hungary
Kolpakov, Aleksandr	Novosibirsk State University `algk@ngs.ru`	Russia
Koskela, Antti	University of Innsbruck `antti.koskela@uibk.ac.at`	Austria
Kuhn, Karen	Graduate School of Computational Engineering, TU Darmstadt `kuhn@gsc.tu-darmstadt.de`	Germany
Kulikov, Gennady	Instituto Superior Técnico `gkulikov@math.ist.utl.pt`	Portugal

Kulikova, Maria	Instituto Superior Técnico `Kulikova.Maria@yahoo.com`	Portugal
Kværnø, Anne	Norwegian University of Science and Technology `anne@math.ntnu.no`	Norway
Lamour, René	Humboldt-University of Berlin `lamour@math.hu-berlin.de`	Germany
Lang, Jens	Technische Universität Darmstadt `lang@mathematik.tu-darmstadt.de`	Germany
Law, Kody	University of Warwick `kodylaw@gmail.com`	UK
Leboucher, Guillaume	Université Rennes 1 `guillaume.leboucher@univ-rennes1.fr`	France
Legoll, Frederic	Ecole des Ponts ParisTech `legoll@lami.enpc.fr`	France
Leitenberger, Frank	Martin Luther University Halle-Wittenberg `leitenbe@web.de`	Germany
Linß, Torsten	FernUniversität in Hagen `torsten.linss@fernuni-hagen.de`	Germany
Mallet, Vivien	INRIA & CEREA `Vivien.Mallet@inria.fr`	France
Marszałek, Wiesław	DeVry University `wmarszalek@devry.edu`	USA
Martínez, Vicente	Universitat Jaume I `martinez@mat.uji.es`	Spain
Mehrmann, Volker	TU Berlin `mehrmann@math.tu-berlin.de`	Germany
Mitsui, Taketomo	Doshisha University `tamitsui@mail.doshisha.ac.jp`	Japan
Mohaghegh, Kasra	University of Hamburg `kasra.mohaghegh@math.uni-hamburg.de`	Germany
Montijano, Juan Ignacio	Universidad de Zaragoza `monti@unizar.es`	Spain
Mraz, Ladislav	CTU in Prague `ladislav.mraz@fs.cvut.cz`	Czech Republic
Mushtaq, Asif	NTNU, Trondheim `asifm@math.ntnu.no`	Norway
Müller, Andreas	Institute of Mechatronics, Chemnitz `andreas.mueller@ifm-chemnitz.de`	Germany

Naumann, Andreas	TU Dresden `Andreas.Naumann@tu-dresden.de`	Germany
Nerger, Lars	Alfred Wegener Institute `lars.nerger@awi.de`	Germany
Niemeyer, Julia	Felix-Klein-Zentrum für Mathematik, TU Kaiserslautern `niemeyer@mathematik.uni-kl.de`	Germany
Niesen, Jitse	University of Leeds `jitse@maths.leeds.ac.uk`	UK
Norton, Terence	University of Bath `tjtn20@bath.ac.uk`	UK
Pandit, Sapna	Motilal Nehru National Institute of Technology Allahabad `sappu15maths@gmail.com`	India
Perminov, Valeriy	Belovo Branch of Kemerovo State University `valerperminov@gmail.com`	Russia
Podhaisky, Helmut	Martin Luther University Halle `helmut.podhaisky@mathematik.uni-halle.de`	Germany
Pulch, Roland	Bergische Universität Wuppertal `pulch@math.uni-wuppertal.de`	Germany
Rang, Joachim	TU Braunschweig `j.rang@tu-bs.de`	Germany
Reich, Sebastian	Universität Potsdam `sreich@math.uni-potsdam.de`	Germany
Rezaeian, Ramezan	Islamic Azad University, Nour Branch, Iran `r.rezaeyan@gmail.com`	Iran
Rossmanith, James	Iowa State University `rossmani@iastate.edu`	USA
Rouhparvar, Hamid	Department of Mathematics, Saveh Branch, Islamic Azad University `rouhparvar59@gmail.com`	Iran
Rouhparvar, Akbar	Peymayesh Rah Abrisham Company, Qhom, Iran `a.rouhparvar@gmail.com`	Iran
Saravi, Masoud	Islamic Azad University, Nour Branch `msaravi2001@yahoo.com`	Iran
Savostianov, Igor	CWI `igor.savostianov@cwi.nl`	The Netherlands

Schierz, Tom	Martin Luther University Halle-Wittenberg `tom.schierz@mathematik.uni-halle.de`	Germany
Schiller, Hagen	Martin Luther University Halle-Wittenberg `hagen.schiller@mathematik.uni-halle.de`	Germany
Schmitt, Bernhard A.	Philipps-Universität, Marburg `schmitt@mathematik.uni-marburg.de`	Germany
Scholz, Lena	TU Berlin `lscholz@math.tu-berlin.de`	Germany
Schranz-Kirlinger, Gabriela	TU Wien `g.schranz-kirlinger@tuwien.ac.at`	Austria
Schröder, Dirk	TU Darmstadt `schroeder@mathematik.tu-darmstadt.de`	Germany
Shcherbakov, Dmitry	University of Wuppertal `shcherbakov@math.uni-wuppertal.de`	Germany
Simeon, Bernd	TU Kaiserslautern `simeon@mathematik.uni-kl.de`	Germany
Sommer, Matthias	Hans Ertel Centre for Weather Research, University of Munich `matthias.sommer@lmu.de`	Germany
Sonar, Thomas	TU Braunschweig `t.sonar@tu-bs.de`	Germany
Steinebach, Gerd	University of Applied Sciences Bonn-Rhein-Sieg `Gerd.Steinebach@h-brs.de`	Germany
Strehmel, Karl	Martin-Luther University Halle-Wittenberg `Karl.Strehmel@t-online.de`	Germany
Thalhammer, Mechthild	University of Insbruck `mechthild.thalhammer@uibk.ac.at`	Austria
Tischendorf, Caren	Inst. of Math., Humboldt University of Berlin `caren.tischendorf@math.hu-berlin.de`	Germany
Tomulik, Paweł	Warsaw University of Technology `ptomulik@meil.pw.edu.pl`	Poland
Trzaska, Zdzislaw	University of Ecology and Management `zdzislaw.trzaska@netlandia.pl`	Poland
Usman, Mustapha	Department of Mathematical Sciences Olabisi Onabanjo University Ago Iwoye Nigeria `usmanma@yahoo.com`	Nigeria
Valášek, Michael	CTU in Prague `michael.valasek@fs.cvut.cz`	Czech Republic

van Brummelen, Harald	Eindhoven University of Technology `e.h.v.brummelen@tue.nl`	The Netherlands
Vandewalle, Stefan	KU Leuven - University of Leuven `Stefan.Vandewalle@cs.kuleuven.be`	Belgium
Vu, Linh	Vietnam National University Hanoi `linhvh@vnu.edu.vn`	Vietnam
Vu Thai, Luan	Department of Mathematics, University of Innsbruck `vu.thai-luan@uibk.ac.at`	Austria
Wandelt, Michele	Bergische Universität Wuppertal `wandelt@uni-wuppertal.de`	Germany
Weber, Steffen	Martin-Luther-University Halle-Wittenberg `steffen.weber@mathematik.uni-halle.de`	Germany
Weiner, Rüdiger	University of Halle `weiner@mathematik.uni-halle.de`	Germany
Weiß, Daniel	University of Tübingen `weiss@na.uni-tuebingen.de`	Germany
Wensch, Jörg	TU Dresden `joerg.wensch@tu-dresden.de`	Germany
Wolke, Ralf	Leibniz Institute for Tropospheric Research `wolke@tropos.de`	Germany
Zakharov, Alexander	National Research Center `zakharov@kiae.ru`	Russia
Zegeling, Paul Andries	Utrecht University `P.A.Zegeling@uu.nl`	The Netherlands
Zhuk, Sergiy	IBM Research `sergiy.zhuk@ie.ibm.com`	Ireland

List of Speakers