The seminar NUMDIFF–11 is jointly organized by the *Institute of Mathematics, Martin Luther University Halle–Wittenberg*, and the *Center for Mathematics and Computer Science* (CWI) in Amsterdam.

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- Martin Arnold (Halle)
- Rüdiger Weiner (Halle)
- Ben P. Sommeijer (Amsterdam)
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We are indebted to the *Martin Luther University Halle–Wittenberg* for making available various university facilities throughout the conference week.

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1 General Information

1. **Conference Location and Lecture Rooms**
   The conference will take place in the lecture rooms of the Computer Science Building situated on the von-Seckendorff-Platz 1. There is a sufficiently large number of free parking places available.

   Opening of the seminar as well as plenary lectures take place in lecture room 3.28.

2. **Conference Office and Registration**
   The conference office is open on Sunday, September 3, 2006 from 4 p.m. to 8 p.m. in the lobby of the Intercity Hotel Halle-Neustadt.

   On the other days it is situated in the Institute of Computer Science in room 1.18, von-Seckendorff-Platz 1. It is open on Monday, Tuesday and Thursday from 8 a.m. to 4 p.m., and on Wednesday and Friday from 8 a.m. to 12 a.m. You can reach the conference office by phone (+49 (345) 5524799) and by fax (+49 (345) 5527004). These lines are active from Monday, September 4, 2006.

   Please register at the conference office after your arrival. There you will also receive your conference documents.

   Participants who did not use the bank transfer pay the conference fee in cash at the conference office. Please note that we cannot accept credit cards or cheques.

3. **Time of Lectures and Discussion**
   Please note that the lecture times as given in the programme already include 5 minutes for discussion.

4. **Coffee and Tea Breaks**
   Coffee and tea are provided during the morning and afternoon breaks.

5. **Lunch Break**
   The *Mensa Weinberg* is a 15 minute walk away. Please ask local participants or the staff in the conference office for further information. A cafeteria is located at the ground floor of the Computer Science building.

6. **E-mail**
   Computers for internet access are available in room 3.03.

7. **Conference Dinner**
   The conference dinner will be held in the Intercity Hotel Halle–Neustadt on Thursday, September 7, 2006 at 7 p.m. One dinner ticket is included in the conference fee; accompanying persons pay EUR 30. The fee for the dinner is payable in cash when registering in the conference office.

8. **Guided Tour on Wednesday afternoon**
   You are invited to an excursion to the town of Freyburg on the banks of the river Unstrut on Wednesday, September 6, 2006 (included in the conference fee). Buses are leaving from the conference venue at 1 p.m. and return to Halle at 7 p.m. On our tour to Freyburg we will visit the Rotkäppchen Sektkellerei and taste the locally produced sparkling wine. You will also have the chance to visit some of the other attractions in Freyburg or walk along the river Unstrut to enjoy the beautiful scenery. Please register at the conference office if you are interested.

9. **Conference Proceedings**
   Selected papers will be published in a Special Issue of the Journal *Applied Numerical Mathematics*. Guest editors are M. Arnold, B.P. Sommeijer, J.G. Verwer and R. Weiner.

   Submitted conference papers must deal with original work not published elsewhere and will be refereed according to the standard journal procedure.
   See `http://www.elsevier.com/locate/apnum` for the statement of objectives and instructions for the authors.

   Papers should be submitted electronically (in pdf or ps format) directly to

   B.P.Sommeijer@cwi.nl

   The deadline for submission is December 1, 2006.

   Authors are encouraged to use the journal style files, see the given web address for instructions. The paper length is restricted to 20 style file pages.

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4 Abstracts

Efficient coupling of micro-macro methods for hierarchical multiscale modeling
Assyr Abdulle
(School of Mathematics, University of Edinburgh, United Kingdom)

Hierarchical multiscale methods based on micro-to-macro approaches have become increasingly popular in multiscale modeling and simulation.
The global behavior of such methods depends on the hierarchy of solvers and on the strategy to couple them. The challenge is thus to couple methods which have the desired properties at the macro level and capable of sampling the microstructure with enough precision at the micro level.
In this talk we will discuss these issues. For finite element methods constructed within the framework of the heterogeneous multiscale method (HMM), we propose a new micro-to-macro approach with robust convergence rates and that is of almost linear complexity in the macro degrees of freedom.

Symmetric Boundary Value Methods for Second Order Initial and Boundary Value Problems
Pierluigi Amodio, Felice Iavernaro
(Dipartimento di Matematica, Università di Bari, Italy)

We introduce symmetric Boundary Value Methods for the solution of second order initial and boundary value problems (in particular Hamiltonian problems). We study the conditioning of the methods and link it to the boundary loci of the roots of the associated characteristic polynomial.
One application will regard the analysis of systems admitting periodic solutions generated by the superposition of both high and low frequencies. The aim is that of exploiting the good stability properties of the symmetric methods to define an efficient filtering procedure (set up by the method itself) in order to cancel out high frequencies (here understood as noise) and correctly reproduce the remaining part of the spectrum.

On the stability of a splitting method for integro-differential equations
Adérito Araújo, J. A. Ferreira
(University of Coimbra, Portugal)

The classical convection-diffusion-reaction equation has the unphysical property that if a sudden change in the dependent variable is made at any point, it will be felt instantly everywhere. These phenomena violate the principle of causality.
Over the years, several authors have proposed modifications in an effort to overcome the propagation speed defect. The purpuse of this talk is to study a modification to the classical model that take in to account the memory effects. Besides the finite speed of propagation, we establish an energy estimate to the exact solution. We also present a numerical method that have the same qualitative property of the exact solution. Finally we ilustrate the theory with some numerical results.

High-order time integration and discontinuities in the right hand side
Martin Arnold
(Martin Luther University Halle-Wittenberg, Germany)

The classical convergence analysis of high-order ODE and DAE time integration methods is based on smoothness assumptions on the right hand side that are often violated in practical applications because of look-up tables, spline interpolation of input data, ... Typically, the numerically observed order of convergence for systems with discontinuities in (derivatives of) the right hand side is, however, substantially larger than the one that is predicted by theory.
In the paper, this problem is studied for differential equations containing polynomial splines. From a practical viewpoint, the most important special cases are linear C^0 splines (spline order $2z+2=2$ with $z=0$) and cubic C^2 splines (spline order $2z+2=4$ with $z=1$).
Classical convergence results for a p-th order method predict an error of size $\mathcal{O}(h^{\tilde{p}})$ with $\tilde{p}=1$ if the right hand side of an ODE or of the differential part of a DAE contains a C^0 spline. In the case of C^2 splines a similar estimate with $\tilde{p}=\min(p,2z)=\min(p,2)$ is obtained. In the paper, a more detailed error analysis is presented that takes into account uniform error estimates for interpolating polynomial splines. An error estimate $\mathcal{O}(h^{\tilde{p}})$ with $\tilde{p}=\min(p,2z+2)$ is proven that improves the classical error bound by a factor of h^2. Similar improvements of classical error bounds are obtained for DAEs up to index 3 containing polynomial splines in their algebraic part. The improved error estimates are in perfect agreement with numerical test results for a benchmark problem from vehicle dynamics.

An alternating direction scheme for the resolution of the non-linear two-dimensional Richards' equation on irregular grids
Andrés Arrarás, L. Portero, J.C. Jorge
(Universidad Pública de Navarra, Spain)

This work is devoted to the study of a new efficient time integrator for simulating two-dimensional isothermal Darcian flows through isotropic and homogeneous porous media. Such phenomena are modelled by a strongly non-linear parabolic partial differential equation (Richards' equation) of the following form:

$$\frac{\partial\theta(\psi)}{\partial t}=\nabla\cdot\left[K(\psi)\nabla\psi(\mathbf{x},t)\right]+\frac{\partial K(\psi)}{\partial z}-S(\psi), \tag{1}$$

where $\psi\equiv\psi(\mathbf{x},t)\,[L]$ is the pressure head, $\theta(\psi)\,[L^2L^{-2}]$ is the volumetric moisture content, $K(\psi)\,[LT^{-1}]$ $(K(\psi)\geq K_0>0)$ denotes the unsaturated hydraulic conductivity, $S(\psi)\,[T^{-1}]$ is a source/sink term (for example, the root water uptake function in soil profiles), $t\,[T]$ is time and $\mathbf{x}\equiv(x,z)\,[L]$ represents the vector of spatial dimensions (see [1]). Suitable initial and boundary conditions are also added.

Concretely, we consider a modified fractionary implicit Euler method for discretizing the time variable, which is combined with a generalized finite difference spatial discretization to deduce the numerical algorithm. As we are dealing with irregular spatial domains, the approximation of the differential operator makes use of logical rectangular grids and stencils which contain nine points (see [2]). The scope of this work is to prove that it is possible to get an unconditionally convergent scheme of alternating direction type. For doing this, we decompose the difference operator in three terms: two of them will have a three-point stencil (in the same way as in the classical ADI schemes), acting in implicit mode, and the third one, which will be treated explicitly, will contain

the coefficients of the stencil corners. In this framework, the calculation of each internal stage is reduced to the resolution of simple sets of tridiagonal linear systems, after the application of an iterative procedure for solving the non-linear systems of equations. Moreover, differing from the classical fractionary implicit Euler discretizations, the source/sink term will also be treated as an explicit term, in order to improve the convergence rate of the iterative procedure previously mentioned (see [1]).

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Moving-Grid Galerkin Methods for Structured Multiscale Models of Biological Systems

Bruce P. Ayati
(Southern Methodist University, USA)

We present methods for continuous models of biological systems where the transport in a variable representing age is computed by the movement of the age grid. Approximation error is the only meaningful source of error in age, resulting in superconvergence properties for the methods. We discuss the role of this computational method for systems with dependence on age, space and time, and provide an overview of the convergence results to date. We close by presenting example computations for Proteus mirabilis swarm colony development, and, if time permits, biofilm growth.

Integro-differential model of percutaneous drug absortion

Silvia Barbeiro, J.A.Ferreira
(University of Coimbra, Portugal)

In this talk we propose a model for percutaneous absorption of a drug which consists in integro-differential equations with appropriate initial and boundary conditions. We study the qualitative properties of the model and its numerical approximation. Simulation of described numerical methods is carried out with various values of the parameters.

PDAE Models and Multirate in Chip-Design: Modeling and Simulation

Andreas Bartel, Michael Striebel and Michael Günther
(University of Wuppertal, Applied Mathematics, Germany)

Commonly, electric circuits are described by systems of time-dependent differential-algebraic equations (DAEs). The effect of down-scaling renders secondary effects more and more important. There are, for instance, thermal-conduction, transmission line phenomena or complex semiconductor behavior. Here more sophisticated models enrich the DAE by spatial systems, which results in a partial differential-algebraic equation (PDAE) depending on both space and time. Both DAE and PDAE exhibit a very strong and pronounced multiscale behavior. Thus, an efficient simulation technique will demand to design a dedicated algorithm to these systems.

Ideally, for heat conduction, only a fast and a slow subsystem exists (on the coarse scale). These can be quasi-decoupled over a communication step. Whereas in the view of a pure circuit, we have not only latent and active variables, but also several levels of activity in between. So we would like to have a kind of distributed time integration scheme. Based on Rosenbrock-Wanner methods an algorithm of a hierachical multirate scheme was developed to allow for a simple generalization to more than two time scales.
In this talk, we discuss the PDAE-setups in chip-design and their properties. Furthermore we give an overview of current developments of multirate methods in this field and we will present and discuss simulation results for the hierachical one-step scheme.

Simulation and Optimization of Partial Differential-Algebraic Equations with a Separation of Time Scales

Paul Barton, Benoit Chachuat
(MIT, USA)

Problems that exhibit multiple time scales arise frequently in many scientific and engineering fields. The modeling and simulation of such systems leads naturally to singular perturbation models. For systems of partial differential-algebraic equations (PDAEs) in time and one spatial dimension, the corresponding quasi-steady-state models yields a reduced set of PDAEs (slow variables), subject to a set of differential-algebraic equations (DAEs) in the spatial dimension (fast variables).
In this presentation, we shall consider a particular class of one-dimensional, quasi-linear PDAEs with a separation of time scales such that (i) the slow variables are lumped (i.e., do not depend on the spatial dimension), and (ii) the hyperbolic variables in the fast subsystem have all their characteristics pointing in the same direction. Under these conditions, the quasi-steady-state model yields two decoupled subsystems, a set of DAEs in time, subject to a set of DAEs in the spatial dimension; hence the name *DAEs embedded DAEs*.
There are several advantages in using the DAEs embedded DAEs approach over the conventional method of lines (MOL) for such problems. First and foremost, this approach guarantees the accuracy of the solution, in the limit of the slow model approximation validity, since rigorous error control can be performed by numerical solvers regarding the time and space steps used in either set of differential equations. This removes the need of choosing a somewhat arbitrary discretization as it is the case with the MOL. Furthermore, the DAEs embedded DAEs approach requires solution of much smaller sets of differential equations than with the MOL approach. Therefore, not only does the proposed approach improve the reliability of the simulations by removing the need of initializing large sets of DAEs, but it also typically outperforms the conventional MOL in terms of computational time whenever the use of fine meshes becomes necessary. This also makes the DAEs embedded DAEs simulation approach particularly well suited for embedding within a mathematical programming formulation for optimization purposes.
The developed approach shall be demonstrated on an application related to the start-up simulation and optimizaton of micro-scale chemical processes for portable power generation.

Implicit TSRK methods of order three and their continuous extensions
Zbigniew Bartoszewski
(Gdansk University of Technology, Poland)

In the talk the construction of implicit two-step Runge-Kutta methods and their continuous extensions that preserve the order of the original TSRK methods will be presented. Similar explicit TSRK methods recently constructed by Z. Bartoszewski and Z. Jackiewicz TSRK are based on approximations to the scaled derivatives of the solution up to the order 3 (Nordsieck vector) and have proved to be quite efficient and robust. The results of the numerical tests of their implicit counterparts carried out on stiff ODEs and DDEs will also be presented in the talk.

Numerical Integration of Field-Circuit Coupled Magnetoquasistatic Simulation with Switching Elements
Galina Benderskaya, Herbert De Gersem, Thomas Weiland
(TU Darmstadt, Institut für Theorie Elektromagnetischer Felder (TEMF), Germany)

The 3D transient field-circuit coupled formulation with the switching elements discretized by the Finite Integration Technique (FIT) represents a system of differential-algebraic equations (DAE) of index 1 and can be solved by any suitable DAE integrator. Standard numerical integration algorithms for DAE systems always assume that the variables being integrated as well as their derivatives stay continuous during the whole simulation time. Mentioned coupled system, however, exhibits hybrid (continuous/discrete) behavior due to the presence of switching elements in the circuit part of the model. The discontinuity handling algorithm presented here consists of three steps: event detection, event location and determination of consistent initial conditions. For the last step, a special technique is proposed by which highly transient phenomena at the circuit side are only resolved by the circuit model avoiding unnecessary evaluations of the field problem.

Recent developments in the time integration of the Maxwell equations
Mike Botchev
(University of Twente, The Netherlands)

The Maxwell equations are used in the modeling of a vast range of electromagnetic phenomena and comprise a class of partial differential equations which can have different properties. Ideally, a choice of a method for the numerical solution of the Maxwell equations should be determined by the properties of the equations for a particular case. It is therefore no surprise that numerics used for time integration of the Maxwell equations is a versatile family of methods based on various ideas and approaches.
In this talk we try to digest some recent developments in the time integration of the Maxwell equations, with an emphasis on high-order methods, symplectic methods and methods involving matrix functions.

Multipliers and the nonlinear stability of linear multistep methods
Bruce Boutelje
(University of Bath, United Kingdom)

The analysis of the stability of A-stable multistep methods for solving nonlinear stiff systems has long been understood. Unfortunately, Dahlquist's second barrier restricts the order of these methods to 2. To analyse the nonlinear stability of higher-order $\mathrm{A}(\alpha)$-stable methods, Nevanlinna & Odeh (1981) imported the idea of multipliers from control theory. We re-examine this work, paying particular attention to the restrictions on the nonlinearity. Results similar to those of Nevanlinna

and Odeh are recovered using a new approach, depending upon $\mathcal{Z}$-transform and convolution methods from control theory. Multipliers are constructed to obtain new stability results, under suitable restrictions on the nonlinearity.

A fourth-order implicit scheme for the two-dimensional sine-Gordon equation
Athanassios Bratsos
(Technological Educational Institution (T.E.I.) of Athens, Greece)

The two-dimensional sine-Gordon (SG) equation is given by

$$u_{tt} = u_{xx} + u_{yy} - \phi\,(x, y) \sin u$$

with $u = u\,(x, y, t)$ in an appropriate region Ω for $t > 0$. A rational approximant of order 4, which is applied to a three-time level recurrence relation, is used to transform the SG equation into a second-order initial-value problem. To avoid solving the resulting nonlinear system an appropriate predictor-corrector (P-C) scheme, in which the predictor is of order 2, is applied. The behavior of the proposed P-C scheme is tested numerically to line and ring solitons known from the bibliography, regarding SG equation and conclusions for both the undamped and the damped problem are derived.
Acknowledgment This research was co-funded 75% by E.E. and 25% by the Greek Government under the framework of the Education and Initial Vocational Training Program - Archimedes, Technological Educational Institution (T.E.I.) of Athens project "*Computational Methods for Applied Technological Problems*".

Discretization of Elliptic Control Problems
Nils Bräutigam, Walter Alt
(Friedrich-Schiller-University Jena, Germany)

We consider linear-quadratic problems of optimal control with an elliptic state equation and control constraints. After a few results of theoretical character we discretize the restriction and the control with the method of Finite Differences. Based on this discretization we develop error estimates for the solution of the discret problem und further we find a feasible control $\tilde{u}$ with

$$\|\bar{u} - \tilde{u}\|_\infty \leq c\, V_0^T \dot{\bar{u}}\, h^2,$$

where $\bar{u}$ stands for the optimal control und c is a constant independent from $\bar{u}$ and h.

Blended Implicit Methods: Theory and Numerics
Luigi Brugnano, Cecilia Magherini
(Universita degli Studi, Firenze, Italy)

The use of implicit numerical methods is mandatory when solving general stiff ODE/DAE problems. Their use, in turn, requires the solution of a corresponding discrete problem, which is one of the main concerns in the actual implementation of the methods. In this respect, Blended Implicit Methods [1,2,6] provide a general framework for the efficient solution of the discrete problems generated by block implicit methods. In this talk, we review the main facts concerning blended implicit methods for the numerical solution of ODE [3] and DAE [5] problems, and their extension for solving second order problems [4]. A few numerical tests obtained with the computational code `BiMD` [7], implementing a variable order-variable stepsize blended implicit method, are also reported, in order to confirm the effectiveness of the approach.

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Order and stability of general linear methods

John Butcher
(The University of Auckland, New Zealand)

The conflict between stability and order of accuracy is well-known and is exemplified by the two Dahlquist barriers as well as the Ehle and Daniel-Moore barriers. Although the famous order star theory is an ideal tool for understanding and settling questions of this type, an alternative approach, based on order arrows, is also available. Some examples of the use of order arrows in the understanding of these barriers will be discussed, with particular application to Padé and generalised Padé approximations. Consider a generalised Padé approximation defined by

$$\Phi(w,z) := P_0(z)w^r + P_1(z)w^{r-1} + \cdots + P_r(z) = 0,$$

where $\Phi(\exp(z),z) = O(z^{p+1})$ with $P(0) = 1$ and the order p is given by

$$p = \sum_{i=0}^{r}(1+n_i) - 1,$$

with $n_i = \deg(P_i)$. Of particular interest is the so-called Butcher–Chipman conjecture, which speculates that $2n_0 - p \in \{0,1,2\}$ is necessary for A-stability.

Runge-Kutta convolution quadrature methods for equations with memory: The non-analytic case

Mari Paz Calvo, E. Cuesta and C. Palencia
(Universidad de Valladolid, Spain)

Runge-Kutta methods, initially designed for the time integration of ODEs, can also be adapted to approximate convolution integrals, at least in case the kernel is sectorial [2]. This leads, in a natural way, to numerical schemes for the time integration of abstract convolution equations of the form

$$u(t) = u_0 + \int_0^t A(t-s)u(s)\,ds, \qquad t > 0.$$

In the present talk we address two main issues. First, we extend the Runge-Kutta convolution quadrature to the non-sectorial framework. Second, in the spirit of [1], we provide a representation of the numerical solution in terms of the continuous one, which allows us to derive interesting qualitative properties of the numerical solution. Numerical results are also provided.

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Optimal load changes of a fuel cell - boundary control of a PDAE

Kurt Chudej, Kati Sternberg, Hans Josef Pesch
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Molten carbonate fuel cells (MCFC) are especially well suited for stationary power plants if their process heat is used to increase their efficiency. MCFCs seem to become soon competitive compared with traditional power plants. The MCFC stationary power plant at the university hospital in Magdeburg reached a worldwide record of 30 000 hours of operation in May 2006. The dynamic behaviour of MCFCs can be modelled mathematically by a hierarchy of systems of partial differential algebraic equations (PDAE) in 1D or 2D. Integral terms appear and the nonlinear boundary conditions are given partly by a DAE system.
These large PDAE systems of dimension between roughly 10 and 30 equations are discretized by the method of lines, yielding huge dimensional DAEs.
We will present new computationally very expensive numerical results of optimal control during load changes for a 2D dynamical MCFC model. Faster load changes are especially welcome, from an economical and operational view point, if the very crucial constraints on the temperature field in the interior of the fuel cell are fulfilled.
Acknowledgement: This research was funded by the BMBF within the project *Optimierte Prozessführung von Brennstoffzellensystemen mit Methoden der Nichtlinearen Dynamik.*
We thank especially Prof. Dr.-Ing. Kai Sundmacher and Dr.-Ing. Peter Heidebrecht (University of Magdeburg / Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg) and Dipl.-Ing. J. Berndt and Dipl.-Ing. M. Koch (IPF Heizkraftwerksbetriebsges. mbH Magdeburg) for their support.
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Continuous Extension of Stochastic Runge-Kutta methods for the Weak Approximation of SDEs

Kristian Debrabant, Andreas Rößler
(TU Darmstadt, FB Mathematik, Germany)

To obtain the solution of an ordinary differential equation at prescribed dense output points, one can use the well-known class of continuous Runge-Kutta methods. In our talk, we extend this idea to a class of stochastic Runge-Kutta methods for the approximation of Itô stochastic differential equations with respect to a multi-dimensional Wiener process.

Advances in Unconditionally Stable Techniques

Hans De Raedt
(University of Groningen, The Netherlands)

We review recent progress in the development of unconditionally stable FDTD algorithms to solve Maxwell's equations. We present a general, unified framework that facilitates the construction of FDTD algorithms (including the Yee algorithm) with specific properties. The approach is constructive and modular: It is a recipe for constructing unconditionally stable algorithms that are tuned to particular problems and that can be combined with other unconditionally stable algorithms to solve more complicated problems. We also review recent progress in the development of one-step algorithms, based on Chebyshev and Faber polynomials, for solving Maxwell's equations.

A fully Lagrangian constrained hydrostatic method for atmospheric flows

Svetlana Dubinkina, J. E. Frank, J. G. Verwer
(CWI, Netherlands)

The hydrostatic primitive equations of motion, which have been used in large-scale weather prediction over the last decades, are considered within a Lagrangian framework. This model is discretized by extending the Hamiltonian Particle-Mesh method of Gottwald et al. (2002), in which the particles represent large masses of fluid. The new model is a 2D hydrostatic one full ideal fluid equations in potential temperature function formulation, such that the particle motion is constrained to preserve a hydrostatic state. The spatial truncation is (at least locally) Hamiltonian, making integration with a symplectic method appropriate. A code for studying the air flow in the atmosphere was made and successfully tested for a two-dimensional problem.

Memory effects and random walks in reaction-transport systems

José Ferreira, P. Oliveira
(University of Coimbra, Portugal)

In this paper we study continuous and discrete models to describe reaction transport systems with memory and long range interaction. In these models the transport process is described by a non Brownian random walk model and the memory is induced by a waiting time distribution of the gamma type. Numerical results illustrating the behavior of the solution of discrete models are also included.

Local conservation and multisymplectic discretizations for Hamiltonian PDEs

Jason Frank, S. Reich, B. Moore
(CWI, Amsterdam, The Netherlands)

Many Hamiltonian PDEs can be given a space-time multi-Hamiltonian structure, as proposed by Bridges [1, 2], among others. The formal structure is

$$J\mathbf{u}_t + K\mathbf{u}_x = \nabla_{\mathbf{u}} S(\mathbf{u}), \tag{1}$$

where J and K are constant, skew-symmetric matrices. Some examples of PDEs that can be cast in this form are classical soliton equations such as the Korteweg-de Vries, nonlinear Schrödinger, and sine-Gordon equations; Maxwell's equations and ideal fluids.

When $S(\mathbf{u})$ is independent of t and/or x, Noether's theorem applied to (1) yields local conservation laws of energy and/or momentum. The above formalism gives easy access to these conservation laws, as noted by Bridges in [1].

Multisymplectic discretizations for (1) as introduced by Reich [3] are constructed by applying symplectic one-step methods to both space and time derivatives. For semi-discretizations, Noether's theorem still implies retention of local conservation laws associated with the *non*discretized coordinates (i.e. spatial semi-discretizations still possess semi-discrete energy conservation laws, etc.) Furthermore, for Gauss-Legendre space-time discretizations of *linear* PDEs, where the conserved densities and fluxes are quadratic, fully discrete energy-momentum conservation laws are admitted.

A question that has been asked before in various contexts is, what is the significance of *local* conservation for numerical discretizations? Is this more than just bookkeeping for conservation of the global quantity? Although we will not attempt to answer this question, some benefits are conceivable: local conservation may be useful in cases where, due to boundary conditions, global conservation fails to hold. Furthermore, locally conservative methods allow construction of conservative schemes on nonuniform grids through a building-block approach.

Recently [4], we have shown that the Gauss-Legendre methods, besides satisfying a local energy conservation law for linear PDEs, also enforce the correct *direction* of energy flow, through preservation of the sign of group velocity. This is certainly also a local property, and it is a necessary condition for the avoidance of internally reflected waves by GL space-time discretizations on nonuniform grids. Methods with this property are necessarily implicit [5].

When $S = S(\mathbf{u}, x, t)$ in (1), neither energy nor momentum is conserved. However, if the dependence on x and t is 'slow' compared to the active frequency/wave number in the solution, the idea of an adiabatic invariant can be generalized to yield a local conservation law of *wave action*, related to translation invariance with respect to phase for the phase-averaged system. Numerical experiments suggest the long time conservation of the total action [6, 7].

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Multi-level Boundary Meshless Techniques

Csaba Gáspár
(Széchenyi István University, Department of Mathematics, Hungary)

The method of radial basis functions is an excellent tool for solving interpolation problems as well as creating meshless methods for various types of partial differential equations. However, it produces large, dense and often severely ill-conditioned systems of linear equations, which causes computational difficulties. This remains the case even if a boundary version of the method is applied. In this talk, the method of radial basis functions is applied in an indirect way by using the direct multi-elliptic interpolation method. Here the interpolation function is created by solving an (at least) fourth order multi-elliptic partial differential equation supplied with the interpolation conditions as a special boundary condition. In practice, this can be performed by applying quadtree/octtree subdivision and multi-level techniques, which results in a robust and computationally stable procedure. However, if the boundary is discretized by relatively few points, this approach fails to work correctly, since it produces boundary singularities. To avoid this phenomenon, the idea of local schemes is applied. Instead of the use of local interpolation based on radial basis functions, however, global interpolation is used based on the direct multi-elliptic interpolation method. This procedure results in re-globalized schemes, the computational cost of which is far less than that of the traditional radial basis function approach. At the same time, the use of large, dense and ill-conditioned matrices are also avoided. The technique becomes especially simple in case of boundary problems, and, in contrast to some previous methods, contains no scaling parameter to be optimized. Numerical examples are also presented.

Stable Iterative Operator-Splitting Methods for Stiff-Problems of Parabolic Equations: Theory and Applications

Jürgen Geiser, István Faragó
(Humboldt-University, Department of Mathematics, Berlin, Germany)

In this paper we present a modified method of the iterative splitting methods, see [1]. We discuss the consistency and stability analysis for the method and present the prestepping and weighting methods, see [2] and [3]. We analyze the local splitting error of the method. Numerical examples are given in order to demonstrate the method.

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A Nonsmooth Newton's Method for DAE Optimal Control Problems
Matthias Gerdts
(University of Hamburg, Germany)

We investigate a nonsmooth Newton's method for the numerical solution of Index-2 DAE optimal control problems subject to mixed control-state constraints. The necessary conditions are stated in terms of a local minimum principle. By use of the Fischer-Burmeister function the local minimum principle is transformed into an equivalent nonlinear and nonsmooth equation in appropriate Banach spaces. This nonlinear and nonsmooth equation is solved by a nonsmooth Newton's method. We prove the global convergence and the locally quadratic convergence under certain regularity conditions. The globalized method is based on the minimization of the squared residual norm.

FE time-stepping using high-order two-step PEER methods
Alf Gerisch, Jens Lang, Helmut Podhaisky, Rüdiger Weiner
(Martin-Luther-Universität Halle-Wittenberg, Germany)

Linearly-implicit two-step PEER methods are successfully applied in the numerical solution of ordinary differential and differential-algebraic equations. One of their strengths is that even high-order methods do not show order reduction in computations for stiff problems. With this property, PEER methods commend themselves as time-stepping schemes in Finite Element calculations for time-dependent partial differential equations (PDEs).
We have included a class of linearly-implicit two-step PEER methods in the Finite Element software Kardos. There PDEs are solved following the Rothe method, i.e. first discretised in time, leading to linear elliptic problems in each stage of the PEER method. In this talk we describe how the PEER methods have been adapted to fit into the Finite Element framework, discuss the starting procedure of the two-step schemes and consider difficulties which arise in the time-step control.
The implementation is tested for PEER methods of orders three to five on a selection of test problems.

The normal spline method for numerical solution of linear singular differential and integral equations

Vladimir Gorbunov, V.Yu. Sviridov
(Ulyanovsk state university, Russia)

The normal spline-collocation (NS) method for linear ODEs, ADEs and integral equations [1, 2, 3] are developing for the problem

$$A(t)\dot{x}(t) + B(t)x(t) - \int_0^\infty K(t,s)x(s)ds = f(t), \quad 0 \le t < \infty,$$

with boundary conditions $x(0) = x^0,\ x(\infty) = 0$. Here $x, f \in R^n$, $A(t)$, $B(t)$, $K(t,s)$ are square n-order arbitrary degenerate matrices. The function $f(t)$ and the matrices coefficients are so smooth as it needs to guarantee appropriate smoothness of the solution $x(t)$ that exists on assumption and belongs to the Hilbert-Sobolev space $W^l_{2,n}[0,\ \infty)$ (l is integer) with norm

$$\|x\|_{l,n} = \left[\sum_{i=1}^{n}\int_0^\infty \left[(x_i(s))^2 + \left(x_i^{(l)}(s)\right)^2\right] ds\right]^{1/2}.$$

Particularly the Laplace transformation's numerical inversion, when the image is determined approximately, is considered.

The NS is based on the construction of the natural system of coordinate function that are generated by reproducing kernel of the used space and by coefficients of the equation to be solved. The problem on the infinite interval $[0, \infty)$ in frame of the NS can be reformulated on the standard segment $[0,\ 1]$ via singular time transformation $\tau = exp(-t)$. In this case a simpler polynomial type norm in $W^l_{2,n}[0,\ 1]$ [2, 3] can be used.

Results of solutions of test problems by different variants of the NS will be presented.

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Numerical Aspects of Modeling and Control of Inverted Pendulum Using Kalman Filtering, DAEs, and Energy Based Lyapunov Functions

Hannes Gruschinski, Bradley T Burchett, Richard A Layton, M. Bikdash
(Rose-Hulman Institute of Technology, Terre Haute, IN, USA)

In this paper a continuous-time extended Kalman filter (EKF) in form of a sequential state estimation technique for nonlinear DAEs is applied to a constrained class of multibody systems formulated as an index 3 Hessenberg DAE system. The filter equations are used to realize a nonlinear Lyapunov based control law which swings up the inverted pendulum. This control law depends on good estimates of non-measurable states including the Lagrangian multipliers. Then the pendulum is stabilized around its unstable equilibrium using linear state feedback. Both the inverted pendulum on the cart and on the disc (Furuta pendulum) are treated. In this talk we discuss numerical aspects of solving the state estimation equations formulated as DAEs and implementation of the control strategy.

Computational Finance - a source of tasks for numerical analysis

Michael Günther, Andreas Bartel, Cathrin van Emmerich, Christian Kahl and Kai Tappe
(Bergische Universität Wuppertal, Fachbereich Mathematik und Naturwissenschaften, Lehrstuhl für Angewandte Mathematik / Numerische Analysis, Germany)

In finance application, one often has to compute the - in some sense - fair price of a financial derivative. For plain-vanilla options and underlyings driven by the geometric Brownian motion, a simple closed solution exists: the famous Black-Scholes formula.
To accomplish this task for more realistic market models and/or exotic options, one has to combine modelling with numerical and stochastic analysis tools. We will review this approach by inspecting different examples which ask for more sophisticated numerical techniques: from pricing Bermudan interest rate derivatives, hedging basket risks in incomplete markets to simulating numerically stochastic volatility models.
This work has been partially funded by ABN AMRO London, UK, NRW Bank Düsseldorf and Sparkasse Leverkusen, both Germany.

A Numerical Model for Diffusion and Reaction in Cells via Homogenization

Michael Hanke, Donald O. Besong, Kristian Dreij, Ralf Morgenstern, Bengt Jernström
(Royal Institute of Technology, Sweden)

When mammalian cells are exposed to foreign and potentially harmful compounds a series of events takes place. Following uptake the substance is distributed in different intracellular compartments by diffusion, absortion and desorption. The majority of the compound is either dissolved in the aqeous phase, the cytoplasm, or in the lipophilic phase, the membranes. Parallel to diffusion and absorption/dissorption bioactivation/biotransformation by different soluble and membrane bound enzymes takes place.
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. If these structures are treated as separate subdomains, any model becomes computationally very expensive. Moreover, due to the natural variations in the cell structures, every individual cell needs its own mathematial model. In order to make the system numerically treatable while at the same time retaining the essential features of the metabolism under consideration, we will develop a way of homogenizing the cytoplasm, aiming at a manageable system of reaction-diffusion equations for the various species.

Symplectic General Linear Methods
Laura Hewitt, Adrian T. Hill
(University of Bath, United Kingdom)

For many applications, a numerical method for the solution of ODEs should ideally be algebraically stable. For general linear methods this is equivalent to a certain matrix $M(G)$ being positive semi-definite; a complicated criterion to work with when searching for methods.
It is conjectured that non-trivial general linear methods cannot be symplectic, however they may be G-symplectic; i.e. $M(G) = 0$. This is simpler to work with than $M(G)$ positive semi-definite and trivially implies algebraic stability. Using the G-symplectic condition in the case $s = r = 2$ and the order equations, we derive our method in terms of systems of equations. We find diagonally implicit general linear methods up to and including total order four, stage order three.

Algebraically stable general linear methods
Adrian T. Hill
(University of Bath, United Kingdom)

Butcher's 1987 BIT paper on nonlinear stability is rich in original and significant insights into the structure of general linear methods. We explore some of the consequences of this extraordinary but neglected paper. New easily testable criteria for algebraic stability are derived, and we discuss the construction of efficient higher order algebraically stable methods.

A Krylov subspace splitting method for the time integration of the Maxwell equations
Róbert Horváth, István Faragó, Mike Botchev
(University of West-Hungary, Hungary)

For the time integration of the Maxwell equations discretized in space with finite differences or finite elements, we analyze several operator splitting schemes where some of the split steps can be done exactly in time, without numerical error. This can be achieved, for example, by employing exponential time integration schemes. Presented analysis and numerical experiments illustrate circumstances under which the proposed scheme appear to be a very efficient tool for time integration of the Maxwell equations.

Unified approach to proving qualitative properties of Runge-Kutta methods with applications
Zoltán Horváth
(Széchenyi István University, Hungary)

In this lecture we consider Runge-Kutta approximations to solutions of IVPs for ODEs, which arise typically from semidiscretization of time dependent PDE problems modeling some physical, chemical, biological processes, e.g. diffusion, linear and nonlinear transport, population dynamics. The focus is on examining whether the discrete version of qualitative properties of the IVP such as positivity, monotonicity, contractivity, boundedness, TVB property were preserved by the RK approximations. We note that the presence of these properties often permits an elegant and powerful analysis of the continuous and discrete time problems both. Moreover, in the talk we shall demonstrate by computational experiments to different type of problems (diffusion-reaction equations, Euler equations of gas dynamics) that violating these qualitative properties may cause break-down of the code.
In this talk we present a unified formulation of the examination of different qualitative properties in terms of dynamical systems with investigating forward invariance of or generalized monotonicity

w.r.t. suitable convex, closed sets. As one of the main result we formulate simple, explicit formulas for the time step size of the RK discretizations under which the examined discrete qualitative property is preserved. Finally, we show how these results apply in the analysis of long term behaviour of population dynamics and computational experiments of some applied problems as well.

A Reliable Adomian Decomposition Method for Ordinary Differential Equations
Mohammad Mahdi Hosseini
(Department of Mathematics, Yazd University, Iran)

In recent years, the studies of initial value problems in the second order ordinary differential equations (ODEs) have attracted the attention of many mathematicians and physicists. A large amount of literature developed concerning Adomian decomposition method, and the related modification to investigate various scientific models. Here, it is attempt to introduce a new reliable modification of Adomian decomposition method. For this reason, a new differential operator is proposed which can be used for singular and nonsingular ODEs. In addition, the proposed method is tested for some examples and the obtained results show the advantage using this method.

Deterministic models of chemical reactions coupled to stochastic reaction kinetics for efficient simulation of cellular systems
Wilhelm Huisinga, A. Alfonsi, E. Cances, G. Turinici, B. Di Ventura
(DFG-Forschungszentrum MATHEON und Freie Universität Berlin, Germany)

When analyzing metabolic networks involving large numbers of molecules, the deterministic model for chemical reaction systems based on the law of mass action has been quite successfully applied in mathematical biology. In the past years, however, it has become evident that in regulatory networks, where often some chemical species are present at very low numbers, stochastic effects play an important role, leading to an increasing in stochastic modelling attempts. When aiming at a thorough investigation of cellular processes involving gene-regulatory networks, signalling pathways and metabolic networks, the question arises how to efficiently and accurately simulate such coupled system.
We present an adaptive and efficient approach for the simulation of hybrid stochastic and deterministic reaction systems. Its algorithmic realization allows for adaptive step-size integration of the deterministic equations while at the same time accurately tracing the stochastic reaction events. The mathematical derivation is given and numerical examples are presented that demonstrate the power of hybrid simulations.

Numerical Simulation of Streamers
Willem Hundsdorfer
(CWI, The Netherlands)

Streamers are conduction channels that are rapidly formed in an isolating medium (e.g. air) under influence of an electric field. When the conducting channel bridges the gap between objects with different charges, an electric discharge follows (e.g. lightning).
The development of streamers can be described by relatively simple models, consisting of convection-diffusion-reaction equations for the densities of charged particles, together with a Poisson equation for the electric potential. The numerical solution of these coupled equations is complicated, however, due to (i) the multiscale character of the problems and (ii) instability of homogeneous states.

In this talk the numerical issues will be discussed. A local grid refinement procedure will be described, together with simulation results of streamers. This work is based on joint research with Carolynne Montijn and Ute Ebert.

Stability of ADI schemes applied to convection-diffusion equations with mixed derivative terms

Karel in't Hout, Bruno Welfert
(University of Antwerp, Belgium)

In many modern application areas, mathematical models are used that involve initial-boundary value problems for convection-diffusion equations in spatial dimensions that are greater than one. The semi-discretization of such equations leads to huge systems of stiff ordinary differential equations that cannot be solved effectively by standard implicit numerical methods, and tailored time-integration methods are required. In the past decades operator splitting schemes of the alternating direction implicit (ADI) type have proven to be a successful tool for efficiently dealing with many of these systems.
In this talk we are interested in multi-dimensional convection-diffusion problems where mixed spatial derivative terms are present. Convection-diffusion problems of this kind arise naturally in various areas, such as in financial mathematics where they appear e.g. when pricing options on a number of correlated assets. The potential use of ADI schemes for the numerical solution of such problems has not yet been explored to great extent in the literature; some promising first results were obtained by McKee & Mitchell (1970), Craig & Sneyd (1988, 1990) and McKee, Wall & Wilson (1996).
In this talk we shall consider three general ADI schemes for the time-integration of semi-discrete multi-dimensional convection-diffusion problems having mixed derivative terms. We investigate the favourable property of unconditional stability and prove that, under appropriate assumptions, all three ADI schemes share this property when applied to these problems. Our results substantially extend those from the literature mentioned above. Numerical experiments are given to illustrate the presence of unconditional stability as well as showing the actual convergence behaviour of the ADI schemes.

Dynamical low-rank approximation of the chemical master equation
Tobias Jahnke, Wilhelm Huisinga
(Freie Universität Berlin, Germany)

Biochemical reaction systems are traditionally modelled by ordinary differential equations (ODEs) representing the concentrations of the substances. The so-called reaction-rate approach, however, is inappropriate if some of the substances are present in a low number of molecules and stochastic fluctuations play an important role for the evolution. In such a situation, a more accurate model is provided by the chemical master equation, which describes the evolution of a probability density on the state space of all possible vectors of molecule numbers.
The chemical master equation can be considered as a difference-differential equation, a "discrete PDE", or as a system of ODEs. For its numerical treatment, the main difficulty is the high number of degrees of freedom. In contrast to the traditional reaction-rate approach which requires only one ODE per *substance*, the chemical master equation consists of one ODE per *state*. Even a rather small system of three species with molecule numbers varying between, say, 0 and 99, contains 100^3 states, and hence 1000000 coupled ODEs have to be solved in order to determine its probability density! As a consequence, the chemical master equation cannot be treated with standard ODE methods unless the problem is extremely small.
In this talk we present a dynamical low-rank approximation of the chemical master equation. The underlying idea is to approximate the solution on a low-dimensional manifold of ansatz functions. The approximation is propagated according to the Dirac-Frenkel-McLachlan variational principle by projecting the derivative onto the tangent space of the manifold. Similar techniques are known in the quantum chemistry community as *multiconfiguration time-dependent Hartree methods* and have been applied with great success to the solution of Schrödinger equations with many degrees of freedom. The performance of the method is demonstrated by applying it to a model problem with bimodal solution density. Moreover, we discuss advantages, drawbacks and possible extensions of the approach.

Explicit parallel two-step peer methods
Stefan Jebens, Rüdiger Weiner
(Martin-Luther-Universität Halle-Wittenberg, Germany)

The construction of explicit s-stage parallel two-step peer methods for the solution of non-stiff initial value problems is considered. In each time step s solutions are computed as approximations at the points $t_{mi} := t_m + h_m c_i$, $i = 1, \ldots, s$. For autonomous scalar equations the methods can be written in the compact form

$$Y_m = BY_{m-1} + h_m AF(Y_{m-1}).$$

In every time step the s evaluations of the right-hand side can be computed in parallel. We consider the construction of methods with optimal zero stability and order $p \geq s$. Criterions for good methods are large stability regions and small error constants. Corresponding parameter sets have been obtained using the differential evolution genetic algorithm.
A numerical comparison between peer methods with $s = 6$ stages and order $p = 6$ and $p = 7$ in a sequential implementation and ode45 in MATLAB shows the efficiency of the peer methods.

Numerical coupling of electric circuits and semiconductor devices
Ansgar Jüngel, Markus Brunk
(Universität Mainz, Germany)

Numerical simulations of highly integrated electric circuits are necessary in order to replace costly experiments and to fulfill the demands due to the technological progress in microelectronics. The high-density circuits show parasitic (for instance, thermal) effects which are usually modeled by equivalent network equations. However, this strategy becomes questionable in modern circuits and the charge transport and thermal effects in the devices need to be described by more precise models. Thermal effects in semiconductor devices can be efficiently modeled on a macroscopic level by energy-transport equations. These equations specify the electron density, the electric potential, and the electron temperature in the device. Therefore, improved models are obtained by coupling the circuit equations and the device models.
In this talk, the numerical coupling of electric circuits (modeled by standard equations from Kirchhoff's laws) and semiconductor devices (modeled by 1-D energy-transport equations) is presented. Together with the circuit equations, the coupled system becomes a system of partial-differential-algebraic equations which are discretized in time by a BDF2 method. The space discretization is performed by an exponentially fitted mixed finite-element method. Numerical examples of a high-frequency bipolar diode and a rectifier circuit consisting of four diodes show the impact of the carrier heating on the semiconductor current.

Deterministic particle methods for high dimensional Fokker-Planck equations
Michael Junk
(Universität Konstanz, Germany)

In the talk, questions are discussed which arise in the construction of Quasi-Monte-Carlo (QMC) methods for high dimensional Fokker-Planck equations. An example which illustrates the need of such methods appears in connection with the bead-spring chain representation of polymer molecules, a classical model used in the study of dynamics of polymeric liquids. The bead-spring chain typically consists of a large number of beads (e.g. 20) and thus the state space V of its configuration, which is essentially the relative position of all the constituent beads, turns out to be high dimensional (for example, dimension 57 in the case of 20 beads). The distribution function governing the configuration of a bead-spring chain undergoing shear flow is a Fokker-Planck equation on V. Classically, Monte-Carlo (MC) methods are used to solve such high dimensional problems. They do not suffer from the curse of dimension but the convergence order is quite low. In order to avoid this disadvantage of MC algorithms it is tempting to consider deterministic QMC algorithms instead because, for a certain class of plain integration problems, they are known to be superior to the MC approach. It turns out, however, that the mutual independence of pseudo random numbers plays a decisive role in MC methods for the solutions of partial differential equations with diffusive terms. Since QMC methods are based on quasi random numbers which are typically highly correlated, a direct substitution of pseudo random numbers with quasi random numbers does not work as in the case of integration problems. Instead, suitable product measures have to be constructed which eventually reduces the efficiency of the QMC approach.

Adaption of Partitioned Integration Strategies for the Simulation of Mechatronic Systems
Daniel Kanth
(Bosch Rexroth AG, Department of Simulation Technology, Germany)

The simulation of mechatronic systems leads to a set of differential or differential-algebraic equations with heterogeneous structure. Due to large differences in eigenvalues these systems are often *stiff*. Using a single integrator for the numerical time integration of stiff systems the step size has to be reduced radically to meet accuracy requirements. As an alternative approach the system can be divided into so called fast and slow subsystems. For each subsystem a specialized time integration methods is used. This approach is called *partitioned integration*.
This paper describes the concept of partitioned integration and emphasizes the advantages of this approach compared to non-partitioned integration. For that purpose two characteristic parameters are derived which represent stiffness and coupling of the system. As a first step so called *elementary systems* are introduced, which represent the smallest decomposable units of a system. If a system has fast *and* slow elementary systems it is said to be stiff. The speed of an elementary system is described by the product of a predicted step size h_{pred} and the norm of the Jacobian matrix. Additionally the numerical effort for the time integration for each elementary system is calculated with $\frac{1}{h_{pred}}$. The coupling of elementary systems is determined by the sensitivity of states. Hence all elementary systems are successively perturbed and the resulting effects in states are measured, after an explicit euler step with h_{pred} was performed. The sensitivity leads to an estimation of the expectable coupling step size H. The expectable numerical effort for automatic coupling step size control and the exchange of coupling data can be estimated with H. The expectable numerical effort of time integration and coupling data exchange leads to the determination whether partitioned integration is superior to non-partitioned integration or not.
By estimating the total numerical effort it is not only possible to determine one or more suitable integration methods but also to determine an optimal granularity for the time integration. Furthermore it is described how efficiency can be improved by using an automatic control of the coupling step size. The functionality is proved by numerical results of a mechatronic system simulation.

Numerical solution of stiff ODEs modelling chemical kinetics
Oleksiy Klymenko, I.B. Svir
(Kharkov National University of Radioelectronics, Ukraine)

Homogeneous chemical processes are described by systems of ordinary differential equations which are often stiff due to greatly differing rates of individual reactions. Special care should be taken during the numerical solution of such systems because of their nonlinearity and the requirement of positivity of the solution. The violation of the latter even within the prescribed tolerance in many cases leads to divergence of the numerical solution. In this work we solve stiff ODE systems describing complex chemical processes using two novel numerical methods the Almost Runge-Kutta method (Butcher J.C., Rattenbury N. Almost Runge-Kutta methods for stiff problems. Appl. Num. Math. 53 (2004)165-181) and the method by Aluffi-Pentini and co-authors (Aluffi-Pentini Ñ., De Fonzo V., Parisi V. A novel algorithm for the numerical integration of system of ordinary differential equations arising in chemical problems. J. Math. Chem. 33 (2003) 1-15) based on the exact solution of linearised ODEs. The performance and stability properties of the two methods are compared.

Implementation of Rosenbrock methods for compressible atmospheric models
Oswald Knoth
(Institute for Tropospspheric Research, Germany)

A new dynamical core for compressible atmospheric models is introduced and evaluated with a suite of standard test cases. The equations are discretized in space in a cartesian or longitudinal-latitudinal grid with height as the z-coordinate. Orography and other obstacles are incorporated by the cut cell approach. In time the spatially discretized equations are integrated by Rosenbrock methods with special chosen approximate Jacobian matrices. This type of approximation allows to split the solution of the linear system in two separate ones, The first linear system is of the advection-diffusion type and the second one is a positive definite Helmholtz system. Both systems are solved by special iterative methods of conjugate gradient type with suitable preconditioning. Rosenbrock methods are linearly implicit time integration methods and fall in the class of the different proposed semi implicit methods found in the literature. Therefore the time step is not restricted by sound and gravity waves. The numerical method is parallelized by nonoverlapping domain decomposition and allows different spatial resolution in different domains. Test cases include warm and cold air bubbles, flow over hills of Agnesi type and flow around buildings.

An Integrated Design Procedure for Design of Smart Structures
Alexander A. Kolpakov
(The Novosibirsk State University, Russia)

In [1] the problem of integrated design of ”smart” structures was formulated and investigated for the simple system described by ordinary differential equation. The recent analysis of the problem leads to some conclusions of general value on the structure of the ”intelligence” [2, 3].
In the present paper, in addition to the results [1-3], new problem of design of smart frameworks (the system described by a system of algebraic equations) is presented.

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The Network Models and Asymptotic of Capacity of a System of Closely-Placed Bodies
Alexander G. Kolpakov
(NGASU, Russia)

In [1, 2] it was demonstrated that boundary value problem in a domain filled with perfectly conducting disks can be approximated with a network model (a system of Kirchhoff type equations). The technique presented in [1, 2] can be used in 2-D case and for circular disks only.
In the paper a newly elaborated technique [3] of network approximation for boundary value problem in a domain filled with perfectly conducting subdomains is presented. It relates the network approximation to capacity of the perfectly conducting subdomains and can be used to analyze problems of arbitrary dimension (the problem demonstrates 2D-3D dimension sensetivity) and for subdomains of arbitrary shape.
The mathematical results are applied to analysis of transport properties of dense-packed high-contrast composites [5].

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Linear Multistep methods for quasi-singular perturbed problems
Felix Kramer
(Vienna University of Technology, Austria)

Stiff behavior occurs in a variety of ODE systems relevant in applications. The notion of stiffness is a phenomenological one, and a stability and error analysis of numerical methods has been based either on simple models or particular problem structures. In particular, stiff initial value problems in standard singular perturbation form are well understood. However, problems of this type exhibit a very simple phase space geometry, namely the stiff eigendirections also behave *stiff* in another sense, i.e., they are almost parallel. This motivates us to consider a more general nonlinear class of stiff ODE systems depending on a small parameter. In particular, we investigate the convergence properties of BDF methods applied to problems of this type, and linear multistep schemes will further be investigated.

Finite Pointset Method (FPM): Meshfree Flow Solver in Continuum Mechanics
Jörg Kuhnert
(Fraunhofer Institut Techno- und Wirtschaftsmathematik, Germany)

FPM is a young CFD tool, developed in the Fraunhofer Institute for Industrial Mathematics, Kaiserslautern. It is a meshfree approach, mainly designed to overcome several drawbacks of classical CFD methods. FPM evolved originally from classical SPH, however it developed towards a general finite difference scheme operating on non-structured point clouds. It is a Lagrangian idea, i.e. the point cloud moves with local fluid velocity. Each point carries relevant information and has to be integrated in time.
We model the incompressible Navier-Stokes equations. Here we employ Chorin's projection idea in order to maintain the incompressible character of the flow. An extension of this idea even leads to more freedom, such that compressible flows can be computed as well. The integration method is implicit in time. That relaxes the CFL-condition (i.e. upper bound for the time step size), however it requires the construction and solution of big, sparse linear systems of equations.
The biggest advantage of FPM is its easy handling of free surfaces and multiphase flows. No additional algorithms have to be employed in order to model free surfaces, as the point cloud itself describes the topology of the free boundaries. The points belonging to a free surface or an interface have to be detected and maintained at each time step.
Another advantage of FPM is its easy handling of flow problems with moving boundaries and complicated geometries. The point cloud perfectly organizes itself through the point movement.
FPM has successfully been employed in various industrial projects, most recently for applications in glass industry. Here, stirring, floating, shrinking and rolling processes are designed and

optimized using FPM. In car industry, FPM is applied for simulation of tank filling and sloshing processes. The most recent idea is to use FPM for cutting processes. Here, of course, the modeling has to be extended to visco-plastic material behavior.

Criticism of Asymptotic Global Error Expansion with a New Extrapolation Theory
Gennady Kulikov
(University of the Witwatersrand, Johannesburg, South Africa)

In this paper we discuss existence of the asymptotic global error expansion for numerical solutions obtained from general one-step methods applied to ordinary differential equations. The asymptotic global error expansion was discovered independently by Henrici, Gragg and Stetter in 1962, 1964 and 1965, respectively. It is an important theoretical background for extrapolation methods. We draw attention to some flaws in that theory and show that such an expansion is likely to fail to work in practice. Therefore we give another substantiation for extrapolation methods. The Richardson extrapolation technique is a key means to explain how extrapolation methods perform. Additionally, we prove that the Aitken-Neville algorithm works for any one-step method of an arbitrary order s under suitable smoothness.

Tractability Index = Strangeness Index +1
René Lamour, Roswitha März
(Humboldt-University of Berlin, Germany)

Once upon a time scientists from various fields tried to solve equations whose essential part consisted of an ODE. There were only a few additional algebraic constraints that would not perturb the power and accuracy of the known robust numerical ODE solution methods. That was the hope - but the hope was dashed. This happened in the late sixties of the last century.
With the observed problems like singularities, drift off, up to divergence every research group started to discover the reasons for such a behavior. They found that, in contrast to classical ODEs, we have to differentiate parts of the right-hand side of such a system of **d**ifferential plus **a**lgebraic **e**quations (DAE) to compute a solution. The quantity of how often you have to differentiate was called the index and it describes the difficulty to solve a DAE.
Every scientist has naturally used her/his scientific background in her/his investigations and, therefore, we have various schools and theories about DAEs. We have the geometric, perturbation, structural, differentiation, strangeness, tractability but also the classical Kronecker index.
We have to compare these different concepts. The easiest one should be the transformation of the (linear) DAE using the different concepts into a canonical form, but these canonical forms are different.
We will focus on a comparison of the tractability and strangeness index for regular DAEs.

The solution of singular Schrödinger problems using a piecewise perturbation method
Veerle Ledoux, M. Van Daele and G. Vanden Berghe
(Ghent University, Belgium)

The piecewise perturbation methods (or PPM in short) were specially devised and shown to be very efficient for the solution of regular Schrödinger problems

$$y''(x) = (V(x) - E)y(x) \tag{1}$$

defined on a finite integration interval $x \in [a, b]$. However many practical problems are defined on an infinite integration interval, i.e. $a = -\infty$ or $b = +\infty$. We discuss an improved truncation

algorithm based on the WKB-approximation which automatically selects good truncation points for a certain E-value. These truncation points are chosen large enough such that the solution in this points may be assumed to be zero. However, for the important class of potentials which behave like a Coulomb potential in the asymptotic region, the truncation algorithm can be improved taking into account the asymptotic form of the Coulomb equation. More precise (truncated) boundary conditions can then be constructed and this allows us to take even smaller cutoff values.
For these Coulomb-like problems another specific problem occurs: the potential is singular near the origin. To deal with this singularity a specially tuned perturbation algorithm is used in a short interval around the origin.

Fast Runge-Kutta approximation of inhomogeneous parabolic equations
María López-Fernández, Christian Lubich, César Palencia, and Achim Schädle
(University of Valladolid, Spain)

The result after N steps of an implicit Runge-Kutta time discretization of an inhomogeneous linear parabolic differential equation is computed, up to accuracy ε, by solving only

$$O\Big(\log N \, \log \frac{1}{\varepsilon}\Big)$$

linear systems of equations. The algorithm is based on a special discretization of the Cauchy integral representation of the Runge-Kutta approximation. We derive, analyse, and numerically illustrate this fast algorithm.

Dynamical low-rank approximation
Christian Lubich, O. Koch and A. Nonnenmacher
(Univ. Tübingen, Germany)

For the low rank approximation of time-dependent data matrices and of solutions to matrix differential equations, an increment-based computational approach is proposed and analyzed. In this method, the derivative is projected onto the tangent space of the manifold of rank-r matrices at the current approximation. With an appropriate decomposition of rank-r matrices and their tangent matrices, this yields nonlinear differential equations that are well-suited for numerical integration. The error analysis compares the result with the pointwise best approximation in the Frobenius norm. It is shown that the approach gives locally quasi-optimal low rank approximations. Further error bounds show the robustness of the approach with respect to the choice of the approximation rank. Numerical experiments with moving images, time-dependent term-document matrices and reaction-diffusion equations illustrate the method and the theoretical results.

Solving Partial Differential-Algebraic Equations in Structural Mechanics: Applications and Enhanced Treatment by Adaptive Mesh Refinement
Christoph Lunk, Bernd Simeon
(Technical University of Munich, Germany)

Computational mechanics and its various applications have experienced a significant development over the last decade. From the numerical analysis point of view, we deal with physical laws of subsystems, e.g. deformable bodies, described by Partial Differential Equations (PDE), which are coupled by physical constraints. Their discretizations and the treatment of constraints are one of the key issues in this problem class. In particular the coupling of time-dependent problems leads to systems of Partial Differential-Algebraic Equations (PDAEs).

In my talk I present a time integrator for this problem class, which combines the plausible scheme of the RATTLE algorithm with the benefit of variable numerical dissipation by the Generalized-α methods. Some key ideas on the convergence proof will be given. For the discretization of the time-depending PDE´s and their algebraic constraints, this scheme is applied to the method of lines and its reversed counterpart. The latter allows us to adapt the spacial mesh at each time integration step, where the step size is also variable. The challenge is the dynamic behavior of entries in the derived saddle point problems. I discuss some aspects on constraint formulations and projection techniques due to the sensitive influence of perturbation.

At the end I give some examples of systems of rigid and deformable bodies (flexible multibody systems). The simulation of pantograph with catenary dynamics demonstrates the potential of our approach. An outlook on further investigations closes the presentation.

The parametrization method for numerical solution of singular differential equations
I.V. Lutoshkin, V.K. Gorbunov
(Ulyanovsk state university, Russia)

The problem to be solved numerically is the initial one for an implicit ordinary differential equation $F(\dot{x}, x) = 0, \quad 0 \leq t \leq T, \quad x(0) = x^0$, where $x \in R^n$ and $F : R^{2n} \to R^n$, smooth transformation, in the case of arbitrary degeneracy of the Jacobi matrix $\partial F(\dot{x}(t), x(t))/\partial \dot{x}$ on the solution $x(t)$. The important particular case is the structured system of DAEs

$$\dot{x}(t) = f(x(t), u(t)), \quad g(x(t), u(t)) = 0,$$

with conditions $x(0) = x^0, \quad u(0)) = u^0$.
The PM is based on the minimization of discrepancy of appropriate differential system and approximation of "control function" $u(t)$ (in the first case $u(t) = \dot{x}(t)$) by splines with moving knots. The first and second derivatives of the discrepancy functional on the spline's parameters can be effectively calculated with help of variational techniques and adjoint variables. The corresponding experience is presented in [1, 2]. Here we present also a simpler techniques for direct approximation of all components of the solution. Comparative analytical and numerical analysis of different variants of the PM will be presented.
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Which ETD method?
Paul Matthews, Hala Ashi
(University of Nottingham, UK)

Exponential time differencing (ETD) methods were originally proposed by Certaine for nonlinear systems with a stiff linear term, and have been re-invented many times since. They generally perform better than the more well-known integrating factor methods (which have larger error constants) and linearly implicit methods (which do not handle the linear term correctly). I will discuss the circumstances under which this generalisation holds. There are many different types of ETD method, and this talk will address their merits in terms of accuracy, stability and ease of use.

Convergence analysis of thin-plate spline interpolation
Jens Markus Melenk, Armin Iske and Maike Loehndorf
(TU Wien, Austria)

Radial basis functions provide a versatile tool for scattered data interpolation. One of the basic questions is the interpolation problem: Given N data point $x_i \in \mathbb{R}^d$, $i = 1, \dots, N$, with corresponding values f_i, find the function If of the form

$$If(x) = \sum_{i=1}^{N} c_i \phi(|x - x_i|) + \pi(x)$$

such that $If(x_i) = f_i$ for $i = 1, \dots, N$. One possible choice of the function ϕ is that of polyharmonic splines, i.e., the function $x \mapsto \phi(|x|)$ is the fundamental solution of the iterated Laplacian Δ^m. The function π is a polynomial of degree $m - 1$. In the case $d = 2 = m$, the function $\phi(r) = r^2 \log r$ is called the thin-plate spline.
Existence, uniqueness, and optimal rates of convergence for quasi-uniformly distributed data points x_i were established in fundamental papers by Duchon and Meinguet. Convergence here means that the interpolation data $f_i = f(x_i)$ originate from a function $f \in H^m(\Omega)$ and the error $f - If$ is considered. We extend this classical theory to functions $f \in H^k(\Omega)$ with $k > m$. Specifically, we show that optimal convergence rates can be obtained for $f \in H^k(\Omega)$ in the range $k \in [m, m+1/2)$. Boundary effects limit the achievable convergence in the regime $k > m + 1/2$; however, we show how further improvements in the convergence rate can be obtained by condensing data points x_i near the boundary. Numerical examples corroborate the theoretical assertions.

Computing Eigenfunctions of Singular Points in Nonlinear Parametrized Two-Point BVPs
Thomas Milde
(Friedrich-Schiller-Universität Jena, Germany)

The iterative computation of singular points in parametrized nonlinear BVPs by so-called extended systems requires good starting values for the singular point itself and the accociated eigenfunction. Using path-following techniques such starting values for the singular points are generated automatically. However, path-following doesn't provide approximations for the eigenfunctions. We propose a new modification of this standard technique delivering such starting values. It is based on an extended system wich can be used for nonsingular as well as singular points.

Adaptivity in mechanical integrators
Klas Modin, Claus Führer and Gustaf Söderlind
(SKF Engineering Research Centre and Lund University, Sweden)

Mechanical integrators are numerical integration methods specifically designed for evolution equations originating from mechanical systems. Typically, the discrete flow introduced by a mechanical integrator share structural properties with the corresponding exact continuous flow, which makes its long time behavior superior to conventional numerical integrators. Examples of structure preserving properties are: reversibility; conservation of momentum maps; conservation of the symplectic form; conservation of energy. A result by Ge and Marsden (1988) asserts that if a symplectic discrete flow exactly conserves energy and momemtum, then it gives in fact the exact solution. Hence, two main branches of mechanical integrators have evolved: symplectic–momentum and energy–momentum conserving. Nevertheless it has been shown, e.g. by Hairer, Lubich and Wanner (2002), that symplectic–momentum methods acquire near conservation of first integrals such as energy.

For evolution equations with alternating dynamics it is classically more efficient to use adaptive numerical integrators with, e.g., varying time-step and/or order of accuracy. The design of adaptive mechanical integrators is non-trivial, since conventional adaptive techniques tend to destroy inherent structural properties. In particular, standard adaptive time-step selection in conjunction with symplectic–momentum methods do not maintain near conservation of first integrals. During the last decade other adaptive time-step techniques, based on dynamic time transformations, have been developed. These techniques allow the construction of variable time-step mechanical integrators.
In this talk further developments and generalizations of adaptive mechanical integrators are presented. More specifically, we show how the framework of variational integrators originating from discrete mechanics – a discrete counterpart to Lagrangian mechanics – can be extended to include integrators with general adaptive objectives. A key point of ours is to analyze adaptivity from a control theoretic point of view, where the input variables of the control system is given by discretization parameters, e.g. the time-step length, and the output variables by local state space measurements, e.g. the local integration error. The art of adaptivity then amounts to the design of suitable feedback laws.

Fractional step Runge-Kutta-Nyström methods for evolution problems of second-order in time
Maria Jesús Moreta, Blanca Bujanda, Juan Carlos Jorge
(Universidad Pública de Navarra, Spain)

As it is well-known, because of their computational advantages, Fractional Step methods are widely used in practice for solving evolutionary problems of first order in time. The application of these methods has been extended to classical second order in time problems like the wave equation. Following the main advantages of these methods, we have developed a new class of methods, called Fractional Step Runge-Kutta-Nyström methods (FSRKN), to solve numerically second-order in time evolutionary problems. As in the case of using Fractional Step Runge-Kutta, the main goal consists of reducing the computational cost of classical implicit methods for solving multidimensional problems of this type. In order to get this, we must split firstly the space differential operator as a sum of simpler operators in a certain sense. After doing this, we integrate in time using a FSRKN method subordinated to such splitting. In this way, only a piece of the splitting acts implicitly at each fractional step.
In this talk the main properties of these methods are shown, as well as the construction of a family of third-order unconditionally stable methods of this class. Finally, we present some numerical results confirming their advantages.

On Multivariate Chebyshev Polynomials; from Group Theory to Numerical Analysis
Hans Z. Munthe-Kaas
(University of Bergen, Norway)

Classical 1-D (univariate) Chebyshev polynomials are ubiquitous in numerical analysis with applications ranging from approximation theory to spectral discretizations of PDEs, signal processing and numerical linear algebra. Chebyshev polynomials have near-optimal approximation properties and enjoy fast expansions via the FFT.
The need for extending the beautiful properties of 1-D Chebyshev polynomials to several dimensions is usually accomplished by considering tensor products on separable (box-shaped) domains. Box-shaped domains are unfortunately not well suited for patching together in domain decomposition and spectral element discretizations of PDEs. There is a need for developing polynomial approximation theory on triangles and higher dimensional tetrahedra.

Multivariate families of Chebyshev polynomials can, however, also be constructed on certain non-separable domains. By applying the theory of Kaleidoscopic mirror groups (or affine Weyl groups) acting on R^n, one obtains families of Chebyshev polynomials living on domains related to triangles and tetrahedra. These were first considered by Koornwinder in 1974. There is a limited literature on the properties of these non-separable multivariate Chebyshev polynomials. However, applications in numerical analysis seem to be absent, and these polynomials are almost unknown in the numerical analysis community.
In this talk we will give an overview of the theory of multivariate Chebyshev polynomials and show how these share the beautiful properties of their univariate cousins, such as near-optimal Lebesgue constants for the interpolation error and the existence of fast transforms for expansions and (pseudo)-spectral differentiation. The goal of the talk is to show that these yield powerful tools that should be available in the toolbox of numerical analysis and scientific computing.
Finally, we will briefly mention some fast symmetry based exponential- and Lie group time integrators obtained from triangle based spectral element discretizations of PDEs.

Numerical integration of the extended plasma fluid equations with SD3 Kurganov-Levy Scheme
Richard Naidoo
(Durban Institute of Technology, South Africa)

The plasma two fluid equations were extended to include the energy equations. We then numerically integrate the new set of conservative equations by means of a recently modified third order semi-discrete scheme for hyperbolic systems due to Kurganov and Levy [SIAM J.Sci.Comp. 22, p1467, 2000]. We illustrate the formation of solitons and shock waves.

On the convergence of the Magnus series
Jitse Niesen, Per Christian Moan
(La Trobe University, Melbourne, Australia)

The solution of a linear nonautonomous differential equation can be given in terms of an infinite series called the *Magnus series*. Specifically, the solution of the equation $y' = A(t)\,y$ can be written as $y(t) = \exp(\Omega(t))\,y(0)$ where exp denotes the matrix exponential and $\Omega(t)$ is given as an infinite series. The Magnus series can be used to design numerical methods for equations of this form.
In this talk, we discuss the convergence of the infinite series for $\Omega(t)$. We mention the connection between the convergence of the infinite series and the convergence of the numerical method. Our main result is that the series converges if $\int_0^t \|A(s)\|\,\mathrm{d}t < \pi$. The constant π is sharp.

A collocation method for solving nonlinear differential equations via hybrid of rationalized Haar functions

Yadollah Ordokhani, Bahman Arabzadeh
(Department of Mathematics,Alzahra University, Iran)

Hybrid of rationalized Haar functions are developed to approximate the solution of the nonlinear differential equations.The properties of hybrid functions which are the combinations of block-pulse functions and rationalized Haar functions are first presented. These properties together with the Newton-Cotes nodes are then utilized to reduce the differential equations to the solution of algebraic equations.The method is computationally attractive,and applications are demonstrated through illustrative examples.

Recent developments in exponential integrators

Alexander Ostermann
(Universität Innsbruck, Austria)

Exponential integrators were first proposed in the 1960s for the numerical solution of stiff differential equations. They later turned out to be efficient for problems where the solution of the linearisation contains fast decaying or highly oscillatory components. In spite of the favourable properties of exponential integrators, there are still few (if any) variable stepsize implementations available in the community.
For higher-order explicit exponential Runge–Kutta methods, it turned out to be difficult to construct reliable and efficient error estimates. Moreover, in contrast to classical time integrators, exponential methods are *not invariant* under linearisation. This results in an error behaviour similar to classical W-methods. Therefore, we have to expect large errors whenever the linear part is not well chosen.
In my talk, I will address these problems. Further, I will discuss alternative approaches for a possible implementation.

On some conservation properties of symmetric methods applied to Hamiltonian systems

Brigida Pace, Felice Iavernaro, Donato Trigiante
(Dipartimento di Matematica, Università di Bari, ITALY)

The use of symmetric schemes has revealed interesting stability properties for the long time simulation of conservative, and in particular Hamiltonian systems. Although in general these methods fail to preserve the energy function and/or the symplecticity property proper of the continuous (Hamiltonian) problem, in many interesting situations, they however display a behavior which is qualitatively close to both symplectic and energy preserving methods. We use a new approach based upon the definitions of *discrete line integral* and *state dependent symplecticity* to specify the terms of such closeness.

A numerical solution of conjugate problem of forest fire initiation

Valeriy Perminov
(Belovo Branch of Kemerovo State University, Russia)

A mathematical model for the description of heat and mass transfer processes at crown forest fire initiation and spread has been designed. Turbulent heat and mass transfer in the forest crown, as well as heat and mass exchange between the near-ground layer of atmosphere and the forest canopy are incorporated in a so-called conjugate formulation. The latter manages to take into consideration the mutual effects of the forest canopy and the atmosphere during forest fires the most accurately.

Based on the model of forest fires, the problems of crown forest fire initiation and spread are studied with due consideration for the effect of a turbulent atmosphere and the actual structure of the forest biogeocenosis. The boundary value problem was solved numerically using the method of splitting according to physical processes. A discrete analog for the system of equations was obtained by means of the control volume method. These results of research provide the foundation for current mathematical forest fire theory, and will be outlined in detail in subsequent models of this paper.

Sensitivity analysis of discontinuous multidisciplinary models
Andreas Pfeiffer
(German Aerospace Center (DLR) Oberpfaffenhofen, Germany)

Multidisciplinary modelling and simulation play an important role in design and analysis of mechatronic integrated systems. Within this subject the object-oriented modelling language Modelica supports automatic model generation for efficient time simulation of DAE-systems in complex technical applications.
Detailed model-based investigations demand not only to compute the solution of model equations but also sensitivites (derivatives) with respect to model parameters. A general numerical approach relies on the simultaneous integration of the nominal system and the sensitivity differential equations. This approach can be extended to hybrid systems with discontinuities in right-hand sides and states. Furthermore, problems will be addressed that solutions remain in crossing function manifolds (Filippov solutions). For the investigated systems it will be discussed, if and under which conditions the parameter sensitivities exist. The numerical computation of sensitivities by automatically generated Modelica models with higher complexity will be introduced, too.
An important application of sensitivity computation is the identification of unknown model parameters in physical systems by optimisiation algorithms. Fast local convergence of gradient based algorithms (e.g. SQP) will only be possible if the gradient information is sufficiently accurate. In general, finite differences (external differentiation) hardly reach this accuracy. The results of SQP-optimisation in combination with sensitivity computation will be demonstrated by a complex six-axis robot model.

Numerical treatment of integro-PDEs for Phytoplankton dynamics
Nguyet Nga Pham Thi, B. P. Sommeijer, J. Huisman
(CWI, The Netherlands)

Modelling the dynamics of phytoplankton is of great importance to many aspects of human interest, since phytoplankton provides the basis of the food chain in lakes, seas and oceans. A particularly interesting aspect is the ability of sinking phytoplankton species to take up CO_2 from the atmosphere, resulting in a downward export of carbon to the bottom of the ocean (the so-called 'biological pump'). By this mechanism, several gigatons per year of carbon dioxide are removed from the atmosphere, thus making a significant contribution to the reduction of the greenhouse problem on earth.
Phytoplankton requires light for photosynthesis. As a result, the production rate, which is determined by the local light intensity, decreases with depth, due to absorption. Furthermore, mortality rates and transport by turbulent diffusion in a water column (mixing) play a role. Also, phytoplankton species often have a specific weight different from that of water, giving rise to vertical transport in the form of sinking or buoyancy. Taking all these processes into account, leads to an integro-partial differential equation of advection-diffusion-reaction type.

Usually, light availability is the major factor limiting phytoplankton growth. In some regions, however, phytoplankton growth is limited by the availability of nutrients, such as nitrogen, iron, and phosphoros. We will consider a model in which *both limiting factors, light and nutrient*, are taken into account. These two factors give rise to contrasting gradients since light is coming from above, whereas nutrients are supplied at the sediment. As a result, the vertical distribution of the phytoplankton population can be quite heterogeneous in the sense that a large aggregation of phytoplankton is formed at a subsurface depth, where both light and nutrient are just sufficiently available to sustain a population. In a certain part of parameter space, it turns out that the biomass (as a function of time) shows an oscillatory behaviour. So far, nutrient limitation of phytoplankton is thought to lead to a stable equilibrium without oscillations.
The above aspect will be illustrated and the underlying algorithms in the numerical simulations will be discussed.

Construction and implementation of peer methods
Helmut Podhaisky, Rüdiger Weiner
(University Halle, Germany)

General linear methods can have favorable properties, in particular the unique combination of

- A-stability,
- high stage order, and
- a diagonally implicit scheme

is possible. However, it seems to be difficult to construct methods which behave robustly enough in a variable stepsize implementation to supersede Runge-Kutta and multistep methods in real applications.
The idea behind a peer methods is to pass all stage values $Y_{mi} \approx y(t_m + c_i h)$, $i = 1, \ldots, s$ from step to step, leading to

$$Y_m = hAf(Y_m) + BY_{m-1}$$

with a 'diagonally implicit' matrix A. The order conditions can easily be satisfied by interpolation and perfect stability at infinity is also automatically guaranteed. The main difficulty is to use the remaining degrees of freedom to find A-stable and 'nice' methods. We will discuss the construction of peer methods and techniques of local error estimation for a variable order implementation.

Wavelet-based Adaptive Grids for Solving Multirate Partial Differential-Algebraic Equations
Roland Pulch, Stephanie Knorr
(Bergische Universität Wuppertal, Germany)

In radio frequency (RF) applications, electric circuits produce oscillatory signals with largely differing time scales. Thus a transient integration of the differential-algebraic equations (DAEs), which describe the circuit, becomes inefficient. Alternatively, a multidimensional signal model yields a system of multirate partial differential-algebraic equations (MPDAEs). A method of characteristics is feasible to solve multiperiodic boundary value problems of the MPDAEs. This technique enables an efficient numerical simulation, if a relatively coarse grid can be used in time domain. In case of digital signal structures, steep gradients or discontinuities may arise near specific time points. In this contribution, we present a technique based on wavelets to construct an adaptive grid in time domain. Consequently, the method of characteristics requires a low number of grid points

in comparison to uniform grids, which achieves the efficiency of the multidimensional approach. Numerical simulations corresponding to benchmark circuits demonstrate the performance of this adaptive construction and the resulting RF signals.

High Resolution Finite Volume Schemes for Solving Population Balance Models
Shamsul Qamar, Gerald Warnecke
(Institute for Analysis and Numerics, Otto-von-Guericke University, Magdeburg, Germany)

Physical modeling of particulate processes has been the subject of intense research over the last half century. It is a fertile area for research and of great importance in a wide range of industries from pharmaceuticals to minerals, food and petrochemicals. Various phenomena involving particle processing are still unclear and a good knowledge of the mechanisms of size changes which occur in particulate processes is useful in product development, waste minimization and quality control.

The mathematical description of the change in particle identities during process such as granulation, crystallization etc. is referred to us as population balance equations. The population balance equation (PBE) is considered to be a statement of continuity and it track the change in particle size distribution as particle are born, die, grow or leave the control volume. The entities in the population density can be crystals, droplets, molecules, cells, and so on.

We focus on the numerical solution of multi-dimensional population balance equations by using semidiscrete high resolution finite volume schemes. The finite volume schemes were originally derived for compressible fluid dynamics. The schemes are derived for general purpose and hence can be applied to any model of hyperbolic type. In this study we concentrate on the population balance models for crystallizatin and aggregation processes. Several one and two-dimensional numerical test problems are considered here. The numerical results are validated against the available analytical solutions and experimental results of our collaborating research group. These numerical simulations prove the versatility, generality and effectiveness of the finite volume schemes.

Numerical solution of a dynamic model for dual methanol reactor
Mohammad Reza Rahimpour
(Shiraz University, Iran)

The present work investigates numerical solution of a dual catalyst bed model for industrial methanol synthesis. A system with two catalyst beds instead of one single catalyst bed is developed for methanol synthesis. In the first catalyst bed, the synthesis gas is partly converted to methanol in a conventional water-cooled Lurgi type reactor. This bed operates at higher than normal operating temperature and at high yield. In the second bed, the reaction heat is used to preheat the feed gas to the first bed. The continuously reduced temperature in this bed provides increasing thermodynamic equilibrium potential. In this bed, the reaction rate is much lower and, consequently, so is the amount of the reaction heat. This feature results in milder temperature profiles in the second bed because less heat is liberated compared to the first bed. In this way the catalysts are exposed to less extreme temperatures and, catalyst deactivation via sintering is circumvented. This system results in outstanding technical features due to the extremely favorable temperature profiles over the catalyst beds. In this work, a one-dimensional quasi-steady plug flow model is used to analyze and compare the performance of dual bed and conventional single bed reactors. The results of this work show that the dual catalyst bed system can be operated with higher conversion and longer catalyst life time.

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Efficient Stochastic Runge-Kutta Methods for the Weak Approximation of the Solution of SDEs

Andreas Rößler, Kristian Debrabant
(TU Darmstadt, Germany)

Stochastic Runge-Kutta (SRK) methods up to order two for the weak approximation of both, Itô and Stratonovich stochastic differential equations (SDEs), have been proposed in recent years. However, if these SRK methods are applied to SDE systems then the number of stages depends linearly on the dimension of the driving Wiener process. This is a significant drawback for the application of such methods in many applications like mathematical finance. In the present talk, a new class of second order SRK methods is presented which overcomes this drawback, i.e. where the number of stages is independent of the dimension of the driving Wiener process. Order conditions for this new class of SRK methods are calculated by the colored rooted tree analysis and some coefficients for explicit and implicit order two SRK methods are determined. The performance of the new methods is confirmed by the results of some numerical examples.

A Simple Method for Solving PDEs on Surfaces using the Closest Point

Steven Ruuth, Barry Merriman
(Simon Fraser University, Canada)

Many applications require the solution of time dependent partial differential equations (PDEs) on surfaces or more general manifolds. Methods for treating such problems include surface parameterization, methods on triangulated surfaces and implicit surface techniques. In particular, implicit

surfaces using level set representations have received recent attention due to their relative simplicity. Level set based methods have several limitations, however. These include the inability to naturally treat open surfaces or objects of codimension two or higher. Level set methods also typically lead to a degradation in the order of accuracy when solved on a banded grid.
This talk describes an approach based on the closest point representation of the surface which eliminates these and other limitations. A noteworthy feature of the method is that it is remarkably simple, requiring only minimal changes to the corresponding three-dimensional codes to treat the evolution of partial differential equations on surfaces.

System of Linear Differential Equations and Differential-Algebraic Equations
Masoud Saravi, E. Babolian, R. England, M. Bromilow
(Department of Mathematics, Islamic Azad University-Noor Branch, Noor, Iran)

In this paper, first we introduce, briefly, pseudo-spectral method to solve linear ODEs and then, extend it to solve a system of linear ODEs and DAEs and compare this method with other using some numerical examples. Furthermore, because of appropriate choice of Chebyshev-Gauss-Raudo points we will show that this method can be used to solve a DAEs whenever some of coefficient functions in constraint are not analytic by providing some examples.

Meshfree Explicit Local Radial Basis Function Collocation Method for Microscopic and Macroscopic Phase Change Simulations
Bozidar Sarler
(Laboratory for Multiphase Processes, University of Nova Gorica, Slovenia)

This paper uses a simple version of the classical meshless radial basis function collocation (Kansa) method for solution of the convective-diffusive solid-liquid phase change problems. The method is structured on multiquadrics radial basis functions. Instead of global, the collocation is made locally over a set of overlapping domains of influence and the time-stepping is performed in an explicit way. Only small system of linear equations with the dimension of the number of nodes included in the domain of influence have to be solved for each node. The computational effort thus grows roughly linearly with the number of the nodes. The applicability of the recently deduced method is shown on several involved numerical test cases, including coupled fluid flow, heat and mass transfer on the microscopic and macroscopic scale. The automatic adaptive redistribution, adding/removing of the collocation nodes is shown on the example of dissolution of different phases in multicomponent aluminium alloys.

A Multirate Time Stepping Strategy For Stiff ODEs
Valeriu Savcenco, W. Hundsdorfer, J.G. Verwer
(CWI, The Netherlands)

To solve ODE systems with different time scales which are localized over the components, multirate time stepping is examined. We introduce a self-adjusting multirate time stepping strategy, in which the step size for a particular component is determined by its own local temporal variation, instead of using a single step size for the whole system. We primarily consider implicit time stepping methods, suitable for stiff or mildly stiff ODEs. Numerical results with our multirate strategy are presented for several test problems. Comparisons with the corresponding single-rate schemes show that substantial gains in computational work and CPU times can be obtained.

Fast and oblivous convolution
Achim Schädle, M. Lopez-Fernandez, Ch. Lubich
(Zuse-Institute Berlin, Germany)

A fast algorithm to evaluate convolution integrals is presented. The convolution $c(t) = \int_0^t k(t-\tau)g(\tau)d\tau$ is discretized by the convolution quadrature $c_n = \sum_{j=0}^n \omega_{n-j} g_j$. c_n is then evaluated with precision ε for all $n = 1, \ldots, N$ with $\mathcal{O}(N \log(N) \log(\varepsilon^{-1}))$ operations requiring $\mathcal{O}(\log(N) \log(\varepsilon^{-1}))$ only active memory. The algorithm requires the evaluation of the Laplace transform of the convolution kernel k, which is assumed to be sectorial, and is based on the numerical inversion of Laplace transforms using contour integrals.
In a simple numerical example the algorithm is used to solve a sub-diffusion equation.
This talk is closely related to the one presented by M. Lopez-Fernandez.

Parameter optimization for explicit parallel peer two-step methods
Bernhard A. Schmitt, Rüdiger Weiner
(University of Marburg, Germany)

Peer two-step methods for time integration use s stages having identical stability and accuracy properties. Explicit parallel peer methods have a very simple structure with s parallel function evaluations followed by one large parallel matrix multiplication. We show that the stability polynomial of a certain subclass with $2s + 1$ parameters has less degrees of freedom and depends linearly on a set of only $s + 1$ new parameters. By using flexible root locus bounds for the stability polynomial we avoid eigenvalue computations and reduce parameter optimization to a linear program which is solved exactly by the simplex method. The size and shape of the stability region serve as constraints under which a certain long-term error constant is minimized. The result carries over to a larger subclass of explicit peer methods where the dependence becomes semilinear with the option to use linear programming as an inner solution method of a Monte-Carlo search. Realistic parallel tests of some peer methods with $s \leq 8$ stages using OpenMP are presented showing nearly optimal speed-up for expensive problems like celestial multi-body systems.

Adaptive Multilevel Techniques for Meshfree Methods
Marc Alexander Schweitzer
(Institut für Numerische Simulation, Universität Bonn, Germany)

In this talk we present an adaptive multilevel solver for the partition of unity method. Core ingredients of our method are a subdomain error estimator to stear the refinement of a particle cloud and a multiplicative multilevel iteration. The results of our numerical experiments in two and three space dimensions indicate that the estimator is efficient and reliable and that the overall solver is of optimal complexity.

An Eulerian-Lagrangian Method for Coupled Parabolic-Hyperbolic Equations
Mohammed Seaid
(Universität Kaiserslautern /AG Technomathematik, Germany)

Coupled parabolic-hyperbolic equations appear in mathematical modelling of many practical applications in physics and engineering. In this contribution, special attention is given to problems in radiation hydrodynamics. The numerical solution of such problems is not trivial due to the different nature of the equation governing the hydrodynamics and radiation and also due to the different time scales. It is well known that fluids flow with speed of sound while radiative signals propagate with the speed of light. Using the same discretization for both dynamics results in an inefficient

solver since the required time steps should be bounded by the fastest speed. Our attempt is to construct numerical time integration schemes for coupled parabolic-hyperbolic equations, which rely on the idea of Eulerian-Lagrangian methods that are stable and second order in time. The methods consist of integrating the hyperbolic equations in the system along the characteristics. This moves many difficulties related to the treatment of convection terms and allows for large time steps in the computational process. The parabolic equations in the system are solved using Eulerian method. The strong relationship between the nature of coupled parabolic-hyperbolic equations and the choice of the most appropriate time marching with large stability region is also highlighted for some of these results.
Numerical results for a class of coupled parabolic-hyperbolic equations demonstrate the ability of our algorithms to better maintain the shape of the solution in the presence of shocks and discontinuities. The robustness, accuracy and efficiency of these methods are illustrated and compared in several benchmark problems from radiation hydrodynamics.

Numerical analysis of a coupled model for the simulation of electrical circuits
Monica Selva Soto
(University of Cologne, Germany)

The goal of this talk is to present a model for the simulation of electrical circuits that consists of a coupled system of differential algebraic and partial differential equations. The partial differential equations describe behaviour of the semiconductor devices in the circuit. For the numerical solution of this model we discretize in space the partial differential equations in the system and solve the resulting differential algebraic equation. During the talk a brief description of the model will be given and some of its properties will be presented. It is also our purpose to discuss some of our simulation results and compare them with those obtained using a different approach, namely the coupling of two simulators.

Some aspects of collocation and least squares method for nonlinear hyperbolic equations
Leonid Semin, Denis Kharenko
(Institute of Theoretical and Applied Mechanics SB RAS, Russia)

In the present study we propose a numerical method for solving nonlinear hyperbolic equation which is based on simultaneous usage of collocation method and least-squares technique. Numerical solution in each grid cell is searched for as linear combination of basic functions. The latter were taken belonging to the space of polynomials. In order to find coefficients of solution expansion by basic functions we use collocation method, i.e. we require boundary conditions, matching conditions between cells, differential equation to be satisfied in specified points. We took the number of these equations greater than number of unknowns. We found a solution of this overdetermined system by least-squares method. The method proposed was applied to problems where the solution has discontinuous derivatives. We developed the variants of the method with basic functions belonging to the space of polynomials of second and third orders, variant for the first order system derived from initial second order equation. The variants were compared numerically. A method of accelerating the convergence of iterations was developed which also gives oscillations damping at discontinuities. This study was supported by RFBR grant Nr. 06-01-00080-a.

Sensitivity Analysis for ODE and DAE systems
Radu Serban
(Lawrence Livermore National Laboratory, USA)

Sensitivity Analysis (SA) is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation. For dynamical systems the most efficient and accurate SA approach is the so-called continuous sensitivity equation which implies generating and solving additional systems, the solutions of which provide either the sensitivities of the states (forward SA) or of some functional of the states (adjoint SA) with respect to model parameters.
We present some of our previous and current work on methods (with emphasis on adjoint SA), implementation (in SUNDIALS, Suite of Nonlinear and Differential/Algebraic Equation Solvers), and applications. We present applications of SA to the assessment of reduced-order models under perturbations and to the approximation of response surfaces for effective sampling for uncertainty quantification.

BS Methods and their Associated Spline
Alessandra Sestini, Francesca Mazzia and Donato Trigiante
(University of Firenze, Italy)

BS methods define a class of Boundary Value Methods for solving general Boundary Value Problems numerically. Their distinguishing property is that the continuous extension of the numerical solution generated by the k–step BS method can be computed with negligible additional computational cost using a $(k+1)$–degree spline having C^k smoothness and sharing with it the approximation order. Both their stability features and an efficient implementation in the setting of general nonuniform meshes have been studied in [1] and [2], respectively. Here we introduce an efficient algorithm devised for the computation of the spline coefficients using the B-spline basis. The continuous extension is useful especially when we deal with nonlinear problems which are solved using a quasi–linearization technique [3]. The hybrid mesh selection strategy introduced in [4] is used in combination with these methods in all the numerical experiments.

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Solving elliptic problems with singularities using finite difference schemes
Vasily Shapeev, Alexander Shapeev
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Boundary-value problems with singularities are solved numerically using high-order finite difference schemes (the sixth- and tenth-order schemes). Two problems were considered. In the first problem

$$\begin{cases} \Delta u(x,y) = 1, \quad 0 \le x \le 1, \;\; 0 \le y \le 1, \\ u|_\Gamma = 0 \end{cases}$$

for the Poisson equation the singularity consists in the discontinuity of solution derivatives at the corner point of the rectangular domain. In the second problem

$$\begin{cases} \beta \left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} \right) + (x-a)\dfrac{\partial u}{\partial x} + (y-b)\dfrac{\partial u}{\partial y} = 0, \quad 0 \le x \le 1, \;\; 0 \le y \le 1, \\ u|_\Gamma = v(x,y) \end{cases}$$

with the small parameter ($\beta = 10^{-4}$) at the highest derivative the singularity consists in a thin inner boundary layer. The solution behaviour and convergence of the numerical solution on a sequence of grids has been analysed with the help of exact solutions. Naturally, the order of convergence was less than the approximation order. However, in both cases the convergence order of high-order method was higher than the convergence order of low-order methods. This allows to gain a good accuracy with a small number of grid nodes. The derivation of the finite difference schemes and the analysis of the solutions were carried out with the help of the computer algebra system Mathematica. (A.V. Shapeev, V.P. Shapeev. Difference schemes of increased order of accuracy for solving elliptical equations in domain with curvilinear boundary. Journal of Computational Mathematics and Mathematical Physics, 2000, 40 (2), p. 223-232.).

One Family of Symmetric One-Step Methods of Order Four
Sergey Shindin, G. Yu. Kulikov
(University of the Witwatersrand, Johannesburg, South Africa, South Africa)

In the talk we present a new family of one-step methods which are sufficiently accurate. These methods are of the Runge-Kutta type. However, they have only explicit internal stages that leads to cheap practical implementation. On the other hand, the new methods are of classical order 4 and stage order 2 or 3. They are A-stable symmetric and conjugate to a symplectic method at least up to order 6. All of these mean that they are applicable to solve both nonstiff and stiff ordinary differential equations (including reversible and Hamiltonian problems) and possess all the necessary practical features making them quite attractive.

Dynamic Contact and Differential-Algebraic Equations
Bernd Simeon
(TU München, Zentrum Mathematik, Germany)

Dynamic frictionless contact is typically modelled by a time-dependent variational inequality. Penalty techniques introduce stiff springs at the contact interface and represent a regularization technique. On the other hand, the Lagrange multiplier approach enforces the impenetrability constraint by unilateral constraint equations. Not surprisingly, this problem class is closely related to the differential-algebraic equations arising in multibody dynamics. Due to the continuum mechanics model, however, we have to deal here with a unilaterally constrained partial-differential-algebraic equation. Several questions arise in this context: What is the connection between the

LBB-condition and the index? What are the requirements for a good time integration method? Is regularization as it is implemented in commercial simulation codes a reliable and efficient approach? The talk will address these questions and discuss some second order integrators, including explicit schemes based on the central difference method and implicit ones based on the midpoint rule. Transition conditions in impact situations will also be covered.

Exponential integrators and spectral element methods
Bård Skaflestad, Anne Kværnø
(NTNU, Norway)

The 'OIFS' framework of Maday and co-workers (1990) uses ideas similar to exponential integrators in the construction of splitting methods for the incompressible Navier–Stokes equations. However, a possible problem with the resulting schemes is an algebraic splitting error stemming from the diffusion operator. Moreover, this error term does not vanish in the case of steady state flows. On the other hand it is not—to the best of our knowledge—known to what extent the splitting error degrades the numerical solution.
Employing exponential integrators for the temporal discretisation, we can eliminate this particular error term. Consequently, we are able to gather empirical evidence on the degradation mentioned above. This talk will show work in progress in this direction.

Adaptive Grids
Gustaf Söderlind
(Numerical Analysis, Lund University, Sweden)

In discretization methods for differential equations there is a trade-off between accuracy and computational effort. Efficiency (the terms of trade) can be improved by using adaptive methods; grid points are not chosen uniformly but are put where they really matter to accuracy. Their number is kept as small as possible subject to keeping the discretization error below a prescribed tolerance. Differential equation solvers use grid adaption and sometimes variable order to increase computational efficiency.
Although technically different, there are similar considerations in initial value ODE solvers, DAE solvers and two-point boundary value problem solvers. Special problems, such as reversible problems and energy conserving systems, may have highly specific requirements.
Grid and order control algorithms have often been heuristic, but today these algorithms can be designed and analyzed using mathematical principles. In particular control theory, signal processing and variational principles are useful in the modern design of adaptive grid algorithms. The techniques extend beyond ordinary differential equations to partial differential equations, where grid refinement and moving mesh algorithms are of importance.
In this talk, we will focus on new techniques for ODEs, DAEs and two-point BVPs. Examples will be given to illustrate
1) Step size control affects computational stability
2) Hamiltonian systems can be solved with both energy conservation and adaptive step size selection; as a result, both accuracy and efficiency increase
3) Grid refinement (or moving meshes) can be constructed based on variational principles

Numerical solution of 1D and 2D shallow water equations in the MATLAB environment
Gerd Steinebach
(University of Applied Sciences Bonn-Rhein-Sieg, Germany)

Many engineering models concerning water flow in rivers or coastal regions are based on the shallow water equations (SWE). These well known hyperbolic equations can be derived from mass- and momentum conservation principles. The main difficulties for numerical solution schemes arise from the friction slope, form variable bed elevations and the drying and rewetting of regions within the computational domain.
These difficulties are analysed and appropriate space-discretization schemes are proposed. A widely open question is the choice of the time-integrator. Numerical comparisons are performed with the default MATLAB integrators and new MATLAB implementations of the ROW-method RODASP, the stabilized Runge-Kutta methods ROCK2 and ROCK4 and combinations of those.
The problem solving environment MATLAB has been choosen for these studies because of it's ease of use. I.e. 2600 lines of code of the FORTRAN implementation of RODASP could be reduced to 320 lines in MATLAB. Moreover, MATLAB is a widely accepted computing platform in the engineering community.

Pattern Formation due to Cell Motion
Angela Stevens
(Max-Planck-Institute for Mathematics in the Sciences, Germany)

Cell motion and reorientation is a fundamental process in early development, tissue organization, and tumor metastasis. Changes of behavior on the microscopic level - singel cell motion - often result in changes of structures on the macroscopic level of cell populations. To undestand these effects in detail, mathematical models for chemotaxis and cellular aligment are discussed and connections between models on different scales derived. Transport type models as well as parabolic models are of interest in this context.

High-order exponential operator splitting methods for the time-dependent Schrödinger equation
Mechthild Maria Thalhammer
(University of Innsbruck, Austria)

In this talk, I am concerned with deducing high-order error bounds for exponential operator splitting methods. The employed techniques are specific to differential equations that involve an unbounded linear operator. In particular, evolutionary Schrödinger equations with sufficiently regular initial values are included in the analysis.

Abstract Differential-Algebraic Equations
Caren Tischendorf
(Universität zu Köln, Germany)

The simulation of complex systems describing different physical effects becomes more and more of interest in various applications, for instance, in chip design, in the development of micro-electro-mechanical systems (MEMS), in structural mechanics, in biomechanics and in medicine. The modeling of complex processes often lead to coupled systems that are composed of ordinary differential equations (ODEs), differential-algebraic equations (DAEs) and partial differential equations (PDEs).

Such coupled systems can be regarded in the general framework of abstract differential-algebraic equations of the form

$$\mathcal{A}(u,t)\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}(u,t)+\mathcal{B}(u,t)=0, \qquad t\in[t_0,T].$$

This equation is to be understood as an operator equation with operators $\mathcal{A}(\cdot,t)$, $\mathcal{D}(\cdot,t)$ and $\mathcal{B}(\cdot,t)$ acting in real Hilbert spaces where $u:\ [t_0,T]\to X$ is the solution belonging to a problem adapted space. For most coupled systems, the operators $\mathcal{A}$ and $\mathcal{D}$ are neither identically zero nor invertible on the time interval $[t_0,T]$.

A general theory of abstract differential-algebraic equations (ADAEs) does not exist and can not be expected to be given considering alone the complexity of problems simulating partial differential equations. However, special classes of ADAEs have recently been successfully analyzed and simulated. We want to give a short overview of treated classes and discuss basic ideas of different approaches to handle coupled problems.

Integration of large stiff systems of ODEs with exponential propagation iterative (EPI) methods

Mayya Tokman
(University of California, Merced, USA)

New exponential propagation iterative (EPI) schemes are designed to efficiently integrate large stiff systems of ODEs over long time intervals. The EPI methods are constructed by approximating the integral form of the solution to a nonlinear autonomous system of ODEs by an expansion in terms of products between special functions of matrices and vectors. The matrix function-vector products are calculated using Krylov subspace projections. For problems where no good preconditioner is available, the EPI integrators can outperform standard methods since they possess superior stability properties compared to explicit schemes and offer computational savings compared to implicit Newton-Krylov integrators by requiring fewer Arnold iterations per time step. We discuss construction of the EPI schemes and present several methods of this type. Performance of the EPI methods is demonstrated using illustrative numerical examples and comparisons with standard explicit and implicit integrators.

Optimal scaling of high index DAEs

Lorenzo Trainelli, Carlo Bottasso
(Dipartimento di Ingegneria Aerospaziale, Politecnico di Milano, Italy)

We develop a new theoretical analysis which justifies the difficulties arising from finite precision arithmetics in the numerical solution of high index differential algebraic equations (DAEs). As it is well known, errors and perturbations pollute the numerical solution causing disastrous effects for small values of the time step size.
Among the remedies presented so far in the literature, the vast majority attack the problem by lowering the differential index to 2 or 1, seeking higher numerical robustness. In this approaches, the governing equations are tipically recast in some convenient form and/or additional constraints and multipliers are introduced, increasing the complexity of the basic framework.
In this work, we take a different route altogether. Based on the previous analysis, we propose a preconditioning strategy consisting of a simple scaling of the unknowns and the equations which completely cures the conditioning and sensitivity to perturbations. As a result, the robustness of the numerical solution is radically enhanced, as confirmed by numerical experiments.

This remarkably plain recipe, that can be trivially implemented in existing codes, leads to perfect time step size independence for the perturbations of all solution fields and condition number, basically making high index DAEs as easy to solve numerically as well behaved ODEs.

Modelling nematode swimming behaviour using the immersed boundary method
Rebecca Tyson, Chris Jordan, Justin Hebert, Lisa Fauci
(University of British Columbia Okanagan, Canada)

How does a given aquatic organism's wiggling result in propulsion? This has been well investigated in fish and in microorganisms such as bacteria where the viscous or inertial terms of the fluid equations can be ignored. Less has been done at intermediate Reynolds' Number, and furthermore, the actual interaction between the organism's musculature and the surrounding fluid is not well understood. In this talk we focus on the swimming behaviour of the nematode, a roundworm The immersed boundary method lends itself very well to the study of organism locomotion in fluid. Movement of passive nematode-like structures has been successfully modeled in complex flows. Active swimming of small organisms has also been sucessfully modelled when the restlength of each muscle segment is prescribed, and an energy minimum for organism configuration obtained. We are interested in modelling the development of swimming motion from rest, when motion is generated by the contraction of innervated muscle segments.
We have developed a three-dimensional model for the body structure of the nematode, which explicitly models the organism's musculature. The immersed boundary method is then used to communicate between the nematode body and the surrounding fluid. This model allows us to study how the nematode musculature and surrounding fluid interact to create propulsion of the nematode.

Exponentially-fitted Obrechkoff methods
Marnix Van Daele, G. Vanden Berghe
(Ghent University, Belgium)

In the last 15 years our research group has done a lot of work on exponential fitting. This research has lead to exponentially fitted linear multistep methods and Runge-Kutta methods. Typically, these methods have coefficients with depend on a parameter and the idea is to choose the parameter in such a way that the method is optimized in some sense.
In the present talk, we consider the construction of exponentially-fitted Obrechkoff two-step methods for second order differential equations. We focus on various aspects, such as the order and the stability of such a method.

A time-parallel time-integration method for ordinary and partial differential equations
Stefan Vandewalle, Martin Gander, University of Geneva
(Katholieke Universiteit Leuven, Department of Computer Science, Belgium)

During the last twenty years several algorithms have been suggested for solving time dependent problems parallel in time. In such algorithms parts of the solution later in time are approximated simultaneously to parts of the solution earlier in time.
A recent method was presented in 2001 by Lions, Maday and Turinici, who called their algorithm the parareal algorithm [1]. The name was chosen for the iterative algorithm to indicate that it is well suited for parallel real time computations of evolution problems whose solution can not be obtained in real time using one processor only. The method is not meant as a method to be used on a one processor computer. One iteration of the method costs already as much as the sequential

solution of the entire problem, when used on one processor only. If however several processors are used, then the algorithm can lead to an approximate solution in less time than the time needed to compute the solution sequentially.
The parareal algorithm has received a lot of attention over the past few years and extensive experiments have been done for fluid and structure problems. In this talk, we will show that the parareal algorithm can be reformulated as a two-level space-time multigrid method with a strong semi-coarsening in the time-dimension. The method can also be seen as a multiple shooting method with a coarse grid Jacobian approximation. These equivalences have opened up new paths for the convergence analysis of the algorithm, which is the topic of the second part of this talk.
First, we will show a sharp linear, and a new superlinear convergence result for the parareal algorithm applied to ordinary differential equations. We then use Fourier analysis to derive convergence results for the parareal algorithm applied to partial differential equations. We show that the algorithm converges superlinearly on bounded time intervals, both for parabolic and hyperbolic problems. On long time intervals the algorithm converges linearly for parabolic PDEs. For hyperbolic problems however there is no such convergence estimate on long time intervals.
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An algebraic multigrid method for high order time-discretizations of the div-grad and curl-curl equations
Stefan Vandewalle, Tim Boonen
(Katholieke Universiteit Leuven, Department of Computer Science, Belgium)

The spatial discretization of time-dependent partial differential equations by finite elements, finite difference or finite volumes leads to systems of ordinary differential equations of very large dimension. Such systems can no longer be solved efficiently by classical ODE software. Their solution requires specialized solvers that take the structure of the problems into account.
When using higher order implicit Runge-Kutta or Boundary Value Method time-discretization schemes, the size of the system to be solved in every time step amounts to a multiple of the number of spatial unknowns. We will show in this talk that these systems can be solved very efficiently, with a complexity that is linear in the number of unknowns when multigrid PDE-algorithms are used.
We will present in particular an algebraic multigrid algorithm fully coupled implicit discretizations of the time-dependent diffusion and curlcurl equations. The algorithm uses a blocksmoother, updating all stage values related to a grid point simultaneously. The multigrid hierarchy can be derived from the hierarchy built by any suitable AMG algorithm for the stationary version of the problem considered. By a theoretical analysis and numerical experiments, we show that the convergence of the algorithm is similar to the convergence of the stationary AMG algorithm on which it is bas

Recent advances in multiscale modeling of the circulatory system
Alessandro Veneziani, L. Formaggia, C. Vergara
(Politecnico di Milano, Italy)

Geometrical multiscale modeling of the arterial tree has been exploited in different contexts, including cases of clinical interest (see e.g. [1,2,3]). This approach relies on the numerical coupling of models with a different level of accuracy, ranging from 3D models in a vascular district of interest to lumped parameters models for the description of the peripheral arteries, the venous system, the heart. These numerical models can be regarded as the outcome of a domain decomposition of the

problem formulated over the whole circulatory system and a model simplification in the regions far from the district of interest. In this approach, there are two main issues:

1. the mathematically sound approximation of defective data problems, i.e. 3D problems with incomplete boundary data (e.g. mean pressure or flow rate), obtained when the simplified models are used for specifying boundary data to the accurate 3D models in an iterative framework;

2. the numerical coupling of the different submodels.

In this talk, we address some recent results concerning the former issue. In particular, we consider a general approach for solving in a reliable way defective boundary problems, based on the solution of suitable control problems.

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General Linear Methods for Index-2 Differential-Algebraic Equations

Daniel Weiß

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General linear methods (GLMs) were introduced approximately thirty-five years ago as a unifying approach for the study of consistency, stability and convergence of the Runge-Kutta and the linear multistep methods. Actually new methods which were neither Runge-Kutta nor linear multistep methods were derived.

Differential-Algebraic equations (DAEs) arise in various simulation problems like chemical reactions, electric circuits, and mechanical multibody systems. They are characterized by their pertubationindex which provides a measure of the sensitivity of the solution to pertubations in the equation. Differential-Algebraic equations of multibody systems have in general Index 3, but in their GGL-Formulation the Index is reduced to 2.

The present talk concerns the consistency, stability and convergence of general linear methods for Index-2 DAEs in Hessenbergform. Furthermore it deals with a special class of GLMs, the so called multistep collocation methods. The convergence of such methods can be improved by a certain projection step.

Calculation of Transient Magnetic Fields Using 3R-Strategies
Georg Wimmer, Thorsten Steinmetz, Daniel Weida, Markus Clemens
(Helmut-Schmidt-Universität Hamburg, Germany)

The discretization of transient magneto-dynamic field problems with geometric discretization schemes such as the Finite Integration Technique or the Finite-Element Method based on Whitney form functions results in nonlinear differential-algebraic systems of equations of index 1. Their time integration with embedded s-stage singly diagonal implicit Runge-Kutta methods requires the solution of s nonlinear systems within one time step. Accelerated solution of these schemes is achieved with techniques following so-called 3R-strategies ("**r**euse, **r**ecycle, **r**educe"). This involves e.g. the solution of the linear(-ized) equations in each time step where the solution process of the iterative preconditioned conjugate gradient method reuses and recycles spectral information of previous linear systems. Additionally, in order to resolve induced eddy current layers sufficiently and regions of ferromagnetic saturation that may appear or vanish depending on the external current excitation a combination of an error controlled spatial adaptivity and an error controlled implicit Runge-Kutta scheme is used to reduce the number of unknowns for the algebraic problems effectively and to avoid unnecessary fine grid resolutions both in space and time. To allow for a transient mesh refinement while avoiding repeated and computationally expensive re-meshing processes an advanced hanging node technique is applied using tree-type data structures. Continuity constraints at the hanging nodes are enforced within the iterative solution process which additionally uses subspace projection deflation-type techniques for further acceleration. First numerical results for 2D nonlinear magneto-dynamic problems validate the presented approach and its implementation.

The scaling and squaring technique for matrices related to the exponential
Will Wright
(La Trobe, Australia)

Exponential integrators require the evaluation of matrices closely related to the matrix exponential. Often the number of the so called φ functions evaluated is related to the order that the exponential integrator can achieve. We will examine what a near optimal choice of the degree of the Padé approximation is and how to scale and square the φ functions efficiently.

Legendre Scaling function for solving of generalized Emden-Fowler equations
Sohrab Ali Yousefi, Ehsan Banifatemi
(Department of Mathematics, Shahid Beheshti University,Tehran, Iran)

A numerical solution of the generalized Emden-Fowler equations as singular initial value problems is presented. We first rewrite Emden-Fowler equation in the form of integral equation by using especial integral operator and then applying Legendre scaling function approximation. The properties of Legendre scaling function are first presented. These properties together with the Gaussian integration method are then utilized to reduce the integral equations to the solution of algebraic equations. Illustrative examples are included to demonstrate the validity and applicability of the technique.

Method of Lines for Stochastic Partial Differential Equations
Mostafa Zahri, Andreas Rößler, Mohammed Seaid
(Fachbereich Mathematik, Johann Wolfgang Goethe-Universitaet, Germany)

We propose a class of numerical methods for solving stochastic boundary-value problems. The methods use the deterministic method of lines to treat the time, space and randomness separately.

The spatial discretization can be carried out using standard finite difference or finite volume methods, while the associated stochastic differential system is numerically solved using an embedded stochastic Runge-Kutta method. The performance of the proposed method is tested for a stochastic heat equation and a stochastic advection-diffusion problem driven with white noise. Numerical results are presented in both one and two space dimensions.

Numerical Solutions of Design Nonplanar Transistor Structures. Hydrodynamics Approach
Alexander Zakharov, Balashov A., Krupkina T.
(Institute of Microtechnologies Russian Research Center "Kurchatov Institute", Russia)

Numerical modeling is a very effective tool for development and optimization of integrated devices that allows to minimize development time and costs. The problems of numerical modeling and simulation of non-planar transistor structures with aid of TCAD have been investigated. The most complicated aspects have been defined and analyzed: modeling of shallow doping profiles and non-planar gate, mesh defining and building, simulation of non-local effects that affect the device performance.

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