The seminar NUMDIFF–10 is jointly organized by the *Institut für Numerische Mathematik, Fachbereich Mathematik und Informatik, Martin–Luther Universität Halle–Wittenberg*, and the *Center for Mathematics and Computer Science* (CWI) in Amsterdam. The members of the organizing committee are

- Karl Strehmel (Halle)
- Rüdiger Weiner (Halle)
- Ben P. Sommeijer (Amsterdam)
- Jan G. Verwer (Amsterdam)

The organizing committee would like to thank

- Ilona Tischler
- Helmut Podhaisky
- Alf Gerisch

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Contents

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1 General Information

1. **Conference Location and Lecture Rooms**
   The conference will take place in the lecture rooms of the Institute of Computer Science situated on the von-Seckendorf-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 also situated in Institute of Computer Science in room 1.18. The conference office is open on Sunday, September 7, 2003 from 4 p.m. to 8 p.m., on Monday and Tuesday from 8 a.m. to 4 p.m., and on Wednesday and Thursday 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 Sunday, September 7, 2003.

   Please register in the conference office after your arrival. You will there also receive your conference documents.

   Participants who did not use the bank transfer can pay the conference fee by cash in 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 discussion time of 5 minutes.

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**
   There will be computers (with Windows 98) for internet access available in room 3.02.

7. **Conference Dinner**
   The conference dinner will be held in the hotel *Magistralen Carré* in Halle–Neustadt on Wednesday, September 10, 2003 at 19.30. One dinner ticket is included in the conference fee; accompanying persons pay EUR 20. The fee for the dinner is payable in cash when registering in the conference office.

8. **Guided Tour on Wednesday afternoon**
   There are no scientific sessions on Wednesday afternoon. Instead you can visit *Buna Sow Leuna Olefinverbund GmbH* (Dow Chemical) in Schkopau near Halle by bus. There will be a guided tour (English). We meet at 2 p.m. in front of the conference office and the tour will take about 1.5 to 2 hours. Please register at the conference office if you are interested.

   You can also use this afternoon to explore the city and its surrounding area with your friends or by yourself.

9. **Conference Proceedings**
   Selected papers will be published in a Special Issue of the Journal *Applied Numerical Mathematics*. Guest editors are B.P. Sommeijer, K. Strehmel, 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.nl/locate/apnum` for the statement of objectives.

   All papers should be sent in triplicate to:
   Dr. B.P. Sommeijer
   CWI
   P.O. Box 94079
   1090 GB Amsterdam
   The Netherlands

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

   The deadline for submission is December 1, 2003.

2 Programme Overview

Monday, 8.9.2003

	Room 3.28
9.00	Opening
9.20–10.10	Spijker
10.30–11.20	Baker
11.20–12.10	Arnold

	Room 1.23	**Room 1.26**	**Room 1.27**	**Room 1.29**
14.00–14.25	Hundsdorfer	März	Lunk	Wolke
14.30–14.55	Horvath, Z.	Lutzenberger	Paternoster	Knoth
15.00–15.25	Ferracina	Lamour	Pfeiffer	Semin
15.45–16.10	Calvo	Schropp	Thalhammer	Fuchs
16.15–16.40	Farago	Balla	Grimm	Backes
16.45–17.10	Kwapisz	Striebel	Van de Vyver	Shapeev
17.15–17.40	Kiriazov	Selva	Rai	
17.45–18.10	Kolpakov, A. A.	Obeng	Boamah	

Tuesday, 9.9.2003

	Room 3.28
8.30–9.20	Ainsworth
9.20–10.10	Ostermann
10.30–11.20	Zennaro
11.20–12.10	Butcher

	Room 1.23	**Room 1.26**
	Minisymposium: *Partial Differential-Algebraic Equations*	Minisymposium: *General Linear Methods*
14.00–14.45	Tischendorf	Podhaisky
14.45–15.20	Simeon	Schmitt
15.20–15.55	Günther	Bartoszewski
16.15–16.50	Debrabant	Moir
16.50–17.25	Lucht	Wright
17.25–18.00	Schulz	Jackiewicz

Wednesday, 10.9.2003

	Room 3.28			
8.30–9.20	Rentrop			
	Room 1.23	**Room 1.26**	**Room 1.27**	**Room 1.29**
9.25–9.50	Chudej	Sommeijer	Pulch	Seaid
9.55–10.20	Bartel	Horvath, R.	Teichelmann	Rahimpour
10.40–11.05	Rang	Wensch	Van Daele	Matviy
11.10–11.35	Schumilina	Gerisch	Perminov	Kolpakov, A. G.
11.40–12.05	Hosseini	Heineken	Smaoui	Liseikin
12.10–12.35	Fosuaa Odoom	Guglielmi	De-Souza	Osei Owusu Ansah

Thursday, 11.9.2003

	Room 3.28	
8.30–9.20	Jackson	
9.20–10.10	Lang	
10.30–11.20	Reich	
11.20–12.10	Hemker	
	Room 1.23	**Room 1.26**
	Minisymposium: *Geometric Methods for PDEs*	Minisymposium: *Discontinuous Galerkin Methods*
14.00–14.45	Munthe-Kaas	Feistauer
14.45–15.20	Cotter	van Raalte
15.20–15.55	Wulff	Schoetzau
16.15–16.50	Leok	Kanschat
16.50–17.25	Hochbruck	Reichenberger
17.25–18.00	Frank	General discussion

3 Scientific Programme

Monday, 8 September 2003

Room 3.28

9.00 **Opening**

Plenary Lectures

9.20–10.10 **Marc Spijker**
Analysis of error growth in numerical initial value problems

10.30–11.20 **Christopher T. H. Baker**, Gennadii A. Bocharov, Christopher A.H. Paul, Fathalla A. Rihan
Computational Modelling with Ordinary and Retarded Differential Equations

11.20–12.10 **Martin Arnold**
Numerical methods for the dynamical analysis of functional virtual prototypes

12.10–14.00 **– Lunch –**

Room 1.23

14.00–14.25 **Willem Hundsdorfer**, Carolynne Montijn
Flux Limiting for Diffusion Discretizations

14.30–14.55 **Zoltán Horváth**
On the positivity step-size threshold of Runge-Kutta methods

15.00–15.25 **Luca Ferracina**
Strongly bounded Runge-Kutta methods

15.25–15.45 **– Break –**

15.45–16.10 **Mari Paz Calvo**, Alf Gerisch
Linearly implicit Runge-Kutta methods and Approximate Matrix Factorization

16.15–16.40 **Istvan Farago**, A. Havasi
Some remarks on the Strang splitting

16.45–17.10 **Marian Kwapisz**
Evaluation of the spectral radius of operators arising in discussion of WR methods for systems of ODE

17.15–17.40 **Petko Kiriazov**
Solving Shooting Equations for a Class of Nonlinear Dynamic Systems

17.45–18.10 **Alexander A. Kolpakov**
Analysis of design problem for ”smart” structures

Room 1.26

14.00–14.25 **Roswitha März**
Boundary value problems resulting from sufficient optimality conditions and their index

14.30–14.55 **Stefan Lutzenberger**
Time integration of structural dynamic DAE

15.00–15.25 **René Lamour**
Index Determination of DAEs without the use of derivative arrays

15.25–15.45 **– Break –**

15.45–16.10 **Johannes Schropp**
Runge-Kutta type methods for differential algebraic equations of high index

16.15–16.40 **Katalin Balla**, Vu Hoang Linh
Adjoint Pairs of Differential-Algebraic Equations and Hamiltonian Systems

16.45–17.10 **Michael Striebel**
Distributed time integration in full chip design

17.15–17.40 **Monica Selva**
Numerical analysis of DAEs from coupled circuit and device simulation

17.45–18.10 **Ernest Obeng**
Solutions to 1st, 2nd and 3rd order differential-algebraic equations

Room 1.27

14.00–14.25 **Christoph Lunk**
Runge-Kutta-Nyström-Methods with Maximized Stability Domain for Stiff Mechanical Systems

14.30–14.55 **Beatrice Paternoster**, Marco Carpentieri
Stability analysis of frequency-dependent one step mixed collocation methods for y"=f(x,y)

15.00–15.25 **Andreas Pfeiffer**, Martin Arnold
Numerical analysis of structure preserving Nyström methods for Hamiltonian systems

15.25–15.45 **– Break –**

15.45–16.10 **Mechthild Thalhammer**
Convergence of variable stepsize linear multistep methods for singular perturbation problems

16.15–16.40 **Volker Grimm**
A Gautschi-type exponential integrator and a related multiple time-stepping method for oscillatory differential equations

16.45–17.10 **Hans Van de Vyver**, Guido Vanden Berghe, Marnix Van Daele
Exponential fitted Runge-Kutta methods of collocation type

17.15–17.40 **A. Sesappa Rai**, U. Ananthakrishnaiah
Adaptive Methods for the Numerical Solution of the General Second Order Differential Equations.

17.45–18.10 **Augustine Boamah**
Applications of Numerical Analysis

Room 1.29

14.00–14.25 **Ralf Wolke**, Oswald Knoth, Aissa-Mounir Sehili, Judit Zoboki
Time-integration schemes for atmospheric multiphase processes

14.30–14.55 **Oswald Knoth**, Aissa-Mounir Sehili, Ralf Wolke
Discontinuous Galerkin methods for the condensation-coagulation equation

15.00–15.25 **Leonid Semin**, Vitaly Belyaev, Vasily Shapeev
On convergence acceleration of collocation and least-squares method for Navier-Stokes equations

15.25–15.45 **– Break –**

15.45–16.10 **Andreas Fuchs**, Martin Arnold
Efficient corrector iteration for implicit time integration in multibody dynamics

16.15–16.40 **Andre Backes**
Necessary conditions for optimal control of DAEs

16.45–17.10 **Vasily Shapeev**
Implicit finite-difference scheme with approximation error $O(\tau^4, h^8)$ for the heat conduction equation

Tuesday, 9 September 2003

Room 3.28

Plenary Lectures

8.30–9.20 **Mark Ainsworth**
Adaptive finite element approximation of Maxwell equations

9.20–10.10 **Alexander Ostermann**
Exponential integrators for parabolic problems

10.10–10.30 **– Break –**

10.30–11.20 **Marino Zennaro**, Nicola Guglielmi
Numerical stability investigations using the joint spectral radius approach

11.20–12.10 **John C. Butcher**
General linear methods for stiff problems

Room 1.23

Minisymposium: Partial Differential-Algebraic Equations

14.00–14.45 **Caren Tischendorf**
Numerical Analysis of PDAEs

14.45–15.20 **Bernd Simeon**
Time Integration of Constrained Variational Problems in Elastoplasticity

15.20–15.55 **Michael Günther**
PDAE models in technical simulation

15.55–16.15 **– Break –**

16.15–16.50 **Kristian Debrabant**, Karl Strehmel
Runge-Kutta Methods for Semi-Linear Partial Differential-Algebraic Equations

16.50–17.25 **Wenfried Lucht**
A special class of PDAEs of second order with convection

17.25–18.00 **Steffen Schulz**
On circuit simulation and Abstract Differential Algebraic Systems

Room 1.26

Minisymposium: General Linear Methods

14.00–14.45 **Helmut Podhaisky**, Rüdiger Weiner, Bernhard A. Schmitt
Two-step W-methods

14.45–15.20 **Bernhard A. Schmitt**, Rüdiger Weiner, Kilian Erdmann
Implicit parallel peer methods for stiff initial value problems

15.20–15.55 **Zbigniew Bartoszewski**
A new approach to construction of two-step Runge Kutta methods

15.55–16.15 **– Break –**

16.15–16.50 **Nicolette Moir**
Improving upon the ARK

16.50–17.25 **Will Wright**
Finding practical general linear methods

17.25–18.00 **Zdzislaw Jackiewicz**, J.C. Butcher
Construction of General Linear Methods with Runge-Kutta Stability

Wednesday, 10 September 2003

Room 3.28

Plenary Lecture

8.30–9.20 **Peter Rentrop**, Sven-Olaf Stoll, Utz Wever
An Adjoint Approach to Optimal Design in Fluid Dynamics

Room 1.23

9.25–9.50 **Kurt Chudej**, Hans Josef Pesch, Kati Sternberg
Indices and Numerical Solutions of Fuel Cell PDAE Models

9.55–10.20 **Andreas Bartel**, Michael Günther
PDAE models for thermal-electric problems in circuit design.

10.20–10.40 **– Break –**

10.40–11.05 **Joachim Rang**, Lutz Angermann
Perturbation index of linear PDAE

11.10–11.35 **Irina Schumilina**
The Definition of DAEs with tractability index 3 and practical index determination

11.40–12.05 **Mohammad M. Hosseini**
A New Reducing Index Method for Linear Semi-Explicit DAEs

12.10–12.35 **Irene Fosuaa Odoom**
Asymptotic expansions for solutions of linear differential-algebraic ordinary differential equations

Room 1.26

9.25–9.50 **Ben Sommeijer**, Jan Verwer
An implicit-explicit Runge-Kutta-Chebyshev scheme for diffusion-reaction equations

9.55–10.20 **Róbert Horváth**, Istvan Farago, Sergey Korotov
On the Discrete Maximum Principle in the Galerkin Numerical Solutions of Parabolic Problems

10.20–10.40 **– Break –**

10.40–11.05 **Jörg Wensch**, Helmut Podhaisky
Krylov-Rosenbrock-Methods for DAEs of index 1

11.10–11.35 **Alf Gerisch**
Elastic matching for images from 2D gelelectrophoresis

11.40–12.05 **Wolfram Heineken**
Excitation wave simulation on ellipsoids using a surface FEM and partitioned W-methods

12.10–12.35 **Nicola Guglielmi**, Ernst Hairer
On the error control in the numerical integration of implicit delay differential equations.

Room 1.27

9.25–9.50 **Roland Pulch**
Multi Time Scale ODEs for Simulating Frequency Modulated Signals

9.55–10.20 **Gunnar Teichelmann**
Modeling and Simulation of German Railway Cable Systems

10.20–10.40 **– Break –**

10.40–11.05 **Marnix Van Daele**, G. Vanden Berghe, H. Vande Vyver
Exponentially fitted quadrature rules

11.10–11.35 **Valeri Perminov**
A numerical study of forest fire initiation

11.40–12.05 **Nejib Smaoui**
Modelling the Dynamics of nonlinear Partial Differential Equations Using Neural Networks

12.10–12.35 **Lloyd Kwame De-Souza**
Algebraic and differential topology

Room 1.29

9.25–9.50 **Mohammed Seaid**
The Method of Characteristics for Transient Radiative Transfer in Scattering and Absorbing Media

9.55–10.20 **M.R. Rahimpour**
Dynamic Simulation of a Recycle Methanol Reactor Loop with Deactivating Catalyst

10.20–10.40 **– Break –**

10.40–11.05 **Oleksandr Matviy**, Igor Cherevko
Approximation of coupled differential-difference and difference equations by ordinary differential equations

11.10–11.35 **Alexander G. Kolpakov**
The net model of a high-contrast composite

11.40–12.05 **Vladimir Liseikin**
Geometric Methods in Numerical Grid Technology

12.10–12.35 **Elvin Osei Owusu Ansah**
Numerical analysis

Thursday, 11 September 2003

Room 3.28

Plenary Lectures

8.30–9.20 **Ken Jackson**, Wayne Hayes
Rigorous Shadowing of Numerical Solutions of Ordinary Differential Equations by Containment

9.20–10.10 **Jens Lang**
Moving Adaptive Finite Elements

10.10–10.30 **– Break –**

10.30–11.20 **Sebastian Reich**
A Fully Lagrangian Particle Method for Large Scale Geophysical Fluid Dynamics

11.20–12.10 **Pieter W. Hemker**
Multigrid iteration for the solution of discontinuous Galerkin discretisations of elliptic PDEs

Room 1.23

Minisymposium: Geometric Methods for PDEs

14.00–14.45 **Hans Munthe-Kaas**
to be announced

14.45–15.20 **Colin Cotter**
Stochastic modelling of unresolved wave motion

15.20–15.55 **Claudia Wulff**, Marcel Oliver, Matt West
Approximate Momentum Conservation for Spatial Semidiscretizations of Semilinear Wave Equations

15.55–16.15 **– Break –**

16.15–16.50 **Melvin Leok**
Foundations of Computational Geometric Mechanics

16.50–17.25 **Marlis Hochbruck**, Ernst-Wolfgang Laedke, Christian Lubich
Time integration schemes for nonlinear Schrödinger equations in optical fiber lines

17.25–18.00 **Jason Frank**
A locally conservative box scheme for micromagnetics

Room 1.26

Minisymposium: Discontinuous Galerkin Methods

14.00–14.45 **Miloslav Feistauer**
Analysis and Applications of Discontinuous Galerkin Methods for Convection-Diffusion Problems

14.45–15.20 **Marc Van Raalte**
Discontinuous Galerkin Discretization with Interior Boundary Conditions

15.20–15.55 **Dominik Schoetzau**
Mixed Discontinuous Galerkin Methods for Saddle Point Problems

15.55–16.15 **– Break –**

16.15–16.50 **Guido Kanschat**
Local error bounds for the interior penalty method

16.50–17.25 **Volker Reichenberger**
Discontinuous Galerkin Methods for Flow and Transport in Porous Media

17.25–18.00 *General discussion on discontinous Galerkin methods*

4 Abstracts

Numerical methods for the dynamical analysis of functional virtual prototypes
Martin Arnold
(Martin–Luther–University Halle–Wittenberg)

Prototypes are the traditional backbone of the development of new vehicles in automotive and railway industry. Today, these classical ”real” prototypes are more and more accompanied or even substituted by extensive computer simulations based on sophisticated models of the vehicle that are called *virtual* prototypes. *Functional* virtual protoypes focus on all aspects of the vehicle's dynamical behaviour and on the interplay of all vehicle components.
From the view point of mathematics, a functional virtual prototype is described by a system of time-dependent differential equations. But these model equations do never occur explicitly in the design process since the high complexity of state-of-the-art functional virtual prototypes makes it mandatory to use computer based industrial simulation packages for the model set-up.
Instead of the mathematical formulae of model equations or some equivalent C or FORTRAN source code these simulation packages offer typically only an interface to their internal formalisms that evaluate the model equations for given input data numerically. Numerical solution methods have to be adapted to these interfaces because a direct access to the mathematical model equations is impossible. In the present talk we will discuss in more detail three numerical problems of this type that have their common origin in vehicle system dynamics.
Modified algorithms for updating the Jacobian in implicit time integration methods reduce significantly the computing time for solving mixed systems of difference equations and differential-algebraic equations. These hybrid systems with discrete and continuous subsystems result, e. g., from discrete controllers that influence the (continuous) dynamics of a vehicle.
Limit cycles are an important phenomenon in the analysis of the long-term running behaviour of railway vehicles. The corresponding periodic solutions of the model equations are computed by a shooting method that requires derivatives of the numerical solution w. r. t. initial values. The BDF integrator DASSL has been modified to evaluate these derivatives with only moderate additional effort during the time integration of the model equations.
The simulation of coupled problems involves often more than one simulation package resulting in *modular* time integration methods for the overall coupled system of model equations. An *overlapping* solution technique will be presented to improve the stability of these modular methods and to avoid a well-known instability phenomenon in the time integration of coupled differential-algebraic equations.

Necessary conditions for optimal control of DAEs
Andre Backes
(Humboldt-University of Berlin)

I consider the linear quadratic optimal control problem for the controlled time-dependent linear DAE

$$A(Dx)' + Bx = Cu \quad , \quad t \in [t_0, T]$$

$$D(t_0)P\left[x(t_0) - x^0\right] = 0 \quad , \quad x^0 \in \mathbb{R}^m \quad , \quad \text{projector} \quad P \in \mathbb{R}^{m\times m}$$

$$J(u) = \frac{1}{2}x^T(T)Vx(T) + \frac{1}{2}\int_{t_0}^{T} x^T Wx + 2x^T Su + u^T Ku\, dt \to \min$$

I use the formulation of the DAE with proper formulated leading term and want to consider the general case, that there is no assumption about regularity or index of the controlled DAE.
A necessary optimality condition for an optimal control can be fomulated with the help of an associated boundary value problem. Beside the controlled DAE this boundary value problem contains also the adjoint DAE. The solvability of the adjoint DAE is no problem in the classical linear quadratic optimal control problem but here it is not clear from the first. The proof can be found with the help of the Behaviour Approach. Therefore we make an assumption to the matrix C appearing in the controlled DAE, otherwise there are examples for which the condition is not necessary.
When investigating the DAE of the boundary value problem for the triple consisting of the state variable, the adjoint variable and the control function, it will be an interesting case that this big DAE is regular with index 1. It turns out that in particular for this case the assumptions for the necessary condition are fulfilled.

Computational Modelling with Ordinary and Retarded Differential Equations
Christopher T. H. Baker, Gennadii A. Bocharov, Christopher A.H. Paul, Fathalla A. Rihan
(University of Manchester)

In this work, the authors aim at a unified approach to the identification of mathematical models (based upon ordinary and retarded differential equations) that can be applied to studies of, in particular, cell proliferation. We employ a hierarchy or family of parametrized neutral delay differential equations in modelling cell dynamics.
For a given model equation, the term 'best fit' is defined by a suitable choice of objective function (which represents quantitative consistency); the quality of fit contributes – along with a measure of parsimony, for example – to an indicator of (in some sense) acceptability.
Since different models, or the same model with different parameters, can be suggested by a given set of observations, we discuss ways of identifying suitable models and discriminating systematically between the various candidates. In particular, we discuss (under assumptions that are precise) the interplay between model evaluation criteria or "model-selection procedures", the choice of objective function, nonlinearity effects, and sensitivity analysis. The models discussed here, which simulate experimental observations, employ retarded differential equations, such as delay differential equations or neutral delay differential equations, incorporating time-lags or memory effects. All the mathematical processes involve advanced computational procedures (in particular, numerical methods for the solution of retarded differential equations) as well as – or in combination with – the more traditional analytical and statistical tools.

Adjoint Pairs of Differential-Algebraic Equations and Hamiltonian Systems
Katalin Balla, Vu Hoang Linh
(Computer and Automation Institute, Hungarian Academy of Sciences)

Recently, differential-algebraic equations (DAEs) of the form

$$A(Dx)' + Bx = f, \tag{1}$$

where $A, D, B : \mathcal{C}([a,b], L(\mathbb{C}^m)),\ f : \mathcal{C}([a,b], \mathbb{C}^m)$, were introduced in [BaMa] and their analysis was launched. A motivation to considering this class of implicit equations was that under very mild conditions the formal adjoint equation

$$-D^*(A^*x)' + B^*x = g, \tag{2}$$

$g : \mathcal{C}([a,b], \mathbb{C}^m)$, shares the basic properties with (1). Now we intend to study ordinary differential equations (ODEs) derived from (1) and (2) in parallel and called inherent ODEs (INHODEs) and essentially underlying ODEs (EUODEs). Assuming $f = 0$ and $g = 0$, we focus on the relationship of the INODEs as well as the EUODEs. Attention will be paid to a subclass of "self-adjoint" equations. We formulate boundary conditions yielding a "self-adjoint" BVP.
[BaMa] K. BALLA, R. MÄRZ, *A unified approach to linear differential algebraic equations and their adjoints*, ZAA, 21(3): 783-802 (2002).

PDAE models for thermal-electric problems in circuit design.
Andreas Bartel, Michael Günther
(Bergische Universitaet Wuppertal, Fakultaet fuer Mathematik, AG Angewandte Mathematik/Numerik, Gauss-Strasse 20, D-42097 Wuppertal, Deutschland)

Semiconducting material is thermally sensitive, since the mobility of charge carriers decreases with temperature. In this way, signals may be delayed over the extension of the circuit. Especially SOI-based (Silicon-on-insulator) technologies suffer from self-heating, since substrate and channel are electrically and consequently thermally separated by an oxide layer. Thus the heat flux to environment is limited, heat is conducted along chip structures and the heat distribution affects the overall behavior of that chip.
For the development of reliable designs, it is important to address the thermal evolution within the circuit simulator. Since heat evolution is secondary and such coupled problem exhibit multiple scales, efficiency is crucial. However, the inter-thermal coupling is usually neglected in circuit simulation.
In this talk the accompanied thermal network model is presented. It is based on distributed 1D and lumped 0D elements, for efficiency, but provides the capability of thermal inter-coupling along the chip's macrostructures. This yields a PDAE (partial differential algebraic equations) model for the coupled thermal-electric system. Then its analytic properties as positivity and passivity are discussed, and an adapted multirate co-simulation technique is outlined to solve that coupled problem. An benchmark from industry concludes the talk.

A new approach to construction of two-step Runge Kutta methods
Zbigniew Bartoszewski
(Gdansk University of Technology, Poland)

A new approach to construction of two-step Runge Kutta (TSRK) methods for ordinary differential equations will be presented. It involves Nordsieck representation of TSRK methods, which results in accurate and reliable estimation of local discretization error and allows an efficient implementation of obtained methods in variable stepsize environment.
Examples of new constructed TSRK methods of third and fifth order will be discussed and the results of some numerical experiments with these methods as well as their comparison with the results of other methods will be presented.

General linear methods for stiff problems
John C. Butcher
(The University of Auckland)

The use of general linear methods, as a practical alternative to Runge-Kutta and linear multistep methods for the solution of stiff problems, is considered. Because of their great generality, GLMs represent a relatively unexplored and somewhat unstructured class of methods. By imposing several constraints on the parameters of a method, it is possible to focus on what seems to be a promising and appropriate sub-class. The constraints are (i) impose the requirements of "inherent RK stability", (ii) demand high stage order, (iii) consider only methods with a diagonally-implicit structure. Imposing these requirements makes it possible to construct A-stable methods, which are relatively inexpensive to implement. This talk will survey some of the properties of these new methods and explain how some of their implementation challenges can be overcome. The research leading to this presentation leans heavily on collaborations, particularly with Shirley Huang, Zdzisław Jackiewicz and Will Wright.

Linearly implicit Runge-Kutta methods and Approximate Matrix Factorization
Mari Paz Calvo, Alf Gerisch
(Universidad de Valladolid)

Linearly implicit Runge-Kutta (LIRK) methods are introduced and a third order LIRK method is considered for the time integration of differential systems arising after the spatial discretization of taxis-diffusion-reaction problems. The use of approximate matrix factorization when solving the linear systems to compute the internal stages leads to a first order behaviour of the method. An explanation for this fact is found and an appropriate modification of the method is proposed in order to increase the order to two. Numerical results obtained with the new procedure are provided and compared with those of other suitable methods.

Indices and Numerical Solutions of Fuel Cell PDAE Models
Kurt Chudej, Hans Josef Pesch, Kati Sternberg
(Universität Bayreuth, Lst Ingenieurmathematik)

Stationary molten carbonat fuel cell stacks (MCFC) produce electrical power in an enviromentaly friendly way. Performance and service life of MCFCs depends on its operating temperature. For higher temperatures material corrosion accelerates greatly, which shortens the stack lifespan. Therefore control of the operation temperature within a specified range and reducing temperature gradients are highly desirable. Based on a hierarchy of spatial 1D and 2D models (P. Heidebrecht & K. Sundmacher, Chem. Eng. Sci. 58, 2003, 1029–1036) of growing complexity we will persent results of 1D and 2D numerical simulations. The 1D PDAE models are solved by the method of lines, which yields DAEs. We will present investigations of the time index, the spatial index and the MOL index.
Acknowledgement: This work is supported by the BMBF within the project *Optimierte Prozessführung von Brennstoffzellensystemen mit Methoden der Nichtlinearen Dynamik.*

Runge-Kutta Methods for Semi-Linear Partial Differential-Algebraic Equations
Kristian Debrabant, Karl Strehmel
(TU Darmstadt)

We consider semi-linear partial differential algebraic equations (PDAEs) of the form

$$A\, u_t(t,\vec{x}) + \sum_{i=1}^{d} B_i\ (u_{x_i x_i}(t,\vec{x}) + r_i u_{x_i}(t,\vec{x})) + C\, u(t,\vec{x}) = f(t,\vec{x},u)$$

with constant non-vanishing but possibly singular matrices A, B_i and C. By discretizing the space variables the PDAE is converted into a system of differential-algebraic equations, which is solved by Runge-Kutta methods. Under appropriate assumptions we prove convergence, where the order of convergence depends on the boundary conditions and the time index. Numerical experiments confirm the theoretical results.

Some remarks on the Strang splitting
Istvan Farago, A. Havasi
(Eotvos Lorand University, Budapest, Hungary)

The splitting method proposed independently by G. Strang and G.I. Marchuk in 1968 is widely used in various fields of applied mathematics. Its main advantage is its second-order local splitting error, and by choosing second order consistent numerical methods for the sub-problems, the resulting numerical model will also be second order consistent. A sufficient condition for higher order is the L-commutativity of the sub-operators. In this talk it is shown that under special assumptions the Strang splitting is convergent, and its local splitting error can sometimes be higher than second order.
We also introduce the so-called weighted Strang splitting method and show its convergence under some assumptions. Again conditions of high order accuracy are found. The consistency property mentioned above is valid also for the weighted Strang splitting method.

Analysis and Applications of Discontinuous Galerkin Methods for Convection-Diffusion Problems
Miloslav Feistauer
(Charles University in Prague, Faculty of Mathematics and Physics)

The subject-matter of this paper is the theory and applications of the Discontinuous Galerkin Finite Element Method for the numerical solution of nonlinear convection-diffusion problems and compressible flow. The sought solution is approximated in space by piecewise polynomial discontinuous functions over a suitable polyhedral mesh. The attention is paid to the approximation of convective as well as diffusive terms, existence of a solution of the discrete problem and qualitative properties of approximate solutions. Particularly, the question of optimal error estimates will be discussed. A further subject is the stabilization of the method in the case of solutions to conservation laws and singularly perturbed convection dominated problems. The method is applied to the solution of compressible flow and technically relevant results will be presented.
The results were obtained in cooperation of the author with V. Dolejší, C. Schwab and K. Švadlenka. The research was supported under the grant No. 201/02/0684 of the Czech Grant Agency and grant No. MSM 113200007.

Strongly bounded Runge-Kutta methods
Luca Ferracina
(Mathematical Institute, Leiden University)

In the context of solving nonlinear partial differential equations, Shu & Osher (1988) introduced representations, of explicit Runge-Kutta methods, which facilitate the derivation of stepsize restriction under which the numerical process is Total-Variation-Diminishing (TVD) - see also e.g. Gottlieb & Shu (1998), Gottlieb, Shu & Tadmor (2001), Shu (2002), Spiteri & Ruuth (2002).
The starting point in these studies is the Total-Variation-Diminishing property of the forward Euler method but, in many applications, this assumption turns out to be too severe - see e.g. Shu (1987), Chockburn & Shu (1989).
In this talk an extension will be presented which improves previous results covering a wider range of situations.
The conclusions that will be presented were obtained in a joint research with Marc Spijker.

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Asymptotic expansions for solutions of linear differential-algebraic ordinary differential equations
Irene Fosuaa Odoom
(Member of Civil Engineering Students Association, KNUST , Ghana)

Asymptotic expansions for solutions of linear differential-algebraic ordinary differential equation with variable matrix coefficients are considered. The solution is being sought in the form of a formal power series. The coefficients of this series satisfies linear infinite-dimensional system of the algebraic equations with triangular matrix of coefficients. Existence and uniqueness theorem is proved for such equations and initial manifolds are described. The Drazin inverse matrices are used to demonstrate the existence of asymptotic expansion.

A locally conservative box scheme for micromagnetics
Jason Frank
(CWI)

The Landau-Lifshitz equation is re-formulated as a multisymplectic PDE. Using this formulation, a box scheme is derived, which, although no longer multisymplectic, still retains an exact discrete energy conservation law [1]. In micromagnetics applications, the LL equation is coupled with Maxwell's equations, for which the box scheme *is* multisymplectic and retains discrete analogs of local energy and momentum conservation laws [2]. An additional attractive property of the box scheme in this context is the absence of parasitic wave solutions [3], as these lead to spurious reflected waves on nonuniform grids.
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Efficient corrector iteration for implicit time integration in multibody dynamics
Andreas Fuchs, Martin Arnold
(DLR German Aerospace Center)

The mathematical description of mechanical systems often leads to stiff differential algebraic equations (DAE's). These equations are solved numerically by implicit integration methods. Thereby, the solution is calculated by a modified Newton method in each integration step. If the mechanical systems are complex in dimension then the computational effort in the dynamical simulation is dominated by the evaluation of the Jacobian of the equations of motion, which is needed for Newton's method. To reduce the computing time, the special structure of this Jacobian has to be exploited in time integration.
For the implicit multistep DAE-solver DASSL with variable order and step-size, the equations of motion are considered in residual form $F(t, y, y') = 0$ such that the Jacobian can be written as

$$J = \alpha \cdot \frac{\partial F}{\partial y'} + \frac{\partial F}{\partial y}$$

with a coefficient $\alpha \in \mathbb{R}$ that depends on the order and step-size.
If J is approximated by finite differences then computing time can be reduced by

- exploiting the sparsity structure of Jacobian J or by
- the separate evaluation of $\partial F/\partial y'$ and $\partial F/\partial y$.

These strategies are very successful for systems with frequent discontinuities and for systems that are linear or only mildly nonlinear. For approximately linear systems the Jacobian is almost constant during the simulation.
Similar savings may be achieved for the important problem class of systems with strongly time-dependent Jacobian J

- updating the time-depending entries of J separately.

The new strategies have been implemented in the industrial multibody system code SIMPACK. Several examples from vehicle simulation will demonstrate the benefits of the new approach.

Elastic matching for images from 2D gelelectrophoresis
Alf Gerisch
(Martin-Luther-Universität Halle-Wittenberg)

2D gelelectrophoresis is an important method for separating a large number of proteins from complex protein mixtures. It is used for uncovering differences in protein expression profiles of the same organism under varied environmental conditions (e.g. stress due to heavy metal vs. no stress conditions) and that way aides in assigning functionality to certain proteins in the organism.
2D gelelectrophoresis images are gray-scale images having a white background with small gray and black dots. Usually more than one experiment is performed under (theoretically) the same environmental conditions leading to a set of images. In order to perform a computer-assisted evaluation of such sets, geometric distortions (due to environmental variations, non-homogeneous gels, or errors introduced during the scanning process) within each set must be filtered out and a master image per set must be selected or generated. For each image in a set the transformation which transforms this images (approximately) to the master image of the set must be known.
We describe how the elastic matching technique based on the equations of linear elasticity can be used for estimating a transformation of one image into another one (e.g. the master image). In order to accelerate the estimation process we make use of a hierarchy of images of increasing resolution. We also present some first results obtained with a code currently under development and outline possible future extensions.

A Gautschi-type exponential integrator and a related multiple time-stepping method for oscillatory differential equations
Volker Grimm
(University of Düsseldorf, Germany)

The talk deals with a numerical method for second-order oscillatory differential equations in which high-frequency oscillations are generated by a linear time- and/or solution-dependent part. The presented results show that the methods admit second-order error bounds which are independent of the product of the step-size with the frequencies. Methods with this property are called long-time-step methods. Applications for which long-time-step methods are intended include molecular dynamics. It is shown that the Gautschi-type exponential integrator applied as multiple time-stepping method is an easy to implement alternative with the same good performance in the field of molecular dynamics. Some results of numerical experiments are included.

On the error control in the numerical integration of implicit delay differential equations.
Nicola Guglielmi, Ernst Hairer
(Dipartimento di Matematica, Università dell'Aquila)

We consider initial value problems of systems of implicit delay differential equations of the form

$$\begin{aligned} M\,y'(t) &= f\Big(t, y(t), y\big(\alpha_1(t,y(t))\big), \ldots, y\big(\alpha_m(t,y(t))\big)\Big), \\ y(t_0) &= y_0, \qquad y(t) = g(t) \quad \text{for } t < t_0, \end{aligned} \tag{1}$$

where M is a constant matrix (possibly singular) and $\alpha_i(t, y(t)) \leq t$ for all $t \geq t_0$ and for all i. The value $g(t_0)$ may be different from y_0, allowing for a discontinuity at t_0. For a numerical treatment of such kind of problems, a sofware tool has been recently developed; such code is called RADAR5 and is based on a suitable extension to delay equations of the 3-stage Radau IIa Runge–Kutta method (the software is available at http://www.unige.ch /math/folks/hairer/software.html). The aim of this talk is that of illustrating suitable error control strategies able to take into account both of the continuous approximation to the solution (which is needed in order to numerically integrate (1)) and of the presence of derivative discontinuities which commonly arise in the solutions of such kind of equations. Numerical examples will illustrate the potential difficulties which are met when using techniques which are straightforward adaptations of the error control

strategies developed for ODEs and how they can be overcome. This is a joint project with Ernst Hairer (Université de Genève).

PDAE models in technical simulation
Michael Günther
(Bergische Universität Wuppertal, Arbeitsgruppe Angewandte Mathematik/Numerik)

The numerical simulation of complex technical systems can be based very naturally on a refined network approach. Here a compact network model is combined with distributed models for parasitic and coupling effects that must not be neglected any more.
This modeling approach results in mixed initial-boundary value problems of partial differential-algebraic equations, for short PDAEs, that combine differential-algebraic network equations with partial differential equations describing the distributed effects.
The numerical simulation of these models, multiscale both in time and space, demands first of all a proper study of well-posedness and a perturbation analysis. Based on these results, numerical schemes can be developed that are suitable for co-simulation or simulator coupling.
In our talk we will discuss the use of PDAE models in chip design. Here one has to consider, for example, thermal effects in SOI devices, transmission lines effects in digital networks and distributed effects of semiconductor devices in HF circuits.

Excitation wave simulation on ellipsoids using a surface FEM and partitioned W-methods
Wolfram Heineken
(O.v.Guericke-Universitaet Magdeburg, Inst. f. Analysis und Numerik)

Excitable media occur in various fields in physics, chemistry, and biology, a famous example being the Belousov-Zhabotinsky reaction. We study efficient numerical methods to solve an underlying reaction diffusion system. For time discretization, several partitioning schemes are investigated. We compare a Krylov-W-method vs. fixed and automatic componentwise partitioning in a W-method, as well as a combination of those methods.
A common phenomenon of excitable media are rotating spiral waves. On nonuniformly curved surfaces, a curvature dependent drift of spiral waves was observed. The wave drift is studied by numerical simulation on several ellipsoids. For spatial discretization, a finite element method on curved surfaces is applied. Curvature and excitability effects on the wave drift velocity are presented.

Multigrid iteration for the solution of discontinuous Galerkin discretisations of elliptic PDEs
Pieter W. Hemker
(CWI)

In this talk we discuss the discretisation of elliptic PDEs by the Baumann-Oden and the symmetric DG method, and the solution of the resulting discrete operators by multigrid iteration. For our purpose we introduce a convenient hierarchical basis for the approximating space.
For the one- and the two-dimensional linear second order elliptic equation, we study the convergence of MG-iteration for cell- and point-wise block-relaxation strategies by means of Fourier analysis.
We show that point-wise block partitioning gives much better results than the classical cell-wise partitioning. Independent of the mesh size, for Poisson's equation, with block-Gauss-Seidel and symmetric block-Gauss-Seidel smoothing, simple MG cycles yield a convergence rate of 0.4 - 0.6 per iteration sweep for both DG-methods studied.
In contrast with higher-order methods, for second order methods are unstable if no interior penalty is applied. We show for the 2nd order methods how convergence depends on the additional penalty parameter. Like with the higher order methods, we find that point-wise block-relaxations give much better results than the classical cell-wise relaxations. Both for the Baumann-Oden and for the symmetric DG method, with a sufficient interior penalty, the block relaxation methods studied (Jacobi, Gauss-Seidel and symmetric Gauss-Seidel) all make excellent smoothing procedures in a classical multigrid setting.

Time integration schemes for nonlinear Schrödinger equations in optical fiber lines
Marlis Hochbruck, Ernst-Wolfgang Laedke, Christian Lubich
(University of Duesseldorf)

The numerical simulation of the pulse propagation in optical fiber lines presents a challenging task even on todays supercomputers. A mathematical model containing damping and second order dispersion for such processes is the nonlinear Schrödinger equations (NLSE)

$$i\frac{d}{dt}\psi(x,t) + \beta\frac{d^2}{dx^2}\psi(x,t) + \epsilon|\psi(x,t)|^2\psi(x,t) = -i\gamma\psi(x,t).$$

Currently, the most promising methods for solving the NLSE appear to be the Crank Nicholson method and split step methods. In order to avoid artificial damping, it is crucial to use schemes which are conservative. The Crank Nicholson scheme and splitting methods fulfill this requirement but they suffer from severe step size restrictions resulting from stability problems, in particular, from the the correct simulation of the so called four wave mixing. Another major problem is that the space interval for the simulation of the fiber line is extremely long, so many Fourier modes have to be used for representing the pulse propagation sufficiently accurate.
In this talk we discuss the problems with the numerical solution of the nonlinear Schrödinger equation and present some ideas for the construction of new time integrators which can be used with time steps much larger those used in splitting methods and which can be implemented efficiently.

On the Discrete Maximum Principle in the Galerkin Numerical Solutions of Parabolic Problems
Robert Horváth, Istvan Farago, Sergey Korotov
(University of West-Hungary)

One of the most important problems in numerical modelling and simulations is the preservation of qualitative properties of solutions of mathematical models. For parabolic partial differential equations, one of such properties is the maximum principle. Fujii [1] proposed a discrete analogue of the (continuous) maximum principle for the linear parabolic problems, and derived the necessary conditions guaranteeing its validity for the piecewise linear finite element approximations built on simplicial meshes. In our paper, we present a necessary and sufficient condition of the validity of the discrete maximum principle in the Galerkin numerical solutions of parabolic problems. As special cases, we deduce sufficient conditions for finite element methods with linear and bilinear elements.
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On the positivity step-size threshold of Runge-Kutta methods
Zoltán Horváth
(Széchenyi István University)

Componentwise non-negativity, shortly positivity of the initial vector of IVPs for ODEs is preserved by the exact exact solution of a large class of IVPs called positive problems, for example the properly semi-discretised advection-diffusion-reaction problems. In this talk we examine the maximal step-size of Runge-Kutta methods for which the numerical approximations are positive whenever the problem and the initial vector are positive.
First we prove that a sufficient condition on the step-size guaranteeing preservation of positivity for *arbitrary* positive initial vector, given by us in an earlier paper, is even necessary for DJ-irreducible and non-confluent methods, i.e. the exact step-size threshold for positivity is determined. We illustrate by numerical experiments that larger step-sizes than the threshold can give very poor numerical results even for accurate and stable methods, such as Lobatto IIIC and Radau IIA (with $s = 2$). Moreover, we point out that the necessity

of this theorem implies step-size barriers for RK-methods with TVD property, which has been examined recently by many authors (e.g. by Spijker, Ferracina, Ruuth).
However, for certain IVPs with some *particular* initial vectors (e.g. some ”smooth” initial vectors in diffusion problems) this step-size threshold is too pessimistic. In the second part of the talk we investigate this phenomenon. More precisely, for dissipative, positive linear problems we define a rather wide subset of positive initial vectors, which forms a positively invariant cone attracting all solutions and we determine the positivity step-size threshold of RK-methods with respect to this cone (or even stronger: the threshold for discrete positive invariance and attractivity of the cone). We remark that this threshold is much less restrictive than that one of the previous paragraph. We display some computational results to illustrate our analysis.

A New Reducing Index Method for Linear Semi-Explicit DAEs

Mohammad Mehdy Hosseini
(Assistant Professor of Mathematics Department, Yazd university, Yazd, Iran.)

It is well known that the index of a DAEs is a measure of the degree of singularity of the system and also widely regarded as an indication of certain difficulties for numerical methods. The DAEs with higher index (> 1) is in a sense ill-posed and a straightforward discretization generally does not work well. An alternative treatment is the use of index reduction methods, whose essence is the repeated differentiation of the constraint equations until a well-posed problem (index-1 DAEs or ordinary differential equations (ODEs)) is obtained. But repeated index reduction by direct differentiation leads to instability for numerical integrations(i.e., drift-off-the error in the original constraint grows). Hence, stabilized index reduction methods were used to overcome the difficulty.
Here, for linear semi-explicit DAEs, a new reducing index method is proposed which has not need to the repeated differentiation of the constraint equations. This method is well applied for DAEs with and without constraint singularities and them is numerically solved by pseudospectral, with and without domain decomposition, methods.The test problems, mentioned in [1,2,3], shows the advantage using the proposed reduction method, compares to some other methods. For more details refer to [1,2,3].

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Flux Limiting for Diffusion Discretizations
Willem Hundsdorfer, Carolynne Montijn
(CWI)

The preservation of monotonicity properties – like positivity, maximum principles and comparison principles – is often essential for numerical schemes to approximate non-smooth solutions in a qualitatively correct manner. For convection equations this has led to the development of 'high-resolution' schemes with flux limiters. The object of this talk is to present a similar technique for diffusion equations. Applications are found in pattern formation problems for reaction-diffusion equations. The 1D Fisher equation

$$u_t = \epsilon u_{xx} + \gamma u(1 - u^2)$$

will be used for numerical illustrations.

Construction of General Linear Methods with Runge-Kutta Stability
Zdzislaw Jackiewicz, J.C. Butcher
(Arizona State University)

We describe the construction of explicit general linear methods of order p and stage order $q = p$ with $s = p + 1$ stages which achieve good balance between accuracy and stability properties. The conditions are imposed on the coefficients of these methods which ensure that the resulting stability matrix has only one nonzero eigenvalue. This eigenvalue depends on one real parameter which is related to the error constant of the method. Examples of methods are derived which illustrate the application of the approach presented in this talk.

Rigorous Shadowing of Numerical Solutions of Ordinary Differential Equations by Containment
Ken Jackson, Wayne Hayes
(University of Toronto)

An exact trajectory of a dynamical system lying close to a numerical trajectory is called a *shadow*. We present a general-purpose method for proving the existence of finite-time shadows of numerical ODE integrations of arbitrary dimension in which some measure of hyperbolicity is present and there is either 0 or 1 expanding modes, or 0 or 1 contracting modes. Much of the rigor is provided automatically by interval arithmetic and validated ODE integration software that is freely available. The method is a generalization of a previously published *containment* process that was applicable only to two-dimensional maps. We extend it to handle maps of arbitrary dimension with the above restrictions, and finally to ODEs. The method involves building n-cubes around each point of the discrete numerical trajectory through which the shadow is guaranteed to pass at appropriate times. The proof consists of two steps: first, the rigorous computational verification of a simple geometric property we call the *inductive containment property*; and second, a simple geometric argument showing that this property implies the existence of a shadow. The computational step is almost entirely automated and easily adaptable to any ODE problem. The method allows for the rescaling of time, which is a necessary ingredient for successfully shadowing ODEs. Finally, the method is local, in the sense that it builds the shadow inductively, requiring information only from the most recent integration step, rather than more global information typical of several other methods. The method produces shadows of comparable length and distance to all currently published results.

Solving Shooting Equations for a Class of Nonlinear Dynamic Systems
Petko Kiriazov
(Institute of Mechanics, Bulgarian Academy of Sciences)

A generic approach for solving multivariable two-point boundary-value problems (TPBVP) is proposed. Dynamic systems are addressed that are nonlinear-in-general, second-order differential systems and their state may depend on some parameters as well. The approach has two main steps. First an appropriate pairing has to be done between the required final states and the unknown initial states and/or the parameters. That can be done by using the corresponding system of sensitivity equations or in many cases with clear physical meaning - merely by intuition. For the pairing to be appropriate it has to be such that a weak condition is fulfilled. That condition is found to be sufficient, and for linear systems - also necessary, for the existence of at least one solution of the required TPBVP. In this way the TPBVP is transformed into a system of shooting equations. The second step is finding their solutions applying a multidimensional bisection algorithm which is numerically stable and globally convergent. The proof of existence and convergence is based on a Borsuk-Ulam theorem and topological degree estimation. The approach has been successfully applied to several dynamic models with control parameters for robotic systems that have to perform optimal in time/energy point-to-point motion tasks.

Discontinuous Galerkin methods for the condensation-coagulation equation
Oswald Knoth, Aissa-Mounir Sehili, Ralf Wolke
(Institute for Tropospheric Research)

The condensation-coagulation equation describes the temporary evolution of particles (aerosol, cloud droplets) in the air. The condensation process which means a transfer of gaseous species to preexisting particles leads to an advection equation. The coagulation process which stands for the merging of particles by collision results in an integro-differential equation. From a physical point of view one is interested in numerical methods which conserve number concentration for condensation and mass concentration for the coagulation process which means that the zeroth and first moment of the number distribution should be conserved. Discontinuous Galerkin methods with polynomial test functions fulfil this rquirement by their construction principles. We report about the implementation of these methods in conjunction with a Rosenbrock-method of second order for the temporal integration and present different test examples.

Analysis of design problem for ”smart” structures

Alexander A. Kolpakov
(Novosibirsk High School)

The paper deals with the design problem for ”smart” structures. The smart structure consists of passive elements (beams, plates and so on), active elements (sensors and actuators) and logical elements (programs). The designer developing the ”smart” structure has to place the actuators in the best positions and provides them with the instruction how to work. As a result the designer arrives at the coupled ”optimal control-structural design” problem [1,2]. In this paper solution of the design problem is given for the problem of shape of structure preservation.

In the paper a ”smart” structure is considered following to the formula:

structural elements (passive elements, active elements) + logical elements (programs)

Note that the usual formula is

passive elements + active elements.

The simplest problem has the form (the ”smart beam”)

$$d^4w/d^4x = F(x,t) + p(x,t)$$

Here F(x,t) is a force applied to the beam (depend on a parameter t), and p(x,t) is a control force.

We seek a control such that

$$|w| -> min$$

Solution $p(x,t) = -F(x,t)$ is the best. But in practice p(x,t) is not arbitrary ($p(x,t)$ belongs to a functional set A) and solution $p(x,t) = -F(x,t)$ is usually impossible. For example, if the control force $p(x,t)$ can be applied in a finite number of points and F(x,t) is continuous function, the equality $p(x,t) = -F(x,t)$ is impossible.

The case described above is most interesting for practice. The problem has the form

$$d^4w/d^4x = F(x,t) + \sum_i^N p_i(t)\delta(x - x_i)$$

One has to find minimal number of actuators N, those positions x_i and control $p_i(t)$, which minimize $|w|$ for $F(x,t)$ from a given set.

If the number of actuators and those positions are given, we have an optimal design problem. In the considered case we must find both optimal control and optimal position of control forces.

Using the Green’s function we can transform the problem into the form

$$\mathbf{u} \rightarrow \mathbf{min}$$

$$\mathbf{u} = \sum \mathbf{L_i p_i}, \mathbf{p_i} \geq \mathbf{0}, \sum \mathbf{L_i p_i} \leq \mathbf{1}$$

This problem can be solved by analizing the positions of the cone

$$K = \{\mathbf{u} : \mathbf{u} = \sum \mathbf{L_i p_i}, \mathbf{p_i} \geq \mathbf{0}, \sum \mathbf{L_i p_{\leq} 1}\}$$

and cube $D(c) = \{\mathbf{u} : |\mathbf{u}| = \mathbf{c}\}$. It is a problem of computational geometry.

The advantage of this analysis is that provides us with the number and positions of actuators (the structural elements) and switching instruction for the actuators (the logical elements).

Examples are given.

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The net model of a high-contrast composite

Alexander G. Kolpakov
(Siberian State University of Telecom and Informatics)

We consider Laplace equation in the domain with the large number of small absolutely conducting randomly distributed fillers. One the method to analyze such the problem is the reduction of the original problem to a "net" model. The method proposed in [1] uses the continuum model of medium. In practice we usually deal with the mixtures formed from homogeneous components and it is impossible adopt the model [1] to describe such kind media.

The continuous problem. In the domain $P = [-1, 1] \times [-L, L]$ the disks $D_i, i = 1, ..., N$ are distributed in a random way; $Q = P \setminus \cup Q_i$. Consider the problem

$$\Delta u = 0 in Q_P,$$

$$u(\mathbf{x}) = t_i on D_i$$

$$\int_{\partial D_i} \partial u / \partial \mathbf{n} d\mathbf{x} = 0, i = 1, ..., N$$

$$u(x, \pm 1) = \pm 1, \partial u / \partial \mathbf{n}(\pm L, x) = 0$$

The effective conductivity of the filled medium is defined as the flux through a boundary:

$$A = (1/2L) \int_{x=\pm 1} \partial u / \partial \mathbf{n} d\mathbf{x}$$

.

The finite-dimensional model. The flux between the pair of disks ($i - th$ and $j - th$) is equal to $g_{ij}(t_i - t_j)$, where $\sqrt{R/\delta_{ij}}$, δ_{ij} is the distance between the disks [2]. We obtain the net $x_i, t_i, g_{ij}; i, j = 1, ..., N$, where x_i are the nodes (corresponding to the disks) and t_i are the potentials, which satisfy the equations (the "net" model)

$\sum g_{ij}(t_i - t_j) = 0, i \in I; t_i = \pm 1, i \in S^{\pm}$ (I means the interior and $S^{\pm}$ means the boundary nodes).

Theorem. The effective conductivity A has the order of $\sqrt{R/\delta}$ as $\delta \to 0$, where $\delta = max \delta_{ij}$ and max is taken for the neighbor disks. The leading term is expressed through solution of the "net" model in the form $A = 1/4 \sum g_{ij}(t_i - t_j)^2$.

The relation with the earlier models. In [2] a periodic structure of the conducting disks was analyzed and the order $\sqrt{R/\delta}$ was predicted for the effective conductivity.

The numerical investigation of high-contrast composites with the "net" model. We use the discrete network to compute A numerically. We compute the dependence of A on the volume fraction of the inclusions V for monodispersed composites and obtained results which are consistent with the percolation theory predictions. For polydispersed composites (random inclusions of two different sizes) the dependence $A(V)$ is not simple and is determined by the relative volume fraction V_r of large and small particles. Some results are published in [3].

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Evaluation of the spectral radius of operators arising in discussion of WR methods for systems of ODE

Marian Kwapisz
(The Academy of Bydgoszcz, Poland)

In the talk we present different approaches to evaluation of the spectral radius of linear operators arising in investigation of the convergence problem for waveform relaxation (WR) methods. The WR method for the linear system

$$B(t)x'(t) + A(t)x(t) = f(t) \tag{1}$$

converges if the spectral radius of the corresponding operator

$$\mathcal{F}_0(x)(t) = D(t)x(t) + \int_0^t Q(t,s)x(s)ds, \tag{2}$$

with some matrix-functions D and Q determined by WR method has the spectral radius $\rho(\mathcal{F}_0)$ smaller than 1. In the general case it is difficult to determine the exact value of $\rho(\mathcal{F}_0)$. Some bounds for $\rho(\mathcal{F}_0)$ will be presented.
In the case of constant matrix B the matrix function D is constant and the spectral radius $\rho(\mathcal{F}_0)$ is equal to the spectral radius of the matrix D.
Some results for the case of differential delay systems will also be presented.

Index Determination of DAEs without the use of derivative arrays

René Lamour
(Humboldt-University of Berlin)

Differential-algebraic equations (DAE) are used to model processes in various fields of applications like electrical networks, chemical reaction or mechanical dynamics. To assess the expected difficulties it is very important to know the index of the DAE.
For a class of differential algebraic equations with properly stated leading terms and nonsmooth data, an index characterization in terms of the original coefficients and their only first partial derivatives is given.
The index characterization is done by means of a matrix sequence, whose realization is discussed.
Examples solved by an algorithm implemented in MATLAB will illustrate the method.

Moving Adaptive Finite Elements

Jens Lang
(TU Darmstadt)

The purpose of this talk is to present a combination of an r–adaptive and an h–adaptive finite element method. r–adaptivity, i.e., moving grid points through the computational domain without destroying the mesh connectivity, is accomplished by a moving mesh method. This method is based on a moving mesh PDE where the gradient or an a posteriori error estimate of the numerical solution is used to indicate the regions requiring higher mesh density. Although moving methods have a good potential to solve non–trivial problems including free boundaries or time–dependent domains, a fixed number of grid points may become a major disadvantage.
Here, h–adaptivity can be useful to insert new grid points in regions where large solution variations have to be resolved and to delete grid points where they are no longer needed. Thus, the main idea is to run the r–method until an h–method is required to keep the estimated discretization error in space below a certain tolerance.
Numerical examples are presented for solving time–dependent PDEs.

Foundations of Computational Geometric Mechanics
Melvin Leok
(California Institute of Technology)

Discrete theories of exterior calculus and connections on principal bundles provide some of the mathematical foundations for the emerging field of computational geometric mechanics.
We will present some recent progress on the construction of a combinatorial formulation of discrete exterior calculus based on primal simplicial complexes, and circumcentric dual cell complexes. Discrete notions of differential forms and vector fields are introduced, and the exterior derivative, wedge product, hodge star, codifferential, sharp, flat, contraction, and Lie derivative are constructed as combinatorial operations on the mesh. In addition, a discrete Poincaré lemma holds.
In this framework, one can systematically recover discrete vector differential operators like the divergence, gradient, curl and the Laplace-Beltrami operator.
For discrete connections, we consider the discrete analogue of the Atiyah sequence of a principal bundle, and relate a splitting of the discrete Atiyah sequence with discrete horizontal lifts and discrete connection forms. Continuous connections can be obtained by taking the limit of discrete connections in a natural way. This yields an isomorphism between $(Q \times Q)/G$ and $\tilde{G} \oplus (S \times S)$. Both the discrete connection and the associated continuous connection are necessary to express the Discrete Lagrange-Poincare operator in coordinates.
Examples spanning the work on exterior calculus and connections is the discrete Levi-Civita connection for a semidiscrete Riemannian manifold, and the curvature of an abstract simplicial complex endowed with a metric on the vertices.

A special class of PDAEs of second order with convection
Wenfried Lucht
(Martin-Luther-Universität Halle)

There are systems in science and technology (especially in fluid dynamics) which are PDAEs of second order with "symmetric" convection terms. For example, if in $d \geq 1$ dimensions the convection terms of the PDAE are written

$$\sum_{j=1}^{d} D_j \frac{\partial u}{\partial x_j}$$

(u a $n-$vector and D_j a $(n,n)-$matrix), then the matrices D_j are symmetric. We use this fact to consider the numerical solution of such PDAEs by means of the vertical method of lines. The semi discrete form is generated by means of standard finite elements. For the semi discrete equations error estimates with respect to the FEM-Parameter h are given.

Runge-Kutta-Nyström-Methods with Maximized Stability Domain for Stiff Mechanical Systems
Christoph Lunk
(Technical University of Munich)

Problems in structural dynamics lead quite often to stiff second order ODEs. Solving them as first order ODE with classical explicit Runge-Kutta methods results in very small stepsizes due to high frequency oscillations and instability. Implicit methods, on the other hand, are not well-suited for real-time applications and very large problems. Thus, there is a need for low order methods that allow relatively large steps and that are computationally not expensive.
In this talk we introduce a class of Runge-Kutta-Nyström methods that meet the requirements above. They are explicit in the position variables and implicit in the velocities. The methods generalize the well-known Störmer's rule and allow a maximization of the stability domain. While the stability domain of standard Runge-Kutta methods reaches at most up to s on the imaginary line where s is the stage number, the method class presented features a domain up to $2s$.

Time integration of structural dynamic DAE
Stefan Lutzenberger
(TU München)

Structural dynamic systems are characterised by a large number of degrees of freedom (Dof). In general, methods that integrate the second order differential equation as the Newmark-β method or the generalized-α method are used for time integration. By applying these time integration schemes to DAE disturbances occur and even the method itself might become unstable.
Structural dynamic DAE can have an index from 1 to 3. The time integration by the α-methods is analysed with respect to the index. So it is possible to derive stability criterias and to analyse appearing effects as high frequent disturbances and consequences of the index reduction by differentiating the constraint.
These insights assist to develop a stable α-method for high index problems. The method makes use of a single index reduction by differentiating the constraint equation. All Dof, their first and second differentiations are free of high frequent disturbances. It can be shown mathematically that a drift-off effect does not exist for this method.
As an application example the differential algebraic formulation of a problem of the vehicle guide way interaction is shown. The vehicle and the bridge are modelled by the Finite Element method. The coupling is done by a constraint. Numerical calculation results will be shown.

Approximation of coupled differential-difference and difference equations by ordinary differential equations
Oleksandr Matviy, Igor Cherevko
(Chernivtsi State University)

Consider the following system

$$x'(t) = f(t, x(t), x(t-\tau_1), \dots, x(t-\tau_p), y(t-\tau_1), \dots, y(t-\tau_p)), \tag{1}$$

$$y(t) = g(t, x(t), x(t-\tau_1), \dots, x(t-\tau_p), y(t-\tau_1), \dots, y(t-\tau_p)), \tag{2}$$

$$t \in [a, T], \quad p \geq 1$$

with the initial conditions

$$x(t) = \varphi_1(t), y(t) = \varphi_2(t), t \in [a-\tau, a], \tag{3}$$

where $\tau = \max\{\tau_i\}$ and the following condition of matching is fulfilled

$$\varphi_2(a) = g(a, \varphi_1(a), \varphi_1(a-\tau_1), \dots, \varphi_1(a-\tau_p), \varphi_2(a-\tau_1), \dots, \varphi_2(a-\tau_p)).$$

Assuming that $f(t, u_0, \dots, u_p, w_1, \dots, w_p)$, $g(t, u_0, \dots, u_p, w_1, \dots, w_p)$ — continious functions which satisfies Lipschitz condition with respect to u_i, w_j uniformly for $t \in [a, T]$, the solution of (1)-(3) has global existence and can be constructed by steps.
In this note we investigate an algorithm of the approximation of given system by system of ordinary differential equations. The method is based on Krasovsky-Repin approximation scheme of differential equations with delay.
The Krasovsky-Repin scheme for system (1)-(3) in different state spaces is constructed and convergence result is established.

Improving upon the ARK
Nicolette Moir
(The University of Auckland)

Although Runge-Kutta methods have been important and useful numerical methods for more than 100 years, it is natural to ask how it is possible to generalise them without destroying their essential properties. Approaches to this have taken the form of pseudo Runge-Kutta methods and two-step Runge-Kutta methods. We believe that Almost Runge-Kutta (ARK) methods also have interesting prospects and potential advantages. Although they pass more than one piece of information from step to step they retain the simple stability properties of traditional Runge-Kutta methods. The information that is passed from step to step is in Nordsieck form, ensuring that changing step-size is cheap and convenient.
A significant advantage of these new methods is that the number of stages required to obtain a certain order is not restrained by the Butcher barrier. Recently a family of methods has been discovered that obtain fifth order with only five stages. Because this family of methods do not satisfy all of the "annihilation" conditions, an order reduction is seen for variable step-size. By carefully implementing the step-size change we can restore fifth order behaviour for variable step-size.
A question to consider is how to identify the best methods within this family. Preliminary investigations have produced a large number of particular choices. We are attempting to assess their relative merits in the hope of obtaining useful general principles.

Boundary value problems resulting from sufficient optimality conditions and their index
Roswitha März
(Humboldt-University Berlin)

Under standard assumptions, if the boundary value problem (BVP)

$$\begin{pmatrix} A(t)(B(t)x(t))' \\ -B(t)^*(A(t)^*\psi(t))' \\ 0 \end{pmatrix} = \begin{pmatrix} C(t) & 0 & D(t) \\ W(t) & C(t)^* & S(t) \\ S(t)^* & D(t)^* & K(t) \end{pmatrix} \begin{pmatrix} x(t) \\ \psi(t) \\ u(t) \end{pmatrix}, \ t \in [0,T], \tag{1}$$

$A(0)B(0)x(0) = y_0,\ B(T)^*A(T)^*\psi(T) = Vx(T)$, has a solution triple x_*, ψ_*, u_*, then u_*, x_* form a minimizer of the quadratic cost function

$$J(u,x) := \frac{1}{2}x(T)^*Vx(T) + \frac{1}{2}\int_0^T \{x(t)^*W(t)x(t) + 2x(t)^*S(t)u(t) + u(t)^*K(t)u(t)\}dt$$

subject to the DAE

$$A(t)(B(t)x(t))' = C(t)x(t) + D(t)u(t),\ t \in [0,T],\ A(0)B(0)x(0) = y_0. \tag{2}$$

Necessary and sufficient index one conditions for the DAE (1) and further relations concerning the index of the DAE (2) and that of the DAE (1) will be discussed. Finally, Hamiltonian properties will be considered.

Exponential integrators for parabolic problems
Alexander Ostermann
(Universität Innsbruck)

Exponential integrators have been developed for the numerical solution of stiff differential equations. More precisely, the are intended for problems where the solution of the linearization contains fast decaying or highly oscillatory components. The construction of exponential integrators is problem-adapted in the sense that essential properties of the exact solution of a prototypic equation are identified and incorporated in the numerical scheme.
In my talk I will discuss the construction of exponential integrators for linear and nonlinear parabolic problems. The resulting integrators are somehow related to Rosenbrock and W-methods. In spite of this similarity, exponential integrators require their own error analysis. This analysis will be carried out in an abstract framework of sectorial operators. Besides convergence properties, also practical issues will be addressed in my talk. In particular, the approximation of the occuring matrix functions by Krylov-type methods will be discussed.
The talk is based on joint work with Marlis Hochbruck.

Stability analysis of frequency-dependent one step mixed collocation methods for y"=f(x,y)
Beatrice Paternoster, Marco Carpentieri
(Dipartimento di Matematica e Informatica, University of Salerno (Italy))

We are concerned with the linear stability analysis of mixed collocation Runge–Kutta–Nyström (RKN) methods for the second order Ordinary Differential Equations $y'' = f(x, y)$, having periodic or oscillatory solutions.
In the case that an accurate estimate of the period or of the dominant frequency is a priori available, it might be advantageous the usage of exponentially–fitted methods, whose parameters depend on the product of the frequency and the stepsize (see for example [1] and references herein contained). Some of them are based on collocation through trigonometric and mixed polynomials [2, 3, 4], which are particularly suitable to reproduce oscillatory solutions.
In this talk we analyze the modification of the stability properties of collocation–based RKN methods, when these methods are reformulated in such a way to fit the predicted frequency through collocation with trigonometric and mixed polynomials [2, 3, 4]. In particular we consider the influence of the collocation nodes on the stability region, analysing in details the case of Gauss–Legendre, Radau and Lobatto mixed collocation methods.

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A numerical study of forest fire initiation

Valeri Perminov

(Belovo Branch of Kemerovo State University)

In the present paper it is planned to develop mathematical model for description of heat and mass transfer processes in overterrestrial layer of atmosphere at crown forest fire spread, taking into account their mutual influence. It will be constructed as a result of an analysis of existing forest fire models. Within the limits of the earlier applied models overterrestrial layer of atmosphere and the combustion front are considered as separate components or otherwise approximate relationships are used for description of their interaction. It doesn't allow to describe nonstationary phenomena proceeding in the environment in a concrete way. The forest canopy is considered as a homogeneous two temperatures, reacting, non - deformed medium. Temperatures of condensed (solid) and gaseous phases are separated out. The first includes a dry organic substance, moisture (water in the liquid-drop state), condensed pyrolysis and combustion products (coke, ash), mineral part of forest fuels components. In the gaseous phase we separate out only the components necessary to describe reactions of combustion (oxygen, combustible products of pyrolysis of forest fuels and the rest inert components). The solid phase constituting forest fuels has no intrinsic velocity, and its volumetric fractions, as compared to the gaseous phase, can be neglected in appropriate equations. It is considered that 1) the flow has a developed turbulent nature, molecular transfer being neglected, 2) gaseous phase density doesn't depend on the pressure because of the low velocities of the flow in comparison with the velocity of the sound, 3) forest canopy is supposed to be non-deformed porous medium. To describe the transfer of energy by radiation we use a diffusion approximation, while to describe convective transfer controlled by the wind and gravity, we use Reynolds equations for turbulent flow. The research is done by means of mathematical modeling of physical processes. It is based on numerical solution of Reynolds equations for turbulent flow taking into account for diffusion equations chemical components and equations of energy conservation for gaseous and condensed (for canopy) phases. In this context, a study - mathematical modeling - of the conditions of forest fire initiation that would make it possible to obtain a detailed picture of the change in the velocity, temperature and component concentration fields with time. To obtain discrete analogies a method of control volume of S.V.Patankar is used. Grid equations, which arose during discretisation, were solved by SIP method. Calculation method and program have been check. The boundary-value problem is solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions are calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting are then integrated. A discrete analog for equations is obtained by means of the control volume method using the SIMPLE like algorithm. The accuracy of the program is checked by the method of inserted analytical solutions. Analytical expressions for the unknown functions are substituted in the system of differential equations and the closure of the equations are calculated. This is then treated as the source in each equation. Next, with the aid of the algorithm described above, the values of the functions are inferred with an accuracy of not less than 1As a result of mathematical modeling the fields of temperatures, mass concentrations of components of gaseous phase, volume fractions of components of solid phase, as well as vectorial fields of velocity at different instants of time with taking into account mutual influence of the overterrestrial layer of atmosphere and a crown fire on each other will be obtained. It allows to investigate conditions of forest fire initiation and spread under influence of various external conditions: a) meteorology conditions (air temperature, wind velocity etc.), b) terrain, c) type (various kinds of forest combustible materials) and their state (load, moisture etc.). The model proposed above is universal the same equations describe the state of the medium inside the forest canopy and in the near-ground layer of atmosphere, while the appropriate components of the database are used to calculate the specific properties of the various forest strata and the near-ground layer of atmosphere. This type of approach substantially simplifies the technology of solving problems of predicting the state of the medium in the fire zone numerically. Using modern computers, current numerical methods, and the model presented above, we can determine fields of velocity, temperature, and component concentration, density, and heat fluxes, and predict the development of a forest fire in a given region with due regard for seasonal changes in the properties of the forest fuels. Since, owing to the requirements of ecological safety,

large-scale experiments under field conditions are rarely permissible, mathematical modeling of forest fires using the model presented above is the very convenient method of studying the nature, limiting conditions of spread, structure and energetic of a forest fire.

Numerical analysis of structure preserving Nyström methods for Hamiltonian systems
Andreas Pfeiffer, Martin Arnold
(German Aerospace Center (DLR) Oberpfaffenhofen , Germany)

Long-term simulations of time depending ordinary differential equations often require numerical integration methods with higher stability and smaller errors than classical methods like Runge-Kutta or BDF. Geometric time integration algorithms preserving structures of the dynamical system are well suited for meeting these requirements [HLW02].
An energy conserving Galerkin type approach of Betsch and Steinmann [BS00] for N-body problems is generalized to modified Nyström methods for Hamiltonian systems. This consideration allows us to transfer existing results for classical Nyström methods such as symmetry or preservation of invariants to the modified versions.
For the modified methods there exist well defined numerical solutions under regularity conditions which also guarantee that there is no order reduction compared to the underlying classical Nyström methods.
As one result we get symmetric and reversible integration methods of any order of convergence which conserve energy, linear and angular momentum. Numerical experiments with many different Nyström methods show the feasibility, the theoretical achieved properties of the numerical solution and the benefits in long-term simulations.
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Two-step W-methods
Helmut Podhaisky, Rüdiger Weiner, Bernhard A. Schmitt
(University Halle)

Space discretization of reaction-diffusion problems yields large stiff systems of ODEs. For 2D and 3D problems implicit integration methods lead to huge linear systems of algebraic equations and Krylov methods have become popular for their solution.
We give an overview of the construction of linearly implicit two-step schemes. We consider schemes with the 'builtin' use of (an approximation to) the Jacobian. In contrast to well known one-step Rosenbrock- or W-methods, we pass additional information from step to step (representing approximations to the solution or its derivative at different timepoints). Potential advantages of this multistage-multistep structure include: (i) high stage order, (ii) accurate predictors, (iii) full order independent of the approximation to the Jacobian (W-method), (iv) parallelism.
For two classes of two-step W-methods we discuss stability properties (zero-, A-, L-stability) and the accuracy of the methods. We describe an implementation using Krylov techniques for the solution of the linear systems. The performance of the methods on large stiff test-problems is discussed and compared with the Krylov-BDF-code VODPK.

Multi Time Scale ODEs for Simulating Frequency Modulated Signals
Roland Pulch
(Technische Universität München)

Radio-frequency (RF) circuits are characterised by quasiperiodic signals with widely separated time scales. In the case of autonomeous time scales, frequency modulation occurs in addition to amplitude modulation. Correspondingly, standard ODE integration techniques demand exorbitant computing time. Based on a multidimensional signal model, an efficient alternative is given by modelling the ODE system as a multi time scale ODE, or MPDE model with periodic boundary conditions.
In this contribution, we present time domain methods for these systems that integrate along characteristic curves, and thus are consistent with the inherent information transport. Since the MPDE model demands the computation of local frequencies, too, additional boundary conditions are necessary. Though different choices are conceivable, we propose a special choice for the boundary condition. Test results confirm that time domain methods based on the multidimensional model are feasible for computing efficiently frequency modulated quasiperiodic signals in RF applications.

Dynamic Simulation of a Recycle Methanol Reactor Loop with Deactivating Catalyst
M.R. Rahimpour
(Shiraz University)

A detailed heterogeneous dynamic model described by a set of partial differential and algebraic equations (PDAEs) was developed to predict the performance of the industrial fixed bed methanol reactor loop in the face of catalyst deactivation. The dynamic recycle models was found to predict the daily observed process data of a methanol plant for four years of operation and good agreement was found. By analyzing the results of the model, it was shown that there is a non-uniform catalyst deactivation along the reactor. Simple model, of the type presented here, represents a useful beginning in the optimization and control of reactor for methanol synthesis loop reactor, since it is capable of describing many of the qualitative trends observed with such reactors. Patterns observed with the two models were quite similar due to the high flow rate of reacting materials through the reactor and in the nature of interaction between phases in the industrial methanol reactor. The dynamic model is explored to examine the effect of catalyst deactivation on the reactor performance. This work shows the influences of catalyst deactivation on the reactor performance. Results of the dynamic simulation of the reactor indicate that the concentrations of all components are time dependent variables at each point along the reactor. Also the results show that there is a non-uniform distribution of catalyst deactivation along the reactor. The reactor model presented here may be used to obtain an optimum strategy in re-using part of the deactivated catalyst from the current run in the next run. Doing so results requires a complex numerical solution which is currently in progress by our research group.
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Adaptive Methods for the Numerical Solution of the General Second Order Differential Equations.
A. Sesappa Rrai Rai, U. Ananthakrishnaiah
(Mahe, University)

The paper deals with Numerical methods , involving higher order derivatives for the numerical integration of the General Second Order initial value problems. The method involves two arbitrary parameters p and q which are dependent on the coefficient of the first derivative of y and y in the given differential equation. The method becomes absolutely stable when applied to linear homogeneous second order differential equations with constant coefficients. Numerical results are presented for the Legendre, Bessel's and Van der pol's equations

Perturbation index of linear PDAE
Joachim Rang, Lutz Angermann
(TU Clausthal)

For numerous problems in science and engineering a refined modeling approach leads to initial-boundary value problems for partial differential-algebraic equations (PDAEs). The paper investigates linear PDAEs from the point of view of weakly differentiable in space solutions. The appropriate treatment of boundary conditions is obtained by the requirement that the spatial differential operator has to satisfy a Gårding-type inequality in suitable function spaces. Based on this, an index concept extending the classical perturbation index is introduced.

A Fully Lagrangian Particle Method for Large Scale Geophysical Fluid Dynamics
Sebastian Reich
(Imperial College London)

In the process of mathematical modelling and/or numerical approximations, a scaling or error analysis identifies small terms. These terms are then neglected on the tacit assumption that small errors in the equations of motion cause only small errors in the solutions to these equations. This assumption is, however, in general untrue. On the other hand, the basic governing equations of geophysical fluid dynamics (GFD) always have an underlying Hamiltonian structure and an associated system of symmetry properties and conservation laws. Recent research on dynamical systems has only reemphasized the importance of these characteristics in determining the large time qualitative behavior of geophysical fluids. Hence the combination of formal accuracy *plus* the proper conservation laws is a better guarantee of an acceptable approximation than is formal accuracy by itself. In numerical analysis this has led to the methodology of *geometric integration*.
Geophysical fluid dynamics – the fluid dynamics of rotating, stratified fluids – is normally described by what are called the *primitive equations*. On a more simplified and abstract level, theorists frequently regard the ocean (or the atmosphere) as a two-layer fluid. This is the model we will also work with during my talk. I will start with a review of the model and some basic GFD concepts such as baroclinic and barotropic motion as well as the geostrophic and rigid-lid approximations. In the second part of my talk I will describe a fully Lagrangian spatial discretization of the two-layer model that results in a finite dimensional set of Hamiltonian equations (with holonomic constraints in the case of the rigid-lid approximation) which can be time-stepped by a symplectic integrator. I will then briefly discuss conservation properties of the numerical method. In the final part of my talk I will present some numerical results.

Discontinuous Galerkin Methods for Flow and Transport in Porous Media
Volker Reichenberger
(IWR, Universität Heidelberg)

We present a discontinuous Galerkin (DG) method based on the method of Oden, Babuska and Baumann for applications in subsurface transport. The method is used for the solution of the elliptic flow equation, where we use a multigrid method for the fast solution of the arising algebraic equations, and for the solution of the transport equation, where we combine the DG space discretization with higher order explicit Runge-Kutta schemes in the convection-dominated case and with diagonally implicit Runge-Kutta schemes in the diffusion-dominated case. Numerical results are presented for single-phase flow in heterogeneous media, solute transport and two-phase flow.

An Adjoint Approach to Optimal Design in Fluid Dynamics
Peter Rentrop, Sven-Olaf Stoll, Utz Wever
(TU München)

Shape design problems in fluid mechanics lead to large optimization problems with pde constraints. We discuss optimization problems governed by the Euler gas equations with the geometry parameters as design variables.
Optimization algorithms like BFGS or SQP require the gradient of the objective function in each iteration step. Therefore it is important to provide this information in an efficient way. Obvious possibilities like finite differences or the discrete and continuous sensitivity equation method are computationally very expensive since they require the solution of one additional partial differential equation per design parameter.
As a way out we use the adjoint method, in which the gradient is computed via the dual problem. The calculation of the gradient then reduces to the solution of the Euler and the adjoint equation and some algebraic computations in each optimization step. We present the properties of the adjoint equations and show some numerical examples.

Implicit parallel peer methods for stiff initial value problems
Bernhard A. Schmitt, Rüdiger Weiner, Kilian Erdmann
(Universität Marburg)

We introduce a new type of implicit multi-stage methods suitable for the parallel solution of stiff initial value problems. The main difference to standard methods is that all s stage solutions are approximations of equal accuracy and no distinguished variable is used (in contrast to Runge-Kutta methods, for instance). The s 'peer' solution approximations for each time step are computed from those of the previous step in parallel. Hence this method has a two-step structure and its stability is influenced by the stepsize ratio of the mesh. We construct methods having order $s-1$ and identify one subclass which is zero-stable and stiffly accurate for variable stepsizes with bounded stepsize ratio. The tool is a structural result on diagonal matrices subject to a Vandermonde similarity transformation. We analyse these schemes on singularly perturbed problems and show that no order reduction occurs. Numerical tests on several problems show that only in critical situations these nonlinear schemes have an advantage over linearly implicit peer methods proposed earlier by the first two authors.

Mixed Discontinuous Galerkin Methods for Saddle Point Problems
Dominik Schoetzau
(University of Basel, Dept. of Mathematics)

We first discuss mixed discontinuous Galerkin methods in the context of incompressible fluid flow problems. The derivation of these methods is explained for velocity-pressure elements of equal and mixed order. It is shown that these elements satisfy a generalized inf-sup stability condition leading to optimal order of convergence. Numerical results demonstrate that the methods perform well for a wide range of Reynolds numbers. We then apply similar techniques in the context of the time-harmonic Maxwell's equations and present a discontinuous Galerkin discretization of the Maxwell operator in mixed form chosen to provide control on the divergence of the electric field. Our theoretical and numerical results indicate that the methods give a promising alternative to standard edge and face elements.

Runge-Kutta type methods for differential algebraic equations of high index
Johannes Schropp
(University of Cologne)

We analyze Runge-Kutta type methods applied to differential algebraic eqautions of index ≥ 3 in Hessenberg form. The convergence properties are analyzed and the geometric features of the numerical and the exact solutions are compared. Finally, numerical examples are provided.

On circuit simulation and Abstract Differential Algebraic Systems
Steffen Schulz
(Humboldt University Berlin)

Today circuit simulation using Differential Algebraic Equations plays a vital role in modern circuit design. When using Partial Differential Equations to model semiconductor devices we have to consider coupled systems of PDEs and DAEs called Partial Differential Algebraic Equations. Considering a simple PDE it will be shown how these equations can be treated as Abstract Differential Algebraic Systems existing in real Hilbert spaces. We put special emphasis on how the tractability index for DAEs can be generalized for these systems.

The Definition of DAEs with tractability index 3 and practical index determination
Irina Schumilina
(Humboldt University, Berlin)

Many technical applications, such as electrical circuit simulation, control theory and other areas, lead to differential-algebraic equations (DAE). The index is an important property of DAEs. There are various index-notions: the differentiation index, tractability index, strangeness index and many others. It is important for the applications the development of sufficient algorithms, that determine practically the index of DAEs.

Numerical analysis of DAEs from coupled circuit and device simulation
Monica Selva
(Humboldt University of Berlin)

We consider a network formed by an RLC circuit and one diode. The mathematical model of this network combines the differential algebraic equations of the circuit with partial differential equations modelling the behavior of the diode. In this work we propose a block–iteration method to obtain an approximate solution to this problem and study the properties of the system of differential–alegraic equations that results from the coupling of the discretized diode equations and the DAE associated to the circuit.

On convergence acceleration of collocation and least-squares method for Navier-Stokes equations
Leonid Semin, Vitaly Belyaev, Vasily Shapeev
(Institute of Theoretical and Applied Mechanics SB RAS)

Two approaches are realized to accelerate iteration convergence for the previously constructed collocation and least-squares method for Navier-Stokes equations (L.G. Semin, V.P. Shapeev. Computational Technologies, 1998, Vol.3, No. 3, p. 72-84). In the multigrid variant of the method, motion through levels of multigrid complex is performed from the coarsest grid to the finest grid. While finding the approximate solution on the immediate level, the iterations are stopped when the difference between two solutions on two sequencing iterations run up to given small value, whereupon the grid is uniformly refined. In the variant realized, the grid step was halved at the grid refinement. The solution found is taken as the initial approximation for further calculations. This allows one to reduce sufficiently the number of iteration and, hence, total calculation time, as compared with the case of finding the solution immediately on the grid fine enough for the necessary accuracy to be obtained.
Another approach for accelerating iteration convergence is based on projecting the solution error of system of linear algebraic equations on the subspace of residuals of previous iterations consequence. Here the coefficients of the error expansion by residuals are found from the requirement of the minimum squared norm of residual. This approach proved to be effective when solving the problems for Navier-Stokes equations, giving iteration number becoming many times smaller. That is why its combination with multigrid technology is of considerable computational interest.

Implicit finite-difference scheme with approximation error $O(\tau^4, h^8)$ for the heat conduction equation
Vasily Shapeev
(Institute of Theoretical and Applied Mechanics SB RAS)

Implicit two-layer difference scheme $DS_{(4,8)}$ with residual term $R(\tau, h) \sim O(\tau^4, h^8)$, where τ and h are grid steps in time and space, is constructed for one-dimensional heat equation. The scheme stencil consists of 10 points: 5 points on the bottom time layer and 5 points on the upper layer. The scheme formulas were find by the method of indefinite coefficients under condition that its residual term $R(\tau, h)$ on solution of the differential problem had the highest possible order of smallness with respect to τ and h [1,2]. In so doing, according to the definition of compact difference schemes, all dependencies between solution derivatives for the heat conduction equation and all its differential consequences were taken into account. Quantities τ and h in the scheme formulas serve as parameters. For particular τ and h it is possible to construct schemes of higher approximation orders.
In solving Dirichlet's problem for approximating heat conduction equation in near-boundary points the scheme $DS_{(4,8)}$ was completed by well-known scheme $DS_{(2,4)}$ on six-point stencil with $R(\tau, h) \sim O(\tau^2, h^4)$. Convergence of the difference solution was tested on problems with known exact solutions. In numerical experiments on a succession of grids at τ and h tending to zero it was found out that difference solution of Dirichlet's problem for scheme $DS_{(4,8)}$ combined with $DS_{(2,4)}$ converges with at least sixth order. Here, for a particular stencil the $R(\tau, h)$ tends to zero corresponding to the approximation order on functions, satisfying the heat conduction equation but not being the exact solutions of the difference scheme. In case of $\tau = ch^2$, $c = 0.16605...$, terms of order $O(\tau^4, h^8)$ in $R(\tau, h)$ are mutually cancelled, and the residual term of the scheme $DS_{(4,8)}$ becomes a quantity of the tenth order of smallness.
It is established that numerical calculations with a given high accuracy by compound scheme $DS_{(4,8)} \bigcup DS_{(2,4)}$ demand much less grid nodes and computational time, than on scheme $DS_{(2,4)}$ alone. The higher accuracy we need, the more advantageous is the first scheme.

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Time Integration of Constrained Variational Problems in Elastoplasticity
Bernd Simeon
(TU München, Zentrum Mathematik)

This talk introduces, implicit Runge-Kutta methods for the dual problem of elastoplasticity. The choice of Runge-Kutta time integration is inspired by the problem structure, which consists of a coupled system of balance equations and unilaterally constrained evolution equations and which can be viewed as infinite-dimensional differential-algebraic equation. Focussing first on the time axis and leaving the space variables continuous, a grid-independent existence and uniqueness result is given for the class of coercive Runge-Kutta methods. Moreover, contractivity preservation and convergence are shown for methods that are in addition algebraically stable. Finally, space discretization by the FEM and time integration are combined and 2d simulation results are presented.

Modelling the Dynamics of nonlinear Partial Differential Equations Using Neural Networks
Nejib Smaoui
(Kuwait University)

The dynamics of two nonlinear partial differential equations (PDEs) known as the Kuramoto-Sivashinsky (K-S) equation and the 2-d Navier-Stokes (N-S) equations are analyzed using Karhunen-Loeve decomposition and artificial neural networks (ANN). For the K-S equation, numerical simulations using a pseudo-spectral Galerkin method is presented at a bifurcation parameter a =17.75, where a dynamical behavior represented by a heteroclinic connection is obtained. We apply K-L decomposition on the numerical simulation data with the task of reducing the data into a set of data coefficients. Then, we use artificial neural networks to model, and predict the data coefficients at a future time. It is found that training the neural networks with only the first data coefficient is enough to capture the underlying dynamics, and to predict for the other remaining data coefficients. As for the 2-d Navier-Stokes equation, a quasiperiodic behavior represented in phase space by a torus is analyzed at a Reynolds number, Re = 14.0. Applying the symmetry observed in the 2-d Navier-Stokes equation on the quasiperiodic behavior, eight different tori were obtained. We show that by exploiting the symmetries of the equation and using K-L decomposition in conjunction with neural networks, a smart neural network model is obtained.

An implicit-explicit Runge-Kutta-Chebyshev scheme for diffusion-reaction equations
Ben Sommeijer, Jan Verwer
(CWI, Amsterdam)

An implicit-explicit (IMEX) extension of the Runge-Kutta-Chebyshev (RKC) scheme designed for parabolic PDEs is proposed for diffusion-reaction problems with severely stiff reaction terms. The IMEX scheme treats these reaction terms implicitly and the diffusion terms explicitly. Within the setting of linear stability theory, the new IMEX scheme is unconditionally stable for reaction terms having a Jacobian matrix with a real spectrum. For diffusion terms the stability characteristics are the same as in RKC. A numerical comparison for a stiff, nonlinear radiation-diffusion problem between an RKC solver, an IMEX-RKC solver and the popular BDF-based solver VODPK, using the Krylov solver GMRES, illustrates the performance of the new IMEX scheme.

Analysis of error growth in numerical initial value problems
Marc Spijker
(Leiden University)

This talk concerns the numerical treatment of systems of ordinary differential equations (ODEs), such as arise when the method of lines is used in the context of time-dependent partial differential equations. We will deal with the analysis of error growth, for linear multistep methods (LMMs) applied to such systems of ODEs. The focus will be on conditions, in terms of the stability regions of these methods, which are to guarantee a mild error propagation (stability).
It is well known that one can arrive at a completely wrong assessment of the actual error propagation mechanism, when performing a standard stability analysis based on the eigenvalues specified by the right-hand member of the ODE. For this reason, in the literature, stability conditions were formulated in terms of epsilon-pseudo-eigenvalues; very interesting results in this direction were obtained notably by Reddy and Trefethen (1990, 1992), Lubich and Nevanlinna (1991), Toh and Trefethen (1999).
In this talk, the natural question will be addressed of whether the known stability results for LMMs, based on the use of epsilon-pseudo-eigenvalues, are best possible. Recent conclusions concerning this question, obtained in a joint research with Karel in 't Hout, will be presented. It will be seen that, rather surprisingly, some of the known results are sharp, whereas others can substantially be improved and extended.

Distributed time integration in full chip design
Michael Striebel
(Infineon Techologie AG München)

In full chip design the verification of the behaviour of large digital circuits and dynamic memories is very important. Charge oriented modified nodal analysis (MNA) usually yields differential or differential-algebraic network equations which are integrated numerically.
Due to the complexity of the underlying circuit the network equations are often given by coupled DAE-systems describing coupled subcircuits. In many applications it can be seen that different subcircuits have got different levels of activity at one time, i.e. latency occurs within the overall system. To fasten up the integration of the network equations one can exploit this effect using multirate schemes which work on different time discretisations, i.e. different stepsizes for different subsystems and deal with the coupling in an appropriate way.
Based on mixed-multirate for ODEs and charge oriented ROW-schemes for index-1 DAEs a first 2-level-multirate-method for special index-1 problems occuring in circuit simulation is presented. To derive order conditions for this ROW-type method MDA-trees and -series, related to the well known B-trees and B-series, are introduced. Finally first approaches towards n-level-multirate-methods will be shown.

Modeling and Simulation of German Railway Cable Systems
Gunnar Teichelmann
(Technische Universität München)

In pursuit of higher speeds and lower costs in railroad traffic the use of computers for the simulation of the catenary's dynamic becomes necessary. High-speed trains in particular require an continuous power supply. Therefore the computation of the nonlinear dynamical interaction of pantograph and catenary is vital for the prediction of mechanical wear and driveable speed. After modelling the systems partial differential algebraic equations a finite element method is applied for semi discretization in space. The Gear/ Gupta/ Leimkuhler - stabilisation then creates a differential algebraic equation of index 2, which can be solved by backward difference formulas. Now numerical results corroborate the gained experience of the last century. Here some examples of these effects will be presented. Especially the influence of stitch wires will be seen with respect to material fatigue of the droppers and also effects of wave propagation and reflection at mass points.

Convergence of variable stepsize linear multistep methods for singular perturbation problems
Mechthild Maria Thalhammer
(University of Innsbruck)

In this talk, we investigate the stability and convergence behaviour of variable stepsize linear multistep methods applied to singularly perturbed problems of the form

$$y' = f(y,z), \qquad \varepsilon z' = g(y,z)$$

involving a small parameter $0 < \varepsilon \ll 1$. Following [3], we extend the convergence estimate given in [1] for linear multistep methods with constant stepsizes to variable stepsizes. Besides, we specify a refined estimate for the widely used class of backward differentiation formulas. Important ingredients in our convergence analysis are stability bounds for non-autonomous linear problems. For the derivation of such stability results, we employ techniques that are similar to those used in [2].

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Numerical Analysis of PDAEs
Caren Tischendorf
(Humboldt University of Berlin)

Motivated by coupled circuit and device simulation, we are interested in the numerical behavior of PDAEs describing coupled systems of parabolic/elliptic PDEs and DAEs. Considering all space-dependent real valued functions $(x,t) \mapsto u(x,t)$ as functions $t \mapsto u(t)$ with values in a suitable Sobolev space, PDAEs can be treated as differential-algebraic systems

$$\mathcal{A}(\mathcal{D}u(t))' + \mathcal{B}(u(t),t) = 0$$

with operators $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{D}$ acting in real Hilbert spaces. We call such systems abstract differential-algebraic systems (ADASs) following the terminology used in the theory of PDEs.
Based on the decoupling approach for DAEs, an analogous concept will be presented for abstract DAEs. This leads to an index definition for abstract systems and informations about suitable initial and boundary conditions for unique solvability of coupled systems.
Finally, we present a Galerkin approach for handling linear ADASs with monotone and bounded operators. The most interesting aspect consists in the choice of basis functions. By a suitable choice, the Galerkin equations are DAEs of index 1 and their solution converges against the solution of the abstract system.

Exponentially fitted quadrature rules
Marnix Van Daele, G. Vanden Berghe, H. Vande Vyver
(Universiteit Gent)

We consider the integral

$$I(f) = \int_1^{-1} f(x)dx \ ,$$

where $f(x)$ shows an oscillatory behaviour, and its computation by means of an N-point quadrature formula, i.e.,

$$I(f) \approx \sum_{k=1}^{N} w_k f(x_k) \ .$$

To derive these methods, we will rely on the formalism of Ixaru [1]. For each number of abscissae N, we will obtain a variety of methods for which the weights w_k and abscissae x_k depend upon a parameter ω, but for $\omega \to 0$, all the quadrature rules considered will reduce to the well known N-point rule of Gauss-type. We will mainly focus onto two questions : (i) what is the behaviour of the nodes and the weights in terms of the frequency and (ii) which methods can be used to compute highly oscillatory integrands?
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Discontinuous Galerkin Discretization with Interior Boundary Conditions
Marc Van Raalte
(CWI)

We introduce a discretization of Discontinuous Galerkin (DG) type for solving a 2-D second order elliptic PDE on a structured regular rectangular grid, while the boundary value problem has a curved Dirichlet boundary. According to the same principles that underlie DG-methods, we adapt the discretization in the cell in which the (embedded) Dirichlet boundary can not follow the gridlines of the orthogonal grid.
The DG-discretization aims at high order of accuracy. We discretize the 2-D Poisson equation, with a curved embedded Dirichlet boundary condition, with tensor products of cubic polynomials. By construction, such a DG discretization is fourth order consistent, both in the interior and on the boundaries. Stability is proved for the one-dimensional Poisson equation with an embedded boundary condition. By experiments we show fourth order convergence.

Exponential fitted Runge-Kutta methods of collocation type
Hans Van de Vyver, Guido Vanden Berghe, Marnix Van Daele
(University Ghent)

Exponential fitted s-stage Runge-Kutta (EFRK) methods of collocation type are methods which exactly integrate a maximum set of $s+1$ linearly independent functions of the form

$$\{1, x, \ldots, x^K, \exp(\pm\omega), x\ \exp(\pm\omega), \ldots, x^P\ \exp(\pm\omega) | \omega \in R \text{ or } i\,R,\ K + 2\,P = s - 2\}.$$

Two stage EFRK methods of collocation type are constructed. Two different classes of EFRK methods are considered: methods with fixed knot points and methods with frequency ω-dependent knot points. For both cases we have obtained extensions of the classical two stage LobattoIIIA, RadauIIA and Gauss methods. For these methods applied to scalar equations, a study of the local truncation error is made, out of which follows a simple heuristic to estimate the ω-value. In the case of a system of differential equations a seperate ω is used for each component such that the EFRK method becomes a partitioned method. Numerical examples reveal important differences between methods with fixed and variable knot points.

Krylov-Rosenbrock-Methods for DAEs of index 1
Jörg Wensch, Helmut Podhaisky
(University Halle)

The derivation of Rosenbrock-Krylov methods for index 1 DAEs involves two well known techniques: a limit process which transforms a singular perturbed ODE to an index 1 DAE and the use of Krylov iterations instead of direct linear solvers for the stage equations. We show that our derived class of Rosenbrock-Krylov schemes is independent of the order in which we apply these techniques. We also conclude that for convergence a rather accurate solution of the algebraic part is always needed.

Time-integration schemes for atmospheric multiphase processes
Ralf Wolke, Oswald Knoth, Aissa-Mounir Sehili, Judit Zoboki
(Institute for Tropospheric Research Leipzig)

The interactions between aerosols, gases and clouds in the troposphere are of increasing importance for the comprehension of atmospheric processes. The model equations resulting from such complex multiphase chemical systems are non-linear, highly coupled and extremely stiff. In the paper, several numerical approaches for treating such processes are investigated for a box model. The particle spectrum is subdivided into several classes. This multi-fractional distribution and the microphysical variables (liquid water content, supersaturation, temperature) are generated simultaneously by a cloud model. In a ”dynamical” approach, the very fast dissociations in the aqueous phase chemistry are described as forward and backward reactions. This leads to large and stiff ODE systems. For the integration of these systems, higher order BDF schemes and the ROS2 method with approximate matrix factorisations and adapted linear system solvers are used. The developed direct sparse solvers exploit the special block structure of the corresponding Jacobian. Furthermore, it is investigated how much an instantaneous treatment of dissociations stabilizes the solution behaviour. This corresponds to a reformulation of the given system of differential equations as a DAE system. The efficiency and accuracy of the time-integration schemes is discussed for four multiphase chemistry systems of different complexity and for a different number of droplet classes.

Finding practical general linear methods
Will Wright
(University of Bergen)

General linear methods with inherent Runge-Kutta stability (IRKS) provide an alternative to the traditional Runge-Kutta and linear multistep methods. The IRKS methods have high stage order, are diagonally implicit and have stability regions identical to those of certain Runge-Kutta methods. One useful property of the IRKS methods is that the methods can be computed using only linear operations. An approach used to find practical IRKS methods is to search for methods where the underlying one-step method (which was developed by Stoffer) has minimal error coefficients. The tools used to construct the underlying one-step method recursively will be explained and numerical evidence will be given.

Approximate Momentum Conservation for Spatial Semidiscretizations of Semilinear Wave Equations
Claudia Wulff, Marcel Oliver, Matt West
(University of Surrey)

We prove that a standard second order finite difference uniform space discretization of the nonlinear wave equation with periodic boundary conditions, analytic nonlinearity, and analytic initial data conserves moentum up to an error which is exponentially small in the stepsize. Our estimates are valid for as long as the trajectories of the full nonlinear wave equation remain real analytic.
The method of proof is that of backward error analysis, whereby we construct a modified equation which is itself Lagrangian and translation invariant, and therefore also conserves momentum. This modified equation interpolates the semidiscrete system for all time, and we prove that it remains exponentially close to the trigonometric interpolation of the semidiscrete system. These properties directly imply approximate momentum conservation for the semidiscrete system.
We also consider discretizations that are not variational as well as discretizations on non-uniform grids. Through numerical example as well as arguments from geometric mechanics and perturbation theory we show that such methods generically do not approximately preserve momentum.

Numerical stability investigations using the joint spectral radius approach
Marino Zennaro, Nicola Guglielmi
(University of Trieste)

The stability analysis of numerical methods for differential equations often leads to study the asymptotic behaviour of the solutions of linear difference equations with variable coefficients. Therefore, it is important to have efficient procedures available for such investigations.
It is known that the asymptotic behaviour of the solutions of a linear difference equation may be described by studying the asymptotic behaviour of the products of the companion matrices associated to the difference equation (as the number of factors goes to infinity). When the difference equation has constant coefficients, there is just one constant companion matrix for which it is sufficient to evaluate the spectral radius. On the contrary, when the coefficients are variable, the companion matrices may be even infinitely many and, in any case, they do not reduce to one constant matrix. Therefore, a satisfactory stability analysis may be done only by evaluating (or, at least, by approximating sufficiently well) the so called joint spectral radius (j.s.r.) of the family of all the companion matrices. In particular, the asymptotic stability of all the solutions is guaranteed by the condition $\mathrm{j.s.r.} < 1$.
In this talk, after outlining some basic results concerning the j.s.r. available in the literature and some new results that we obtained recently, we illustrate how the j.s.r. approach may be successfully applied to analyze the stability properties of some numerical methods for ordinary and delay differential equations.

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