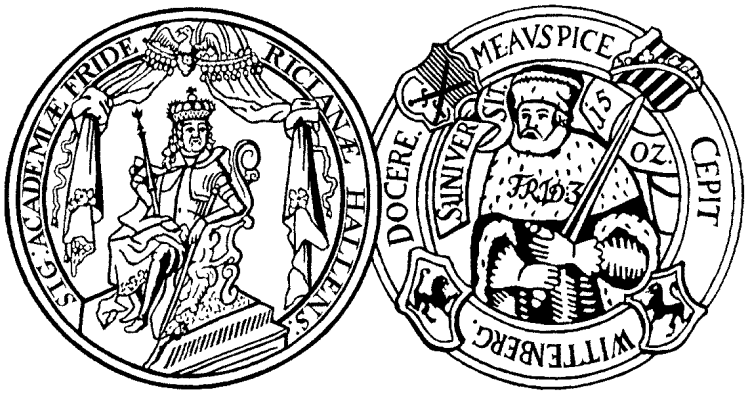
MARTIN–LUTHER UNIVERSITÄT
HALLE–WITTENBERG
FACHBEREICH MATHEMATIK UND
INFORMATIK



9th Seminar on
Numerical Solution of Differential and
Differential–Algebraic Equations

NUMDIFF–9

4 September — 8 September, 2000
Halle (Germany)

Programme and Abstracts

The seminar NUMDIFF–9 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)
- Pieter J. van der Houwen (Amsterdam)
- Ben P. Sommeijer (Amsterdam)
- Jan G. Verwer (Amsterdam)

The organizing committee would like to thank

- Ilona Tischler
- Alf Gerisch
- Helmut Podhaisky

for their committed assistance in preparing the seminar.

Acknowledgements

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- Kultusministerium des Landes Sachsen–Anhalt
- Deutsche Forschungsgemeinschaft

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- ComTelco
- Daimler Chrysler AG
- Sun Microsystems GmbH

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

Contents

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1 General Information

1. **Conference Location and Lecture Rooms**
   The conference will take place in the lecture rooms A, B, and Z on the ground floor of the *Melanchthonianum* situated on the *Universitätsplatz* in the centre of Halle.

   Opening and closing of the seminar as well as plenary lectures (Monday to Friday morning, except Tuesday) take place in lecture room B. In addition, the lecture rooms A and Z are used for minisymposia (Tuesday morning) and contributed talk sessions (Monday, Tuesday, and Thursday afternoon).

2. **Conference Office and Registration**
   The conference office is also situated in the *Melanchthonianum*. The conference office is open on Sunday, September 3, 2000 from 4 p.m. to 8 p.m., on Monday, Tuesday and Thursday from 8 a.m. to 4 p.m., and on Wednesday and Friday from 8 a.m. to 12 a.m. You can reach the conference office by phone (+49 (345) 5521045 or +49 (345) 5521048) and by fax (+49 (345) 5521047). These lines are active from Sunday, September 3, 2000.

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

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**
   A cafeteria is located in the *Juridicum* down the steps of the *Universitätsplatz*. Further, the *Mensa Harz* is a 5 minute walk away and around the *Marktplatz* there are different restaurants. Please ask local participants or the staff in the conference office for further information.

6. **E-mail**
   There will be a computer with telnet and internet access available in the conference office.

7. **Conference Dinner**
   The conference dinner will be held in the hotel *Steigenberger Esprix* in Halle–Neustadt on Thursday, September 7, 2000 at 19.30. The meal is included in the conference fee; participating students and accompanying persons pay DM 25. 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 the *Archäologisches Museum* of the university in the *Robertinum*. 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 to 1.5 hours.

   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 94097
   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, 2000.

2 Programme Overview

Monday, 4 September 2000

	Room B	Room A	Room Z
9.00	Opening Address		
9.20 – 10.10	Jan G. Verwer		
10.30 – 11.20	Claus Führer		
11.20 – 12.10	Wenfried Lucht		
14.00 – 14.25	Marc Spijker	Makky Jaya	Christian Grossmann
14.30 – 14.55	Amelia Garcia	Julia Novo	Zoltán Horváth
15.00 – 15.25	Jörg Wensch	Mansour A. Al-Zanaidi	Larisa Piddubna
15.45 – 16.10	David J. Lopez	Javier de Frutos	Marian Kwapisz
16.15 – 16.40	Guido Vanden Berghe	Andy Georges	Zbigniew Bartoszewski
16.45 – 17.10	Volker Grimm	Vasily P. Shapeev	Mohammad R. Rahimpour
17.15 – 17.40	Hans-Eberhard Scholz	Natalia Borovykh	Vadim Azhmyakov

Tuesday, 5 September 2000

	Room B	Room A	Room Z
8.30 – 12.50	Minisymposium: Partial Differential-Algebraic Equations	Minisymposium: Atmospheric Transport-Chemistry Problems	Minisymposium: Parallel Methods for Differential Equations
14.30 – 14.55	Roland England	Alexander Ostermann	Lidia Aceto
15.00 – 15.25	Inmaculada Higueras	Karel in ’t Hout	Angel Duran
15.45 – 16.10	Frank Cameron	Alf Gerisch	Valeri A. Perminov
16.15 – 16.40	René Lamour	Róbert Horváth	Faisal Fairag
16.45 – 17.10	Jürgen Sand	Hrant Hovhannissian	Zdzislaw W. Trzaska
17.15 – 17.40	Katalin Balla		Sergey Nurmagambetov

Wednesday, 6 September 2000

	Room B
8.30 – 9.20	Thomas Sonar
9.20 – 10.10	Roswitha März
10.30 – 11.20	Zdzislaw Jackiewicz
11.20 – 12.10	Stefan Vandewalle

Thursday, 7 September 2000

	Room B	Room A	Room Z
8.30 – 9.20	Marlis Hochbruck		
9.20 – 10.10	Philippe Chartier		
10.30 – 11.20	Ken R Jackson		
11.20 – 12.10	Cesar Palencia		
14.00 – 14.25	Renate Winkler	Mari Paz Calvo	Felice Iavernaro
14.30 – 14.55	Johannes Schropp	Mechthild Thalhammer	Ivonne Sgura
15.00 – 15.25	Caren Tischendorf	Roland Pulch	Marnix Van Daele
15.45 – 16.10	Carmen Arevalo	István Faragó	Tanja Van Hecke
16.15 – 16.40	Brahim Benhammouda	Joerg Sautter	Manouchehr Parsaei
16.45 – 17.10	Yauheni Sonets	Muhammed I. Syam	Alex Kolpakov

Friday, 8 September 2000

	Room B
8.30 – 9.20	Willem Hundsdorfer
9.20 – 10.10	David F. Griffiths
10.30 – 11.20	Gerhard Starke
11.20 – 12.10	Gerald Warnecke
12.10	Concluding Address

3 Scientific Programme

Monday, 4 September 2000

Room B

9.00	**Opening Address by Karl Strehmel** **Welcome by the rector of the Martin–Luther–University Halle–Wittenberg Magnifizenz Prof. Dr. W. Grecksch**
	Plenary Lectures
9.20 – 10.10	**Jan G. Verwer** Numerical Time Integration of Air Pollution Models
10.10 – 10.30	**— Break —**
10.30 – 11.20	**Claus Führer** & Carmen Arevalo & Monica Selva Variable Stepsize Extension of Multistep Formulas - A Review and new Approaches
11.20 – 12.10	**Wenfried Lucht** On quasi–linear PDAE's with convection
12.10 – 14.00	**— Lunch —**
	Contributed Talks
14.00 – 14.25	**Marc Spijker** Are the Stability Estimates, in the Kreiss Matrix Theorem, Sharp ?
14.30 – 14.55	**Amelia Garcia** & Pablo Martin New methods for oscillatory problems based on classical codes
15.00 – 15.25	**Jörg Wensch** Extrapolation methods in Lie groups
15.25 – 15.45	**— Break —**
15.45 – 16.10	**David J. Lopez** & Pablo Martin & Amelia Garcia A variable-stepsize variable-order multistep method for the integration of perturbed linear problems
16.15 – 16.40	**Guido Vanden Berghe** & L. Ixaru & H. De Meyer Exponentially-fitted Runge-Kutta methods: construction and implementation
16.45 – 17.10	**Volker Grimm** Exponential Integrators for Classical Molecular Dynamics
17.15 – 17.40	**Hans-Eberhard Scholz** Implicit Taylor series methods and stiff semi-linear initial value problems

Room A *Contributed Talks*

14.00 – 14.25 **Makky Jaya** & Claus-Dieter Munz
Modular Implementation of Navier-Stokes Equation Solver on Arbitrary/Hybrid Unstructured Meshes

14.30 – 14.55 **Julia Novo** & Javier de Frutos
Postprocessing the linear finite element method

15.00 – 15.25 **Mansour A. Al-Zanaidi** & M. M. Chawla
A linearly implicit one-step time integration scheme for second order nonlinear hyperbolic equations

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Javier de Frutos** & Julia Novo
A posteriori error estimation for evolutionary dissipative equations

16.15 – 16.40 **Andy Georges** & Marnix Van Daele
Acquiring a solution of the time-dependent Schrödinger equation using CP methods

16.45 – 17.10 **Vasily P. Shapeev** & Leonid G. Semin
Adaptive Collocation and Least-Squares Method for Navier-Stokes Equations

17.15 – 17.40 **Natalia Borovykh**
Stability in the numerical solution of the heat equation with nonlocal boundary conditions

Room Z *Contributed Talks*

14.00 – 14.25 **Christian Grossmann** & Zoltán Horváth
Two-sided enclosures for IVPs by means of bounding operators I: Construction of bounding operators and convergence properties

14.30 – 14.55 **Zoltán Horváth** & Christian Grossmann
Two-sided enclosures for IVPs by means of bounding operators II: Application to PDEs

15.00 – 15.25 **Larisa Piddubna** & Igor Cherevko
Approximations of coupled differential and difference equations by ordinary differential equations

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Marian Kwapisz**
On delay dependent error estimates for waveform relaxation methods for differential-functional equations

16.15 – 16.40 **Zbigniew Bartoszewski**
Numerical verification of delay dependent error estimates for WRM for differential-functional equations

16.45 – 17.10 **Mohammad R. Rahimpour** & A. Azrapour
Numerical Solution of a Nonlinear Model of Urea Hydrolysis Reactor

17.15 – 17.40 **Vadim Azhmyakov**
Newton-Type Method for Solving Non-regular Equations

Room B

Minisymposium: Partial Differential–Algebraic Equations (Karl Strehmel)

8.30 – 9.05 **Volker Mehrmann** & Thilo Penzl & Fredi Tröltzsch
Control of heterogeneous systems of partial and differential algebraic systems

9.05 – 9.40 **Martin Arnold**
Distributed time integration of coupled differential-algebraic systems

9.40 – 10.15 **Michael Günther**
Generalized descriptor formulation in electrical network analysis

10.15 – 10.30 **— Break —**

10.30 – 11.05 **Wieslaw Marszalek**
A boundary value problem for linear PDAEs

11.05 – 11.40 **Bernd Simeon**
A weak descriptor form for constrained motion in elastodynamics

11.40 – 12.15 **Jens Lang**
Adaptive Multilevel ROW-Methods for Nonlinear PDAEs

12.15 – 12.50 **Werner M. Seiler**
Involution Analysis of Semi-Discretisations of a Class of Linear Partial Differential Systems

12.50 – 14.30 **— Lunch —**

Contributed Talks

14.30 – 14.55 **Roland England** & René Lamour
Integration of Index-One Differential-Algebraic Equations using Dichotomically Stable One-Step Formulae

15.00 – 15.25 **Inmaculada Higueras**
On numerical contractivity for DAEs

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Frank Cameron** & Mikko Palmroth & Robert Piché
Low-order SDIRKS for DAEs

16.15 – 16.40 **René Lamour** & Diana Estevez Schwarz
The Computation of Consistent Initial Values for Nonlinear Index-2 Differential-Algebraic Equations

16.45 – 17.10 **Jürgen Sand**
On Implicit Euler for High-Order High-Index DAEs

17.15 – 17.40 **Katalin Balla**
Transfer equations and linear boundary value problems for DAEs

Room A

Minisymposium: Atmospheric Transport–Chemistry Problems (Jan G. Verwer)

8.30 – 9.05 **Martin Berzins** & A. Tomlin & S. Ghorai
Unstructured Adaptive Mesh Solvers for Atmospheric Dispersion Problems

9.05 – 9.40 **Mike Botchev** & Jan G. Verwer
Improving Approximate Matrix Factorizations for implicit time integration in Air Pollution Modelling

9.40 – 10.15 **Oswald Knoth** & Ralf Wolke
Coupled integration of chemistry and transport in microscale air quality modelling

10.15 – 10.30 **— Break —**

10.30 – 11.05 **Stig Skelboe**
Partitioning techniques for decoupled integration of chemical reaction equations

11.05 – 11.40 **Bruno Sportisse** & Rafik Djouad
Simulation of aqueous-phase chemistry in Air Pollution Modeling

11.40 – 12.15 **Ralf Wolke** & Oswald Knoth
Time-Integration of Multiphase Chemistry in Size-Resolved Cloud Models

12.15 – 12.50 **Zahari Zlatev**
Large-scale computations in air pollution modelling

12.50 – 14.30 **— Lunch —**

Contributed Talks

14.30 – 14.55 **Alexander Ostermann**
Stability of W-methods with applications to operator splitting

15.00 – 15.25 **Karel in 't Hout**
On the contractivity of implicit-explicit linear multistep methods

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Alf Gerisch** & Jan G. Verwer
Operator Splitting and Approximate Factorization for Taxis-Diffusion-Reaction Models

16.15 – 16.40 **Róbert Horváth**
On the Monotonicity Conservation of the Numerical Solution of the One-Dimensional Heat Equation

16.45 – 17.10 **Hrant Hovhannissian**
Five-pointed difference schemes for the equations of parabolic type

Room Z

Minisymposium: Parallel Methods for Differential Equations (Rüdiger Weiner)

8.30 – 9.05 **Luigi Brugnano** & Cecilia Magherini & Donato Trigiante
Blended Block Implicit Methods for the Numerical Solution of ODEs

9.05 – 9.40 **Francesca Mazzia** & Felice Iavernaro
Generalized Backward Differentiation Formulae for parallel implementation

9.40 – 10.15 **Jason Frank** & Pieter J. van der Houwen
Parallel Extended BDF Methods

10.15 – 10.30 **— Break —**

10.30 – 11.05 **Bernhard A. Schmitt** & Rüdiger Weiner & Helmut Podhaisky
On the stability of two-step-W-methods

11.05 – 11.40 **Helmut Podhaisky** & Bernhard A. Schmitt & Rüdiger Weiner
Numerical Experiments with parallel Two-step W-methods

11.40 – 12.15 **Nguyen Cong** & Nguyen Thi Hong Minh
Parallel PC iteration of pseudo RKN methods for nonstiff initial-value problems

12.15 – 12.50 **Dana Petcu**
Experiments with parallel methods for ODEs

12.50 – 14.30 **— Lunch —**

Contributed Talks

14.30 – 14.55 **Lidia Aceto**
The Pascal matrix and its relations with numerical methods for ODEs

15.00 – 15.25 **Angel Duran** & Miguel A. Lopez Marcos
Numerical behaviour of stable and unstable solitary waves

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Valeri A. Perminov**
Numerical modeling forest fire spread initiation

16.15 – 16.40 **Faisal Fairag**
A Two-level Finite Element Method for the streamfunction form of the Navier-Stokes Equations

16.45 – 17.10 **Zdzislaw W. Trzaska**
Solving Partial Differential Equations with Using Power Polynomials

17.15 – 17.40 **Sergey Nurmagambetov**
Quantum motion numerical calculation for axial channeling

Room B

Plenary Lectures

8.30 – 9.20 **Thomas Sonar**
From Finite Volume Approximations to Meshless Collocation for Hyperbolic Conservation Laws

9.20 – 10.10 **Roswitha März**
On properly formulated differential-algebraic systems

10.10 – 10.30 **— Break —**

10.30 – 11.20 **Zdzislaw Jackiewicz**
Construction and Implementation of General Linear Methods for Ordinary Differential Equations

11.20 – 12.10 **Stefan Vandewalle**
Multigrid dynamic iteration methods for delay differential equations

Room B

Plenary Lectures

8.30 – 9.20 **Marlis Hochbruck**
Exponential integrators

9.20 – 10.10 **Philippe Chartier** & R.P.K. Chan & A. Murua
Post-projected methods for index-2 DAEs

10.10 – 10.30 **— Break —**

10.30 – 11.20 **Ken R Jackson** & Ned Nedialkov
Validated Methods for IVPs for ODEs

11.20 – 12.10 **Cesar Palencia**
On the numerical recovery of holomorphic mappings and some applications to ill-posed problems

12.10 – 14.00 **— Lunch —**

Contributed Talks

14.00 – 14.25 **Renate Winkler**
Structural analysis for stochastic DAEs in circuit simulation

14.30 – 14.55 **Johannes Schropp**
Qualitative Properties of Discretizations for Index 2 DAE's

15.00 – 15.25 **Caren Tischendorf**
DAE Structure and Index in Dependence on MOSFET Modelling in Circuit Simulation

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Carmen Arevalo** & Steven Campbell
Unitary Coordinate Partitioning for General DAE Integrators

16.15 – 16.40 **Brahim Benhammouda**
A Partial Differential-Algebraic Equations Approach for Elastic Rods

16.45 – 17.10 **Yauheni Sonets** & V. V. Bobkov
Multistage algorithms for numerical solution of ODEs

Room A *Contributed Talks*

14.00 – 14.25 **Mari Paz Calvo** & Cesar Palencia
Avoiding the order reduction of Runge-Kutta methods for linear initial boundary value problems

14.30 – 14.55 **Mechthild M. F. Thalhammer** & C. Gonzalez & A. Ostermann & C. Palencia
The dynamical behaviour of Runge-Kutta time discretizations for nonlinear parabolic problems near an equilibrium point

15.00 – 15.25 **Roland Pulch**
A method of characteristics for solving multirate partial differential equations in radio frequency application

15.25 – 15.45 **— Break —**

15.45 – 16.10 **István Faragó** & C. Palencia
Sharpening the stability bound in the maximum-norm of the Crank-Nicolson scheme for one-dimensional heat equation

16.15 – 16.40 **Joerg Sautter**
Strategies for the Numerical Solution of the Navier-Stokes Equations

16.45 – 17.10 **Muhammed I. Syam**
Path Following-Collocation Method for Solving Burger's Equation

Room Z *Contributed Talks*

14.00 – 14.25 **Felice Iavernaro** & Francesca Mazzia
Block Boundary Value Methods used as General Linear Methods

14.30 – 14.55 **Ivonne Sgura** & Francesca Mazzia
Numerical Approximation of Nonlinear BVPs by means of BVMs

15.00 – 15.25 **Marnix Van Daele** & J. R. Cash
A new method to solve first order Systems of nonlinear two-point boundary value problems

15.25 – 15.45 **— Break —**

15.45 – 16.10 **Tanja Van Hecke** & Marnix Van Daele
Accuracy improvement with RKN methods

16.15 – 16.40 **Manouchehr Parsaei**
Coupled High Order Boundaries in Numerical Solution of Hyperbolic Equations

16.45 – 17.10 **Alex Kolpakov**
A second-order differential-finite-differences model

Room B

Plenary Lectures

8.30 – 9.20	**Willem Hundsdorfer** Splitting with Stabilizing Corrections
9.20 – 10.10	**David F. Griffiths** & I. Garrido & B. Ayuso Mixed finite element models: instability and its consequences
10.10 – 10.30	**— Break —**
10.30 – 11.20	**Gerhard Starke** Galerkin Least-Squares Methods for Parabolic Problems: Adaptivity in Space and Time
11.20 – 12.10	**Gerald Warnecke** Multiscale Problems in Numerics for Hyperbolic Conservation Laws
12.10	**Concluding Address**

4 Abstracts of Plenary Lectures

Post-projected methods for index-2 DAEs
Philippe Chartier & R.P.K. Chan & A. Murua
(INRIA, Campus Universitaire de Beaulieu, RENNES, France)

A new projection technique for Runge-Kutta methods applied to index-2 differential algebraic is presented in which the numerical approximation is projected only when an output is required. It is shown that for methods that are strictly stable at infinity, the order of convergence is unaffected compared to standard projected methods. Gauss methods, for which this technique is of special interest when some symmetry is to be preserved, are studied into more detail.

Variable Stepsize Extension of Multistep Formulas - A Review and new Approaches
Claus Führer & Carmen Arevalo & Monica Selva
(Lund University, Centre of Mathematical Sciences, Sweden)

Multistep methods are classically constructed by specially designed difference operators on an equidistant time grid. To make them practically useful, they have to be implemented by varying the step size according to some error control algorithm. It is well known how to extend Adams and BDF formulas to a variable step size formulation. In this talk we will discuss various possibilities to extend k-step methods of order $k+1$ in general. We will start from ideas developed by Skeel in the 70s and present some new results and approaches.

Mixed finite element models: instability and its consequences
David F. Griffiths & I. Garrido & B. Ayuso
(University of Dundee, UK)

This talk will address several issues relating to stability of mixed finite element approximations of elliptic systems. We will extend recent work of Babuška and Narasimhan on a one-dimensional problem and give simple proofs establishing the relationship between instability in the Babuška–Brezzi sense and rates of convergence. This model also allows clear illustrations of different stabilization techniques and their effects on convergence rates.
The second part of the talk will focus on mixed finite elements for the Stokes equations. We shall look at the way in which the one-dimensional results may be interpreted in this setting, on the influence of boundary data in unstable situations as well as the relationship between the spectra of continuous and discrete operators associated with questions of stability.

Exponential integrators
Marlis Hochbruck
(Mathematisches Institut, Heinrich-Heine Universität Düsseldorf, Germany)

An alternative to implicit methods for solving large systems of stiff or oscillatory differential equations is using exponential integrators. In contrast to implicit schemes, no solution of nonlinear systems of equations is required; only function evaluations and matrix vector products with the Jacobian. In this talk we intend to give an overview on several variants of exponential integrators. We start from a general purpose code constructed for the solution of large systems of time-

dependent differential equations. The basic idea of our exponential integrators is to solve a typical prototype of differential equation exactly. For instance, the general purpose code integrates affine linear equations $y' = Ay + b$ exactly. The implementation requires approximating the product of a matrix function, in this case an exponential function, and a vector. In our codes, suitable Krylov subspace methods are used for this task.
For special applications leading to oscillatory problems (e.g. second-order differential equations in which high-frequency oscillations are generated by a linear part, and Schrödinger equations with time-dependent Hamiltonian) we show that suitable exponential integrators allow time steps much larger than the inverse of the highest frequency and we present convergence results which are independent of the smoothness of the solution.

Splitting with Stabilizing Corrections
Willem Hundsdorfer
(CWI, The Netherlands)

In this talk several splitting methods are discussed that are based on Stabilizing Corrections, leading to splitting schemes with internal consistency for initial-boundary value problems for PDEs. Due to the internal consistency, given boundary data can be used directly in the scheme and steady states of the PDE remain steady states of the numerical scheme.
The most simple method of this kind consists of combinations of Euler and Trapezoidal Rule steps. For the heat equation with dimensional splitting these methods are related to classical ADI schemes of Douglas, Gunn and others. In this talk more general splittings for convection-diffusion-reaction equations are considered.
To obtain more accuracy and a better treatment of explicit terms several extensions of the simple Stabilizing Correction scheme will be regarded and analyzed. The relevance of the theoretical results is tested for convection-diffusion-reaction equations.

Construction and Implementation of General Linear Methods for Ordinary Differential Equations
Zdzislaw Jackiewicz
(Arizona State University, USA)

In the first part of this lecture we will give the overview of different approaches to the construction of diagonally implicit multistage integration methods for both nonstiff and stiff differential systems of ordinary differential equations. The identification of high order methods with appropriate stability properties requires the solution of large systems of nonlinear equations for the coefficients of the methods. For low orders these systems can be generated and solved by symbolic manipulation packages such as MATHEMATICA or MAPLE. For moderate orders these systems can be generated symbolically in FORTRAN format and then solved by algorithms based on the homotophy appoach such as PITCON, ALCON, or HOMEPACK. For high orders the approach to the construction of such methods is based on the computation of the coefficients of the stability function by a variant of the Fourier series method and then solving the resulting large systems of polynomial equations of high degree by least squares minimization with the aid of MINPACK subroutines based on Levenberg-Marquardt algorithm. Using these approaches both explicit and implicit methods were constructed up to the order eight with good stability properties (Runge-Kutta stability for

explicit methods, A-stability and L-stability for implicit methods).
In the second part of this talk we will address different issues related to the implementation of general linear methods. They include selection of initial stepsize and starting values, computation of Nordsieck representation, efficient and reliable estimation of the local discretization errors for nonstiff and stiff equations, step size ond order changing strategies, construction of continuous interpolants, and updating vector of external approximations to the solution. Experiments with variable step variable order experimental Matlab codes for both nonstiff and stiff differential systems on interesting test problems will be presented and compared with appropriate codes from Matlab ODE suite. These experiments demonstrate the high potential of diagonally implicit multistage integration methods, especially for stiff systems of differential equations.

Validated Methods for IVPs for ODEs
Ken R. Jackson & Ned Nedialkov
(Computer Science Dept., University of Toronto, Canada)

Compared to standard numerical methods for initial value problems (IVPs) for ordinary differential equations (ODEs), validated methods have two important advantages: if they return a solution to a problem, then

1. the problem is guaranteed to have a unique solution, and
2. an enclosure of the true solution is produced.

We survey validated methods for the numerical solution of IVPs for ODEs, describe several methods in a common framework, and identify areas for future research.
Papers on which this talk is based can be found at `http://www.cs.toronto.edu/~krj`

On quasi–linear PDAE's with convection
Wenfried Lucht
(Martin-Luther-Universität Halle-Wittenberg, Germany)

In the lecture, some aspects of systems of partial differential algebraic equations (PDAEs) for u of quasi–linear type with convection terms,

$$Au_t + Bu_{xx} + C[u]u_x + Du = f(t,x), \quad t \in I_t := (0,t_e), \quad t_e > 0, \quad x \in \Omega \subseteq \mathbb{R},$$

will be discussed. u and f are of type $u, f : I_t \times \Omega \to \mathbb{R}^n, \ n > 1$, where f (supposed to be sufficiently smooth) is given. $A,\ B,\ C[u]$ and D are real $(n,n)-$matrices where, for simplicity, $A,\ B$ and D are assumed to be constant. All matrices may be singular, but $A,\ B \neq 0$ (in particular, there is at least one time derivative of a component of u in the system). $C[u]$ may depend on u. Furthermore, it is supposed that there is $z \in \mathbb{R}^n$ such that $C[z] \neq 0$ (i.e. there is at least one derivative of first order with respect to x of some component of u). Typically, when $C[u]$ is linear in u, the vector $C[u]u_x$ describes physical convection. Terms of this form appear, e.g., in (one–dimensional) models based on continuum mechanics. An example used for illustration comes from plasma physics where $n = 4$ and $\mathrm{rank}(A) = \mathrm{rank}(B) = 2, \quad \mathrm{rank}(C(z)) = 3$.
For systems given above we consider initial boundary value problems (IBVPs) (with $\Omega = (0,1)$) and initial value problems (IVPs) (with $\Omega = \mathbb{R}$). In both cases appropriate initial values written in

the form $u(0,x) = \Phi_a(x) + \Phi_c(x), \quad x \in \overline{\Omega}$ or $x \in \Omega$, must be added, and for IBVPs, boundary values of a similar form, $u(t,x) = \Psi_a(t,x) + \Psi_c(t,x), \quad t \in \overline{I_t}, \quad x \in \partial\Omega,$ are needed. The data which can be prescribed arbitrarily are in $\Phi_a,\ \Psi_a$. The consistent data are collected in $\Phi_c,\ \Psi_c$.

First, the problem of determination of indexes of the PDAE is discussed. Since the methods of linear PDAEs (based on Fourier and Laplace transformations) cannot be applied to the PDAE given, we determine the index by means of the invertibility of certain differential operators. The method is illustrated by the PDAE from plasma physics.
Furthermore, some methods for the numerical solution of IBVPs by means of finite differences are developed. First, a functional iteration for a semidiscretization of the system with time index $\nu_t = 1$ is considered. It is shown by a fixed point argument that the method converges under definite assumptions. However, the convergence is only local in time. Second, we consider the numerical solution of IBVPs or IVPs by means of operator splitting methods combined with factorizations. These methods are generalizations of fractional step techniques well known for the numerical solution of classical time dependent partial differential equations. Among others, the splitting methods are investigated for PDAEs with indexes $\nu_t = 1$. Some theoretical results concerning stability are given. The more difficult case $\nu_t = 2$ is also mentioned.

In the last part of the lecture some results of numerical experiments are presented.

On properly formulated differential-algebraic systems
Roswitha März
(Humboldt-Universität zu Berlin, Institut für Mathematik, Germany)

Beyond the scope of the formal integrability theory, an equation

$$f(x'(t), x(t), t) \tag{1}$$

with an everywhere singular leading Jacobian $f'_y(y,x,t)$ is somehow inaccurately formulated. A priori, neither an appropriate function space which the solutions should belong to nor properties of the respective map representing the equation emerge from this. However, thinking on possible generalizations such as PDAEs and control problems with (generalized) DAEs to be controlled one should clear up the fundamental background rigorously.
Equations of the form

$$f((Dx)'(t), x(t), t) = 0 \tag{2}$$

with well-matched matrices $f'_y(y,x,t)$ and $D(t)$ are said to be properly formulated DAEs. The matrix function D precisely figures out all those derivatives of the unknown function that are actually involved in the equation. Naturally, a solution should be a continuous function $x(.)$ having a continuously differentiable part $(Dx)(.)$.
Note that there is no need at all for $D(t)$ to be a projector matrix. However, previous reformulations of (1) like $f((Px)'(t) - P'(t)x(t), x(t), t) = 0$ by means of projector functions $P(t)$ are of type (2).
Quasilinear equations $A(t)x'(t) + b(x(t),t) = 0$ are often rewritten as

$$(Ax)'(t) + b(x(t),t) - A'(t)x(t) = 0, \tag{3}$$

or, equivalently, in type (2) form

$$R(t)(Ax)'(t) + b(x(t), t) - R(t)A'(t)x(t) = 0,$$

where $R(t)$ denotes a projector onto im $A(t)$.
Recent results on DAEs of the form (2) will be reported. In particular, a unified approach to linear DAEs $A(Dx)' + Bx = 0$ and their adjoint equations $D^*(A^*y)' - B^*y = 0$ (instead of $Ax' + Bx = 0$ and $(A^*y)' - B^*y = 0$ formerly) is possible now. A consequence for an optimal control problem will be discussed.

As far as numerical integration methods applied to (2) are concerned, it will be shown whether resp. why a qualitatively correct reflection of the asymptotic solution behaviour may be expected.

On the numerical recovery of holomorphic mappings and some applications to ill-posed problems
Cesar Palencia
(Universidad de Valladolid, Spain)

A method for the numerical reconstruction of an analytical mapping from knowledge of approximate values at a finite set of nodes is presented. This algorithm is shown to be helpful for the numerical treatment of a variety of ill-posed problems: the backwards heat equation, the one side heat equation and some problems in potential theory.

From Finite Volume Approximations to Meshless Collocation for Hyperbolic Conservation Laws
Thomas Sonar
(TU Braunschweig, Germany)

We describe the design of essentially non-oscillatory and weighted essentially non-oscillatory finite volume approximations to hyperbolic conservation laws on triangular meshes. Emphasis is laid on the recovery process which is essential not only for high order of accuracy but also for stability. This class of methods is now fairly well understood from a computational point of view, although a convergence analysis for general hyperbolic systems is still missing.
In contrast, meshless collocation methods are still in a state of infancy. Basic questions concerning conservativity, order of accuracy, etc. are unanswered. However, in employing modern tools from numerical analysis like nonlinear anisotropic dissipation terms and multiscale analysis of discrete data there is hope that this class of schemes can be developed into numerical workhorses in the near future.

Galerkin Least-Squares Methods for Parabolic Problems: Adaptivity in Space and Time
Gerhard Starke
(University of Essen, Germany)

In this talk, a class of Galerkin least-squares methods for parabolic initial-boundary value problems is presented and analyzed. These methods are based on the minimization of a least-squares functional for an equivalent first-order system over time and space with respect to suitable discrete

spaces. One of the most important features of the least-squares methodology is the built-in a posteriori estimator for the approximation error. This is a consequence of the least-squares functional to the consistency error associated with a time-step, measured in an appropriate norm. For our presentation, we focus our attention to the specific combination of piecewise linear, not necessarily continuous, functions for the flux with continuous piecewise linears for the scalar variable for the time discretization. The discretization in space uses standard $H(div)$ and H^1 conforming finite element spaces, respectively. A detailed convergence analysis of these methods will be given for linear parabolic problems. Moreover, we address the problem of identifying the components in the least-squares functional associated with the discretization error in time and space, respectively. This leads to adaptive strategies for the proper balance of time-step choice and spatial mesh refinement.

Multigrid dynamic iteration methods for delay differential equations
Stefan Vandewalle
(Katholieke Universiteit Leuven, Dept of Computer Science, Belgium)

The dynamic iteration method, also called waveform relaxation method, extends the applicability of classical iterative methods, such as Jacobi, SOR, and multigrid, to systems of differential equations. The method offers great potential for good parallel performance. It has been applied primarily to solve systems of equations derived by discretization of parabolic PDEs. The convergence theory of the method for that type of problem is nowadays well understood.
Recently, the method was applied to delay ordinary and partial differential equations. Such equations arise for example in population dynamics, in numerical control, and in the study of nonlinear materials with memory. Earlier work concentrated on Jacobi- and Gauss-Seidel type iterations. In this talk we will concentrate on the multigrid acceleration.
First the type of equation that is considered will be defined. It will be shown that delay PDEs exhibit quite different stability characteristics than classical partial differential equations. Then, the application of waveform relaxation and its multigrid acceleration will be illustrated by means of a number of examples. Special emphasis will be put on techniques for variable coefficient problems. Finally, the convergence of the method will be studied by using a two-level Fourier analysis technique.

Numerical Time Integration of Air Pollution Models
Jan G. Verwer
(Center for Mathematics and Computer Science (CWI), The Netherlands)

Partial differential equations of the advection-diffusion-reaction type lie at the heart of all modern air pollution models. These PDEs are used to describe advective transport in given wind fields, turbulent/diffusive transport, chemical reactions, emissions and depositions of many natural and anthropogenic atmospheric species. The equations are time-dependent, three-space dimensional and nonlinearly coupled through the chemical reactions. Numerical research is of high relevance since modern models require excessive amounts of computer time so that efficient, state-of-the-art numerical algorithms are needed.
In this lecture we will first introduce the application field. After this introduction, several of the most important numerical algorithms in use will be discussed, including the popular operator split-

ting method and a Rosenbrock method from the stiff ODE field which provides an alternative to operator splitting by means of approximate matrix factorization. The performance of these methods will be illustrated using data from a real model. If time permits we will also discuss the Rosenbrock method for the spherical Shallow Water Equations. The SWEs are an important prototype for numerical research into atmospheric circulation.

Multiscale Problems in Numerics for Hyperbolic Conservation Laws
Gerald Warnecke
(Otto-von-Guericke-Universität Magdeburg, Germany)

There is an increased demand for numerical calculations of solutions to problems modeled by hyperbolic systems of conservation laws with additional dissipative terms and stiff source terms. These type of problems arise for instance when considering inviscid flows with combustion or mixing multi-phase flows. These problems a characterized by the presence of widely varying length and time scales, e.g. characteristic speeds, shocks, boundary layers, reaction zones. Small scales may only be present locally in the solution. The choice of minimal spatial mesh lengths and time steps leads to a cut-off of smaller scales. Adaptive methods, here not being restricted to mesh refinement only, are needed to take small scale information into account incase this influences the larger scales being resolved in the numerical calculation.

The talk will focus on the use of adaptive methods for overcoming well known problems arising in numerical calculations. Typical unwanted features are wrong shock speeds and the appearance of unphysical states. Depending on the nature of the applications and various priorities, different ways of handling these problems must be considered in order to guarantee correct and efficient calculations. The use of mesh adaptive methods employing a posteriori error estimation techniques for unsteady problems is just one possible option. Substructured solvers may be an alternative in some instances.

A fundamental goal in numerics is to guarantee *accuracy* as well as *efficiency*. This is also what is essentially behind the issue of stiffness. Numerical methods may become highly inefficient if the problem changes due to a small parameter. Numerics has to react to a singular limit once the limit is reached within prescribed accuracy, whereas the underlying analytical problem only changes in the limit. This is where especially error estimation, stability analysis and solver adaption play an important role.

An adaptive numerical scheme contains two main elements. The first is the *adaption criterion* which tells us if and where we want to modify our numerical solution. This could be an a posteriori error indicator, a stiffness detector or a feature detector, e.g. shock indicator or a symmetry indicator. The criterion itself usually tells us very little about how we want to modify the solution in order to overcome a detected problem. This is the second element in an adaptive algorithm, namely the *adaption method*. There is a wide range of possibilities. We know various forms of local or global mesh adaption. One can adapt the solution space, for instance to modify the order of the method. One can adapt solvers, e.g. by using flux limiters or by explicit/implicit switching. An important question is whether the adapted solution just looks good or is actually better. A long term goal of numerical analysis for CFD is to give us reliable criteria and to link these to the methods employed, i.e. to prove that the solution is generally improved by the adaptive method.

The theory of a posteriori error estimation using residuals is a key element of the validation of

numerical calculations as well as useful tool in adaptive algorithms. By 'a posteriori' we mean that the information given by the estimator is calculated from the computed solution. Assuming that the model equations adequately represent the physical problem, we need such a tool in order to assess whether solutions to the equations are well approximated by the scheme used. We need it to detect stiffness. We also need it in adaptive algorithms in order to efficiently distribute the workload in demanding calculations. Though adaptive methods based on heuristic error indicators are highly successful in CFD, the mathematical theory is still in its infancy. The concepts are generally inferred from the better developed theories for elliptic and parabolic problems, where a rigorous theory is possible.

The presentation will expand on the issues raised above and present recent work on adaptive flow calculations as well as a solver for detonation waves that avoids wrong shock speeds and spurious physical states.

5 Abstracts of Minisymposia Talks

5.1 Atmospheric Transport–Chemistry Problems

Unstructured Adaptive Mesh Solvers for Atmospheric Dispersion Problems
Martin Berzins & A.Tomlin & S.Ghorai
(The University of Leeds, UK)

It has been shown that the accuracy of solution for atmospheric pollution dispersion problems is highly dependent on the computational mesh and in particular the degree of resolution. Coarse meshes cannot resolve the underlying structure and uniformly fine meshes are prohibitively expensive for reactive flow problems with a large number of chemical species.
A solution to this problem is to provide extra resolution of the mesh where large solution errors or steep concentration gradients exist, leaving a coarse resolution elsewhere. In this way computational resources are utilised where they provide significant gains in accuracy. This talk presents a 3-D finite volume reactive flow model based on a transient adaptive unstructured mesh. The use of tetrahedral mesh elements allows fully 3-D adaptivity and the flexibility to enable the code to handle complex structures arising from source terms of very different spatial scales. The underlying algorithm makes use of positivity preserving finite volume methods, fast iterative solvers, mesh adaptation and parallel computing.
Preliminary studies of dispersion from a single source in stable, unstable and neutral boundary layers have been carried out. The results show the efficiencies of using adaptive grids in order to represent the accurate structures of the plume in the boundary layer and also the advantage of this method compared to fixed methods for mesh refinement. Some comments about the interpolation of input data such as wind fields onto unstructured meshes are also made.
Examples will be described for a number of different pollution dispersion problems covering a range of meteorological conditions. Results will demonstrate that the adaptive model is capable of achieving accuracy close to that of fixed high resolution meshes at a fraction of the computational cost.

Improving Approximate Matrix Factorizations for implicit time integration in Air Pollution Modelling
Mike Botchev & J.G.Verwer
(CWI, Amsterdam, The Netherlands)

For a long time operator splitting was the only computationally feasible way of implicit time integration in large scale Air Pollution Models. A recent attractive alternative are Rosenbrock schemes combined with Approximate Matrix Factorization (AMF) [1]. With AMF, linear systems arising in implicit time stepping are solved approximately in such a way that the overall computational costs per time step are not higher than those of splitting methods [1,2].
We propose and discuss two new variants of AMF. The first one is aimed at yet further reduction of costs as compared with conventional AMF. The second variant of AMF provides in certain circumstances a much better approximation to the inverse of the linear system matrix than standard AMF and requires the same computational work.
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Coupled integration of chemistry and transport in microscale air quality modelling
Oswald Knoth & Ralf Wolke
(Institute of Tropospheric Research, Leipzig, Germany)

We compare different time integration methods for modelling atmospheric chemistry transformations inside urban street canyons. The necessary wind and dispersion fields are simulated simultaneously by a microscale atmospheric fluid model with a spatial resolution between 1-5 m or taken as a snapshot from this model. Since the transport time scale for this model application is in the range of 1 second integration schemes proposed for mesoscale or long range transport may be not appropriate. We will focus on low order implicit methods with an iterative solution of the resulting linear systems. Depending from the time scales and stiffness of the different processes involved the use of approximate Jacobian matrices is investigated. Parallel implementation aspects are discussed.

Partitioning techniques for decoupled integration of chemical reaction equations
Stig Skelboe
(University of Copenhagen, Denmark)

The chemical reaction equations are often partitioned into subsystems to permit more efficient numerical solution. A partitioned system can be solved using various strategies such as the Euler Backward Iterative method (block Gauss-Seidel) or waveform relaxation.
While these methods iterate until convergence and therefore give identical results to the underlying integration formulas, the decoupled implicit Euler and BDF2 methods presented in this talk avoid the relaxation until convergence. This strategy is, in general, more efficient than the two above mentioned methods or classical implementations. However, a poor partitioning will jeopardize the accuracy or even the stability of the discretization.
This talk presents partitioning techniques which permit the use of just one or two relaxation iterations in the decoupled integration formula while maintaining accuracy and stability.
The partitioning techniques and decoupled implicit integration formulas will be demonstrated for a system of 56 chemical reaction equations in an air pollution model.

Simulation of aqueous-phase chemistry in Air Pollution Modeling
Bruno Sportisse & Rafik Djouad
(ENPC- CEREVE, France)

Regional Air Pollution Models describe the time and space evolution of some trace gases through Reaction-Diffusion-Advection PDEs subject to appropriate Boundary Conditions.
We describe here the simulation of aqueous-phase chemistry. The interfacial transfer between gaseous and aqueous phases has indeed to be taken into account since this may strongly influence the concentrations of gas-phase species.
We focus on numerical and mathematical issues: what is the validity of the lumped parameter

assumption (due to the large values of molecular diffusivities) ? How to solve the set of coupled stiff ODEs ? How to reduce this system ? What is the sensitivity wrt some physical parameters (such as the radius of aqueous droplets) ?

Time-Integration of Multiphase Chemistry in Size-Resolved Cloud Models
Ralf Wolke & Oswald Knoth
(Institute of Tropospheric Research, Leipzig, Germany)

An important subject of atmospheric chemistry is to assess with more accuracy the role of clouds on pollutants. The existence of cloud drops leads to a transfer of chemical species between the gaseous and aqueos phases. Species concentrations in both phases are modified by chemical reactions and by this phase transfer. The model equations resulting from such multiphase chemical systems are nonlinear, highly coupled and extremely stiff depending on the time of the day. In the paper we investigate several numerical approaches for treating such processes. The droplets are subdivided into several classes. The very fast dissociations in the aqueous–phase chemistry are treated as forward and backward reactions. The aqueous–phase and gas–phase chemistry, the mass transfer between the different droplet classes among themselves and with the gas phase are integrated in an implicit and coupled manner by the second order BDF method. For this part we apply a modification of the code LSODE with an adapted step size control and a special linear system solver. This direct sparse solver exploits the special structure of the equations. Furthermore we investigate an approximate matrix factorization which is related to operator splitting at the linear algebra level. The sparse Jacobians are generated explicitly and stored in a sparse form. The efficiency and accuracy of our time–integration schemes is discussed for four multiphase chemistry systems of different complexity and for a different number of droplet classes.

Large-scale computations in air pollution modelling
Zahari Zlatev
(National Environmental Research Institute, Roskilde, Denmark)

Air pollution models are described mathematically by systems of partial differential equations (PDEs). By using different discretizations of the spatial derivatives and different splitting techniques, the systems of PDEs are reduced to several large systems of ordinary differential equations (ODEs), which have to be treated numerically at every time-step. The number of equations in every ODE system is equal to the product of the number of grid-points and the number of chemical species. This number is normally very large; up to several millions. If the time-interval is long, then the number of time-steps is also very large; up to several thousands. Finally, many scenarios with different values of some key parameters have to be run. This explains why the use of efficient numerical methods and parallel computers is crucial in the treatment of large-scale air pollution models. The choice of the numerical methods and the organization of the parallel computations will be discussed in this talk.

5.2 Partial Differential–Algebraic Equations

Distributed time integration of coupled differential-algebraic systems

Martin Arnold
(DLR German Aerospace Center, Vehicle System Dynamics Group Oberpfaffenhofen, Germany)

The term *partial differential-algebraic equation* (PDAE) summarizes various types of coupled instationary differential equations (ordinary and partial differential equations, differential-algebraic systems). The increasing interest in the analysis and efficient numerical solution of such coupled systems is mainly motivated by complex technical applications that require the coupled simulation of qualitatively different physical phenomena.

Typically the overall system consists of a (small) finite number of subsystems that are coupled by source terms and/or boundary conditions. The numerical solution of PDAEs combines space discretization (performed, e. g., by FEM or FDM) and time discretization. In the talk we focus on the *time* integration of the coupled system that may be based on a coupling of standard time integration methods for the subsystems.

In this modular approach the time integration for the overall system is *distributed* to several separate integration methods for the individual subsystems. Classical techniques from the theory of ordinary differential equations are the use of different time steps in different subsystems (multi-rate approach), the coupling of different time integration methods (multi-method approach), and the iterative refinement by waveform relaxation or dynamic iteration methods.

In the application to more complex coupled systems like coupled differential-algebraic systems or PDAEs these classical techniques may, however, result in exponential instability. Additional projection steps may be necessary to satisfy some *contractivity conditions* that guarantee stability and convergence of the distributed time integration.

The results of the error analysis are applied to the dynamical simulation of coupled mechanical systems.

Generalized descriptor formulation in electrical network analysis

Michael Günther
(Universität Karlsruhe (TH), Fachbereich Mathematik, IWRMM, Germany)

To cover parasitic and second order effects in network analysis, a refined description based on models of partial differential equations can overcome problems due to higher and high index descriptor formulations, which are caused by coupling controlled sources of arbitrary type. This ansatz generalizes the descriptor formulation to initial-boundary value problems of coupled systems of partial differential (PDEs) and differential-algebraic (DAEs) equations, for short systems of partial differential algebraic equations (PDAE systems). With interconnected electrical circuits as an example in mind, we analyze the analytical properties of these systems with respect to existence, uniqueness and sensitivity. Connections can be derived to dynamic extended saddle-point problems, with constraint currents in the role of Lagrangian multipliers. Generalizing the concepts of perturbation index for DAEs and a-priori estimates for PDEs, we can analyze the impact of semidiscretization on the approximate DAE systems. We will see that some companion models for interconnects, which can be regarded as a-priori non-adaptive semidiscretizations with respect to space, lead to an artificial deregularization or regularization, resp., of the underlying PDAE system.

Adaptive Multilevel ROW-Methods for Nonlinear PDAEs
Jens Lang
(ZIB Berlin, Germany)

In this talk, we concentrate on nonlinear PDAEs which can be written in the form

$$B(x,t,u)\partial_t u = \nabla \cdot (D(x,t,u)\nabla u) + F(x,t,u,\nabla u)$$

with suitable boundary and initial conditions. The vector–valued solution $u = (u_1, \ldots, u_m)^T$ is supposed to be unique and temporally smooth, at least after an initial transition phase. In order to solve such systems efficiently, an adaptive algorithm is proposed, where linearly implicit methods of Rosenbrock–Wanner type in time are coupled with multilevel finite elements in space. A posteriori error estimates are used to assess the local discretization errors and to choose time steps and mesh sizes automatically during the integration.
Practically relevant applications that arise in today's semiconductor–device fabrication, fluid dynamics, and porous media modelling are presented to illustrate the performance of the proposed method.

A boundary value problem for linear PDAEs
Wieslaw Marszalek
(DeVry Institute of Technology, USA)

We analyze a boundary value problem for linear partial differential algebraic equations, or PDAEs, by using the method of separation of variables. The analysis is based on the Kronecker-Weierstrass form of the matrix pencil $[A, -\lambda_n B]$. This BVP PDAE problem differs in many ways from the conventional BVPs considered in the literature on DAEs. A new theorem is proved and two illustrative examples are given.

Control of heterogeneous systems of partial and differential algebraic systems.
Volker Mehrmann & Thilo Penzl & Fredi Tröltzsch
(Fakult. f. Mathematik, TU Chemnitz, Germany)

We consider control problems for generalized state-space systems

$$E\dot{x}(\tau) = Ax(\tau) + Bu(\tau)$$

with output equation

$$y(\tau) = Cx(\tau)$$

arising from the semi-discretization of heterogeneous systems of partial differential equations and algebraic equations.
Here $E, A \in R^{n,n}$, $B \in R^{n,m}$, and $C \in R^{q,n}$, are large and sparse , and the input/output dimensions m and q are small.
We use model reduction techniques based on the balanced truncation method to derive a small scale model from which we compute the optimal feedback control and then use this feedback control for the large scale problem.

The necessary Lyapunov equations are solved iteratively and approximately by the low rank cyclic Smith method which is justified by the large decay of the singular values of the solution of the Lyapunov equation.

Involution Analysis of Semi-Discretisations of a Class of Linear Partial Differential Systems
Werner M. Seiler
(Universität Mannheim, Germany)

We study a class of non-normal, linear, first order systems of partial differential equations. Typical representatives consist of a hyperbolic evolution system and some elliptic constraints (like Maxwell's equations of electrodynamics). We compare the completion to involution of the original system of partial differential equations with the completion of differential algebraic equations arising from it by semi-discretisation. Somewhat surprisingly, it turns out that the condition for involution are the same in both cases. Thus the stronger concept of involution and not just formal integrability (i.e. the absence of integrability conditions) is decisive for the numerical integration of general systems of partial differential equations.

A weak descriptor form for constrained motion in elastodynamics
Bernd Simeon
(University of Karlsruhe, Germany)

Constrained mechanical systems including both rigid and elastic bodies are a focus of current research in computational mechanics. They meet the increasing demand for refined simulation in vehicle dynamics, robotics, and in air- and spacecrafts. While rigid bodies form discrete systems in space and are easily modelled by differential-algebraic equations, their elastic counterparts satisfy the partial differential equations of elastodynamics. Mutual coupling is accomplished by constraints formulated for isolated spatial points or parts of the boundary.
The talk presents a general framework for the treatment of constraints in elastodynamics and introduces the notion of a *weak descriptor form* which comprises both rigid body systems and mixed systems and which can be considered as a descriptor form model in both space and time. With respect to space discretization, there is a connection to mixed and hybrid finite element methods and to domain decomposition techniques. Using these techniques, a convergence proof for the space discretization is given.

5.3 Parallel Methods for Differential Equations

Blended Block Implicit Methods for the Numerical Solution of ODEs
Luigi Brugnano & Cecilia Magherini & Donato Trigiante
(Universitá di Firenze, Italy)

Currently, a great variety of numerical methods for differential equations is available. In particular, when dealing with the numerical solution of stiff problems, there are a lot of stable - high order methods. As a consequence, the definition of new methods is relevant only if they do posses good features for their actual implementation. In such a category, for example, fall many families of

Runge-Kutta methods and, more recently, Block BVMs. A more recent instance, is obtained by considering a suitable ”blend” of (possibly different) block methods [1,2], for which a natural nonlinear splitting is defined. In the talk, some of the most recent results concerning this approach are presented, which seems to be promising, even for the construction of parallel solvers.

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Parallel PC iteration of pseudo RKN methods for nonstiff initial-value problems

Nguyen Cong & Nguyen Thi Hong Minh

(Faculty of Mathematics, Mechanics and Informatics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam, Vietnam)

This talk discusses parallel iteration schemes for pseudo RKN for solving special second-order nonstiff initial-value problems. By using pseudo RKN methods as correctors, the resulting parallel PC Methods can be well provided with high-order predictors without additional costs, and require for a given order of accuracy, less computational efforts, less number of processors when compared with the parallel PC iteration process applied to classical Gauss-Legendre RKN correctors.

Parallel Extended BDF Methods

Jason Frank & P.J. van der Houwen

(CWI, The Netherlands)

The extended backward differentiation formulas (EBDFs) for solving ordinary differential equations were introduced in the 1980s by J. Cash. These methods are stiffly accurate; and L-stable methods are known to exist up to order 6. Furthermore, recent experience with the ‘Testset for Initial Value Problems’ shows a variable stepsize variable order method based on the EBDFs to be quite efficient compared to other popular methods from the literature. We have studied a number of possible modifications to these methods which make them suitable for implementation on shared memory parallel computers.

As originally formulated, the EBDFs area general linear methods(GLMs) having a lower triangular coefficient matrix A. In the serial case, a desirable property of A is a constant diagonal entry, since this allows reuse of the iteration matrix in all stages. From the parallel point of view, the defective spectrum of A precludes diagonalization, the standard approach to parallelizing GLMs. In our investigations we consider two alternatives: (1) iterating with an approximation to A which *is* diagonalizable, and (2) reformulation of the EBDF methods on a staggered grid such that A does have a complete spectrum.

Tests with these methods using a fixed stepsize code indicate that a reasonable speedup can be obtained in parallel on 3-4 processors.

Generalized Backward Differentiation Formulae for parallel implementation
Francesca Mazzia & Felice Iavernaro
(Dipartimento di Matematica, Universitá di Bari, Italy)

Generalized Backward Differentiation Formulae (GBDFs) are a class of Boundary Value Methods that numerically solve the m dimensional Initial Value Problems

$$\begin{cases} y'(t) = f(t,y), & t \in [t_0, t_0+T], \\ y(t_0) = y_0. \end{cases}$$

by means of the following nonlinear system

$$(A_i \otimes I_m)Y^{(n-1)} + (A_f \otimes I_m)Y^{(n)} - h(I_N \otimes I_m)F(Y^{(n)}) = 0,$$

where A_i and A_f are square matrices of dimension N, $I_s,\ s = N, m$, is the identity matrix of size s, h is the stepsize of integration, $Y^{(n)} = (y_1^{(n)}, \ldots, y_N^{(n)})^T$ and $Y^{(n-1)}$ contain the approximations to the true solution computed at step n and $n-1$ respectively, $F(Y^{(n)}) = (f(t_1^{(n)}, y_1^{(n)}), \ldots, f(t_N, y_N))^T$ and $b^{(n)}$ depends on the solution computed at step $n-1$.
By definition GBDFs are L-stable methods; giving to the matrices A_i and A_f a suitable structure (e.g. block-diagonal), we obtain A-stable (A_α-stable) methods that achieve an high degree of parallelism. In finite precision arithmetic, the ill-conditioning of a matrix related to the method may destroy its convergence properties, giving rise to loss of accuracy due to a saturation threshold; this question is also faced.

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Experiments with parallel methods for ODEs
Dana Petcu
(Western University of Timisoara, Romania)

We study from a practical point of view the issue of applying parallelism across method in solving initial value problems for ordinary differential equations. Three computational environments are considered: a parallel computer with distributed memory, a cluster and a workstation network. Two different numerical ODE solving tools are used: EpODE (ExPert system for ODEs, available at http://www.info.uvt.ro/˜ petcu) and D-NODE (ODE solver based on a distributed version of Maple) both allowing parallel and distributed computations. We benchmark several known parallel methods, with accent on Runge-Kutta type methods. Test ODE systems are derived from real problems (like semi-discretized convection-diffusion problems). The goal of our test is twofold: to

investigate to what extent the theoretical parallelization can be achieved in practice, and to compare the code performances on parallel computers relative to those on distributed environments.

Numerical Experiments with parallel Two-step W-methods
Helmut Podhaisky & Bernhard A. Schmitt & Rüdiger Weiner
(Martin-Luther-Universität Halle-Wittenberg, Germany)

We present numerical experiments on a shared memory machine for the recently introduced class of parallel two-step W-methods. These methods are especially designed for large stiff ODE systems. For small test problems where the linear equations in the stages can be solved by LU decomposition we compare our methods with the parallel method PSIDE.
For the solution of large semidiscretized parabolic test problems we discuss our methods with Krylov approximation and compare our code with the sequential Krylov-code VODPK.

On the stability of two-step-W-methods
Bernhard A. Schmitt & Rüdiger Weiner & Helmut Podhaisky
(Universität Marburg, Germany)

Two-step-W-methods for stiff initial value problems possess s linearly-implicit external stages which may processed in parallel. The stability analysis of these methods has to deal with the difficulty that additional recursions for the stages are used besides the one for the approximate solution, similar to general linear methods. Hence, the stability function of these methods is a matrix function even for scalar problems. In this talk we discuss A-stability in a strong sense by constructing G-norms in which the stability matrix of certain methods is bounded by one in the left complex halfplane for scalar problems. By the von-Neumann theorem this bound carries over to norm estimates for linear dissipative systems of ODEs. With respect to the notion of L-stability, on the other hand, it is preferable to apply certain restrictions to the solution component of the recursion only.

6 Abstracts of Contributed Talks

The Pascal matrix and its relations with numerical methods for ODEs
Lidia Aceto
(Universitá di Firenze, Italy)

The Pascal matrix has been known since ancient times, and it was mentioned in Chinese mathematical texts dating from 1303. Nevertheless only recently it has been carefully studied (**[2]**, **[4]**, **[5]**, and **[6]**). Such matrix arises in probability, numerical analysis, surface reconstruction, and combinatorics; we came across it while studying stability properties of numerical methods for solving ordinary differential equations **[1]**. In this talk we present some of the nice properties of the Pascal matrix and show how it is related to other matrices associated with great names such as Vandermonde, Stirling, etc.. Moreover, we shall consider the existing relations between this matrix and the following classes of methods: Generalized BDF (GBDF), GAMs and ETRs **[3]**.

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A linearly implicit one-step time integration scheme for second order nonlinear hyperbolic equations
Mansour A. Al-Zanaidi & M. M. Chawla
(Department of Mathematics and Computer Science, Kuwait University, Kuwait)

We present a linearized *linearly implicit* version of the well-known (*functionally implicit*) Newmark method for initial-value problems for second order ODEs; the linearized method has the same local truncation error and stability properties as the Newmark method. We then employ the linearized method to obtain a linearly implicit one-step time integration scheme for second order nonlinear hyperbolic equations: $u_{tt} = c^2 u_{xx} + p(x,t,u)$; the resulting scheme is unconditionally stable and it obviates the need to solve nonlinear systems at each time step of integration. We demonstrate the computational performance of the linearly implicit scheme for nonlinear ODEs and for nonlinear hyperbolic equations, including the sine-Gordon equation.

Unitary Coordinate Partitioning for General DAE Integrators
Carmen Arevalo & Steven Campbell
(Universidad Simon Bolivar, Venezuela)

Many physical problems are most easily initially modeled as a nonlinear implicit system of differential and algebraic equations (DAEs),

$$f(x', x, t) = 0$$

with $f_{x'} = \partial f / \partial x'$ identically singular. Many of the problems in constrained mechanics are initially formulated as index two and three DAEs. However, DAEs of index up to six naturally occur in mechanics if actuator dynamics, joint flexibility, and other effects are included.
Numerical methods for DAEs based directly on classical approaches require that the systems have special structure, such as being a mechanical system with holonomic constraints or have indices of only one or two. There is a need for more general higher index DAE integrators. Three somewhat related constraint preserving approaches have been proposed for general higher index DAEs. Here we examine the Implicit Coordinate Partitioning (ICP) approach. In particular, we examine how to chose a good local coordinate system. In Unitary Coordinate Partitioning (UCP) this is done by orthogonal transformations as opposed to permutations.
We see this approach as being especially useful in the early stages of design and simulation when various computer generated models are being used to investigate system behavior. It will also be useful as a truth model for investigating other integration methods and the validity of various simplified models.

Newton-Type Method for Solving Non-regular Equations
Vadim Azhmyakov
(EMA University of Greifswald, Institute of Mathematics and Computer Sciences, Germany)

Newton methods are widly used for receiving the approximate solutions for differential and differential-algebraic equations in Hilbert space. We consider nonlinear operator equations with expanding left-hand side. For such systems the problem of searching the zero solution is examined. We assume in addition that the Frechet derivative of operator is singular. The existence of solution for operator equations with expanding operators is proved.
A new quadratically convergent method is introduced for differential equations in Hilbert space with nonregular, expanding right-hand side. The obtained Newton-type method is the theoretical basis for effective numerical procedures for solving the differential and differential-algebraic equations.

Transfer equations and linear boundary value problems for DAEs
Katalin Balla
(Computer and Automation Research Institute, Hungarian Academy of Sciences, Hungary)

As it was proven recently by R. März and the author, an index equal to 1 or 2 may be assigned to the implicit differential equation of the form

$$A(Cx)' + Dx = f, \quad (*)$$

provided the matrix functions $A, B : I \to L(R^n)$ are well-matched on I and together with $D : I \to L(R^n)$ have sufficient (low) smoothness. It was shown that a homogeneous equation (*) ($f = 0$) and its properly defined adjoint equation are solvable simultaneously [1]. These results allow considering the transfer of boundary conditions with some invariant. Properties of the transfer equation and its use in BVP will be discussed.

[1] K. Balla, R. März: An approach to linear differential algebraic equations and their adjoint equations in a unified way. *Manuscript*

Numerical verification of delay dependent error estimates for WRM for differential-functional equations

Zbigniew Bartoszewski
(The Faculty of Applied Physics and Mathematics, The Technical University of Gdansk, Poland)

In the paper there is given a numerical illustration of the theoretical results presented by M. Kwapisz in his talk given at this conference. The theoretical results have been tested on a number of examples and it was observed a good agreement between the theoretical error estimates and numerically obtained results despite the fact that numerical realization of waveform relaxation methods introduces discretization errors.

A Partial Differential-Algebraic Equations Approach for Elastic Rods

Brahim Benhammouda
(United Arab Emirates University, UAE)

The equations of motion of inextensible elastic rods form a system of partial differential-algebraic equations (PDAEs) of index three. Elastic rods are used to model many practical problems such as solitons or DNA loops. A semidiscretization of these equations yields a system of differential-algebraic equations (DAEs) of index ≥ 3. Such DAEs are known to cause serious difficulties for numerical integration methods.

In this paper, we describe a new index reduction technique to lower the index from three to one while preserving all constraints. The resulting index-1 PDAE system is discretized in space by Galerkin method to lead to an index-1 DAE system for the coefficients of the Galerkin solution. This system can be integrated in time efficiently by DASSL.

Stability in the numerical solution of the heat equation with nonlocal boundary conditions

Natalia Borovykh
(Mathematical Institute, Leiden University, The Netherlands)

In this talk we deal with numerical methods for the solution of the heat equation with integral boundary conditions. Finite differences are used for the discretization in space. The matrices specifying the resulting semi–discrete problem are proved to satisfy a sectorial resolvent condition, uniformly with respect to the discretization parameter.

Using this resolvent condition, unconditional stability is proved for the fully discrete numerical process generated by applying $A(\theta)$ –stable one–step methods to the semi–discrete problem. This stability result is established in the maximum norm; it improves some previous results in the literature in that it is not subject to various unnatural restrictions which were imposed on the boundary

conditions and on the one–step methods.

Avoiding the order reduction of Runge-Kutta methods for linear initial boundary value problems

Mari Paz Calvo & Cesar Palencia
(Universidad de Valladolid, Spain)

A new strategy to avoid the order reduction of Runge-Kutta methods when integrating linear, autonomous, non-homogeneous initial boundary value problems is presented. The solution is decomposed into two parts. One of them can be computed directly in terms of the data and the other satisfies an initial value problem without any order reduction. This idea applies to practical problems, where spatial discretization is also required, leading to the full order both in space and time. Numerical illustrations are given.

Low-order SDIRKS for DAEs

Frank Cameron & Mikko Palmroth & Robert Piché
(Pori School of Technology and Economics, Finland)

Our purpose is to design and test low-order integrators for the class of implicit index 1 initial value DAE problems typically represented by

$$F(y',\, y, t) = 0\,, \;\; y(t_0) = y_0\,, \;\; y'(t_0) = y'_0$$

where $y : \mathbf{R} \to \mathbf{R}^N$ and $F : \mathbf{R}^N \times \mathbf{R}^N \to \mathbf{R}^N$ [2]. We study SDIRKs because their ease of implementation makes them attractive for use in software for simulating engineering processes, for which low-order methods often suffice. Our design goal is an embedded SDIRK pair with local orders 4(3) together with an interpolator and a predictor for providing starting values to the iterative method used to solve the nonlinear stage equations. We introduce some properties akin to stage-order that can be used with SDIRKs to reduce the number of order conditions that need to be explicitly handled. In addition to order conditions, our SDIRK design also takes into account stability, truncation error coefficients and some measures of error estimate quality. We present several new SDIRKs. Numerical tests are presented comparing different predictors and comparing our SDIRKs with the Radau IIA method from Hairer and Wanner [1, pg. 74,123].

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A posteriori error estimation for evolutionary dissipative equations
Javier de Frutos & Julia Novo
(University of Valladolid, Spain)

In [2] we introduce a postprocess of the spectral element method for time-dependent dissipative two dimensional equations.
In this talk we will show that the postprocessed method can be used as an a posteriori error estimator for evolutionary dissipative equations [1]. More precisely, we will show that the error achieved using the spectral element method can be accurately estimated by calculating the L^2 or H^1 norm of the difference between the spectral element approximation and the postprocessed approximation that can be obtained f rom it. The postprocessed method, used as an a posteriori error estimator, reveals itself not only cheap and easily computable, but also able to give local and global information on the error of the numerical solution.

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Numerical behaviour of stable and unstable solitary waves
Angel Duran & Miguel A. Lopez Marcos
(University of Valladolid, Spain)

Classical analysis of numerical methods for integrating time-dependent differential equations is based on the search of small approximations errors. However, a numerical scheme can have many other important properties. In particular, conservation properties would be pointed out. Almost every problem possesses physical quantities such as mass, energy, etc that remain constant during the evolution of the system. It is not always true that these quantities keep invariant through numerical integration. Then, we can distinguish between conservative and nonconservative numerical methods.
On the other hand, conservative integrators reveal successful for the numerical integration of certain class of solutions. In this talk we study this situation in the case of solitary wave problems for the gRLW equation. This equation has a remarkable property: the stability of the shape of solitary wave solutions depends on their velocity. We pretend to describe the different behaviour of the numerical approximations by using conservative and nonconservative methods, depending on the velocity of the wave.

Integration of Index-One Differential-Algebraic Equations using Dichotomically Stable One-Step Formulae
Roland England & René Lamour
(The Open University, UK)

The first author has previously established the need for dichotomic stability when solving stiff boundary-value problems (BVPs) in ordinary differential equations (ODEs), with potentially sharp boundary layers at each end of the interval. He has implemented a dichotomically stable implicit

Runge-Kutta method, of order 4, in a variable step-size initial-value integrator (SYMIRK). The 3-stage Lobatto IIIA method may be written as a single formula:

$$\mathbf{X}_{i+1} - \mathbf{X}_i - h\left[\tfrac{1}{6}\mathbf{X}'_{i+1} + \tfrac{2}{3}\mathbf{F}\left\{\tfrac{1}{2}(\mathbf{X}_{i+1} + \mathbf{X}_i) - \tfrac{1}{8}h(\mathbf{X}'_{i+1} - \mathbf{X}'_i)\right\} + \tfrac{1}{6}\mathbf{X}'_i\right] = \mathbf{0},$$

where the system of ODEs is written as $\mathbf{x}' = \mathbf{F}(\mathbf{x}) \in I\!R^n$. An explicit, 4-step, third-order, extrapolation formula is used, both as a predictor, and to provide a local error indicator. This has the correct asymptotic behaviour, both for small and for large step sizes.
For differential-algebraic equations (DAEs) of the form $\mathbf{F}(\mathbf{x}', \mathbf{x}, t) = \mathbf{0} \in I\!R^n$, the Lobatto IIIA formulae must be solved simultaneously for the derivatives $\mathbf{X}'_{i+\frac{1}{2}}$, $\mathbf{X}'_{i+1}$. The Newton iteration matrix is then non-singular for an index-one system. Predictors are also needed for the derivatives, and at the off-step points.
The ODE integrator (SYMIRK) has been adapted in this way, for the solution of index-one DAEs, and the resulting integrator (SYMDAE) has been inserted into the multiple-shooting code (MSHDAE) developed by R. Lamour for differential-algebraic BVPs. Tests on a few stiff boundary-value problems have shown that, at least in some cases where the standard BDF integrator in MSHDAE fails to integrate across the interval of interest, the dichotomically stable integrator SYMDAE encounters no difficulty. What is more, the modified version of MSHDAE produces an accurate solution in such cases, and within limits imposed by computer word length, the efficiency of the solution process improves with increasing stiffness. For some non-stiff problems, the solution is also entirely satisfactory.

A Two-level Finite Element Method for the streamfunction form of the Navier-Stokes Equations
Faisal A. Fairag
(King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia)

to be submitted

Sharpening the stability bound in the maximum-norm of the Crank-Nicolson scheme for one-dimensional heat equation
István Faragó & C. Palencia
(Eötvös Lorand University, Budapest, Hungary)

The maximum norm stability constant C_s of the numerical solution of the one-dimensional heat equation, via the Crank-Nicolson method, is considered. It is known that the method is contractive, i.e. that $C_s = 1$, only for $\mu \in (0, 1.5]$, where $\mu = \frac{\tau}{h^2}$. Moreover, it is also known that $C_s \leq 23$ for any value of $\mu > 0$. In this talk, using the Laurent expansion and the theory of sectorial operators, we sharpen the existing estimates to $3 \leq C_s \leq 5$, for $\mu \geq 1.5$.

New methods for oscillatory problems based on classical codes
Amelia Garcia & Pablo Martin
(University of Valladolid, Spain)

The numerical integration of differential equations with oscillatory solutions is a very common problem in many fields of the Applied Sciences. Some methods have been special devised for this

kind of problems, such as those of Bettis [1], Gautschi [2], Gonzalez *et al.* [3], Martmn *et al* [4], van der Houwen and Sommeijer [5] ... In most of them the calculation of the coefficients needs more computational effort than the classical codes because the mentioned coefficients depend on the frequency of the problem in a not simple manner. On the contrary, in this work we present new algorithms specially designed for oscillatory problems whose coefficients have a simple frequency dependence. The methods obtained are competitive when comparing with classical and special codes.

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Acquiring a solution of the time-dependent Schrödinger equation using CP methods

Andy Georges & Marnix Van Daele
(University of Ghent, Belgium)

The time-dependent Schrödinger equation (TDSE) can be solved as a partial differential equation of the parabolic type, e.g. by using a Cranck-Nicholson scheme. Another approach can be as follows. We take constant approximations to the potential in the time dimension. Then one can use the Separation of Variables method in eacht time interval in order to solve the TDSE. The solution Ψ in each such interval can be written as a linear combination of the solutions to the time-independent Schrödinger equation: ψ_E multiplied with an appropriate exponential factor. These ψ_E can be efficiently calculated using CP methods. In the movement through time, we can calculate the coefficients to the solutions ψ_E of the next time interval by imposing a matching condition at the meshpoints in time.

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Operator Splitting and Approximate Factorization for Taxis-Diffusion-Reaction Models
Alf Gerisch & Jan G. Verwer
(Martin-Luther-Universität Halle-Wittenberg, Germany)

We consider the numerical solution of 2D systems of certain types of taxis-diffusion-reaction equations from mathematical biology. By spatial discretization these PDE systems are approximated by huge systems of positive, nonlinear ODEs (Method of Lines). We are especially interested in the numerical integration of these large ODE systems for low to moderate accuracy by means of splitting techniques. An important consideration is maintenance of positivity. We apply operator splitting and approximate matrix factorization using low order explicit Runge-Kutta methods and linearly implicit Runge-Kutta-Rosenbrock methods. As a reference method the general purpose solver VODPK is applied.

Exponential Integrators for Classical Molecular Dynamics
Volker Grimm
(Heinrich-Heine-Universität Düsseldorf, Germany)

A problem in integrating molecular dynamic systems is the presence of high-frequency oscillations, which restricts the integration step-size. In many cases an explicit separation of the forces into fast forces and slow forces is available in such a way that the fast forces are nearly linear and contain all of the high-frequency part of the solution. Exponential integrators are considered which overcome the step-size barrier.

Two-sided enclosures for IVPs by means of bounding operators I: Construction of bounding operators and convergence properties
Christian Grossmann & Zoltán Horváth
(TU Dresden, Germany)

Monotonicity properties of the originally given initial value problem are applied to derive discretization methods which generate guaranteed upper and lower bounds for the unknown solution. The main idea of our discretizations is to replace the right hand side of the problem by upper and lower bounds respectively using the concept of bounding operators similar to a technique originally proposed for 2-point boundary value problems. The solution of the modified initial value problem constitute upper and lower solutions respectively in case when the original problem is monotone. Further, monotonicity assumptions may be relaxed by means of monotone splitting.
Finally a rather general class of bounding operators is introduced and two basic principles of construction of bounding operators are studied . The first one is based on interpolation of the right hand side while the second one rests on numerical methods of dense and smooth output, which are considered as solution methods for the original initial value problem. The bounding operator technique can be viewed as a correction process of this underlying method.

On numerical contractivity for DAEs
Inmaculada Higueras
(Universidad Publica de Navarra, Spain)

In the theory of ODEs, different models have been introduced in order to study the numerical stability of the methods. One of these models are the contractive problems and the interesting methods in this context are the algebraically stable methods.

Given a DAE, similar questions can be made. In this talk we discuss about what do we mean by contractivity in the context of DAEs and its numerical counterpart.

On the Monotonicity Conservation of the Numerical Solution of the One-Dimensional Heat Equation
Róbert Horváth
(University of West Hungary, Institute of Mathematics, Hungary)

It is very important to choose such numerical methods in the applications which are not only convergent, but they conserve some characteristic properties of the described process. Some of these properties are the nonnegativity conservation, concavity conservation, sign-stability and others in the case of the heat conduction.
In this lecture we introduce the notions of the totally monotone and monotonicity conserving one-step vector iterations. We analyse their conditions. The results are applied in the qualitative investigation of numerical solutions of the one-dimensional heat equation. We give the necessary and sufficient conditions of the monotonicity conservation.

Two-sided enclosures for IVPs by means of bounding operators II: Application to PDEs
Zoltán Horváth & Christian Grossmann
(Széchenyi István College Györ, Hungary)

Here the basic principle of bounding operator discretizations discussed in the preceding talk (Grossmann, Horváth: Two-sided enclosures for IVPs by means of bounding operators I: Construction of bounding operators and convergence properties) will be studied more in detail for two specific classes of problems. These problems arise in semidiscretization of initial-boundary value problems for partial differential equations of parabolic type and of first order hyperbolic type, respectively. First, we investigate the relevant characteristics of the obtained methods for these problem sets and discuss numerical results. Further, for selected applications of the methods under consideration we derive guaranteed a posteriori error estimates in case of underlying continuous ODE solvers.

Five-pointed difference schemes for the equations of parabolic type
Hrant Hovhannissian
(The Engineering State University of Armenia, Armenia)

The fourth-power parabolic type of equation, given in the orginal and the boundary conditions is observed in the research.For the mentioned problem is studied the second and the fourth-power accuracy indeterminate, five-pointed difference schemes, which for each layer (beginning from the second) are linear algebraic system of equations with five-diagonal matrix.

The obtained linear algebraic system of equations with five-diagonal matrixes is solved by the Thomas's algorithm, right, left and according to the methods of opposing displacement. For five-pointed difference schemes are proved:

- maximum of source
- theorem of comparison
- theorem of existence and uniqueness
- majorants.

Block Boundary Value Methods used as General Linear Methods
Felice Iavernaro & Francesca Mazzia
(Dipartimento di Matematica, Universitá di Bari, Italy)

The numerical solution of the initial value problem

$$\begin{cases} y'(t) = f(t,y), & t \in [t_0, t_0+T], \\ y(t_0) = y_0, \end{cases}$$

by means of a block-Boundary Value Method (block-BVM), generates, at step n of the integration procedure, the following nonlinear system of equations:

$$\begin{cases} \displaystyle\sum_{j=0}^{k} \alpha_j^{(i)} y_j^{(n)} = h \sum_{j=0}^{k} \beta_j^{(i)} f_j^{(n)}, & i = 1, \ldots, k_1 - 1, & \text{initial methods,} \\ \displaystyle\sum_{j=-k_1}^{k-k_1} \alpha_{j+k_1} y_{n+j}^{(n)} = h \sum_{j=-k_1}^{k-k_1} \beta_{j+k_1}^{(i)} f_{n+j}^{(n)}, & n = \nu, \ldots, N-k+\nu, & \text{main method,} \\ \displaystyle\sum_{j=0}^{k} \alpha_{k-j}^{(i)} y_{N-j}^{(n)} = h \sum_{j=0}^{k} \beta_{k-j}^{(i)} f_{N-j}^{(n)}, & i = N-k+k_1+1, \ldots, N, & \text{final methods,} \end{cases}$$

where $k_1 \leq k$ is the number of initial methods and h is the stepsize of integration. The integer N defines the dimension of the discrete problem as well as the time interval over which the approximation is computed, namely $[t_0^{(n)}, t_f^{(n)}]$, with $t_f^{(n)} = t_0^{(n)} + Nh$. In details, $y_i^{(n)},\ i = 0, \ldots, N$, are approximations to the true solution at the time $t_i^{(n)}$ while $f_i^{(n)} = f(t_i^{(n)}, y_i^{(n)})$. The initial and final methods are necessary to approximate the boundary conditions needed by the main methods, that is

$$y_0^{(n)}, \ldots, y_{k_1-1}^{(n)}, \qquad y_{N-k+k_1+1}^{(n)}, \ldots, y_N^{(n)}.$$

An alternative approach is to neglect the initial methods and use information from the previous computed solution to approximate the left boundary condition. This reduces the dimension of the system to $N - k_1$, and change the stability and convergence properties of the overall block-BVM.

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On the contractivity of implicit-explicit linear multistep methods

Karel in 't Hout

(Leiden University, Mathematical Institute, The Netherlands)

This talk is concerned with the class of implicit-explicit (IMEX) linear multistep methods for the numerical solution of initial value problems for systems of ordinary differential equations. These numerical methods have been considered by various authors in the literature, especially in the recent years. In this talk, we are interested in the stability properties of IMEX linear multistep methods. We will analyze their stability by considering certain linear autonomous systems of ordinary differential equations. First we present a theorem on contractivity, which can be regarded as a matrix-valued version of a theorem of von Neumann for several variables. Next, we determine the so-called contractivity regions of some popular IMEX linear multistep methods. Finally, we give a result based on the stability regions of IMEX linear multistep methods, yielding strong stability.

Modular Implementation of Navier-Stokes Equation Solver on Arbitrary/Hybrid Unstructured Meshes

Makky Jaya & Claus-Dieter Munz

(Institute for Aerodynamics and Gasdynamics, University of Stuttgart, Germany)

We describe the modular implementation of Navier-Stokes equation code using the Finite-Volume discretization scheme in Fortran 90. By the current implementation, object-oriented models of mesh, primitive and conservative variables and related objects concerning on Riemann problem and higher order computation are modularly contsructed and employed. Due to the high flexibility and independency of each module (object), the end solver of Navier-Stokes equation is achieved by unifying all modules in the main driver code. By this way, the overall structure of the new implementation may be implicitly viewed as a kind of black-box. Despite of being able to design a black-box solver for Navier-Stokes equation, the achieved code embodies rather a group of dynamic modular libraries which can be used in any part of the main driver code. Detailed analysis of the performance and strategy of the current modular implementation, and the result of numerical tests from simple to highly complex geometries are presented.

A second-order differential-finite-differences model

Alex Kolpakov
(Siberean State Universiti T&I, Russia)

The paper is devoted to numerical analysis of a differential-finite-differences model describing, in particular, a filamentary composite [1]. The numerical analysis is based on fundamental solutions of the system.

The model under consideration has the form

$$d^2w_i/dt^2 + D_+(G_i(t)D_-w_i) = 0$$

where $D_+f_i = f_{i+1}f_i, D_-f_i = f_{i-1}f_i$ are the operators of finite differences.

$dw_i/dt(t_k) = 0$ if the i-th fiber in broken at the point t_k.

$G_i(t) = 0, t \in [t_1, t_2]$ if the matrix between the (i+1)-th and the i-th filaments is broken at the interval $[t_1, t_2]$.

Combining the broken fibers and matrix layers, we can obtain a hole.

The fundamental solutions

The problem above has two types of the fundamental solutions:

- corresponding to an expansion center (or broken fiber);
- corresponding to a pair of forces applied to adjacent fibers.

The first solution was obtained in [2]. The second solution is found by the author. Both the solutions can be written in explicit forms (as series).

Transformation of the initial problem Using the fundamental solutions we can transform the initial problem to a system of integral-algebraic equations, which involves point where the fibers or/and the matrix are broken. This system is less in dimension then the initial problem.

Numerical analysis

The integral-algebraic system was solved numerically. Some interesting from the mechanics point of view models were analyzed. There were among them the problems about concentration of stresses near a broken matrix and near a hole.

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On delay dependent error estimates for waveform relaxation methods for differential-functional equations

Marian Kwapisz
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In the paper we deal with the iterative processes

$$\begin{aligned} x'_{k+1}(t) &= F(t, x_{k+1}(t), x_k(t), x_k(\cdot)), \quad k = 0, 1, \dots, \quad t \in J = [0, T], \\ x_{k+1}(t) &= g(t), \quad t \in J_0 = [-h, 0], \quad h > 0, \quad x_0 \text{ - given}, \end{aligned}$$

for solving the initial value problems

$$\begin{aligned} x'(t) &= f(t, x(t), x(\cdot)), \qquad t \in J \\ x(t) &= g(t), \quad t \in J_0, \end{aligned}$$

where $g \in C(J_0, R^n)$, $f \in C(J \times R^n \times C_g(J_T, R^n), R^n)$, $J_T = [-h, T]$, and $C_g(J_T, R^n)$ denotes the space of continuous functions defined on J_T and being equal to g on J_0.
For the splitting function F, $f(t, x, y(\cdot)) = F(t, x, x, y(\cdot))$, we assume the one-sided Lipschitz condition

$$(F(t, x, y, z) - F(t, \bar{x}, y, z), x - \bar{x}) \leq m(t)\|x - \bar{x}\|^2$$

and the Lipschitz conditions with respect to the last two arguments

$$\|F(t, x, y, z) - F(t, x, \bar{y}, \bar{z})\| \leq K(t)\|y - \bar{y}\| + L(t)\|z - \bar{z}\|_{\beta(t)}$$

It is assumed that β is continuous, nondecreasing, and satisfies $0 \leq \beta(t) \leq t$ and $\|y\| = \max_{-h \leq s \leq t} \|y(s)\|$ for $t \in J$. Let $u_k(t) = \max_{0 \leq s \leq t} \|x_*(s) - x_k(s)\|$, where x_* is the exact solution of the initial value problem under consideration. Under suitable conditions on the given functions m, K, L, u_0, we will present delay dependent estimates for the errors $u_k(t)$.

The Computation of Consistent Initial Values for Nonlinear Index-2 Differential-Algebraic Equations
René Lamour & Diana Estevez Schwarz
(Humboldt-University of Berlin, Germany)

The computation of consistent initial values for differential–algebraic equations (DAEs) is essential for starting a numerical integration. Based on the tractability index concept a method is proposed to filter those equations of a system of index–2 DAEs, whose differentiation leads to an index reduction. The considered equation class covers Hessenberg-systems and the equations arising from the simulation of electrical networks by means of Modified Nodal Analysis (MNA). The index reduction provides a method for the computation of the consistent initial values. The realized algorithm is described and illustrated by examples.

A variable-stepsize variable-order multistep method for the integration of perturbed linear problems
David J. Lopez & Pablo Martin & Amelia Garcia
(University of Valladolid, Spain)

In 1971 Scheifele [3] wrote the solution of a second order equation as an expansion in terms of the G-functions. This set of functions extend the classical monomials in the Taylor series of the solution, and it show interesting properties when integrating perturbed problems. Recently, Martín and Ferrándiz [2] constructed the SMF code, based on the Scheifele G-functions for oscillatory problems, which was generalized by López and Martín [1] to the linear multistep LM method. However, the remarked codes are constant steplength methods, and efficient integrators must be able to change the steplength. In our work we extend the ideas of Krogh for the Adams methods

to the LM algorithm, removing the G-functions, with a special attention in the computacional cost of the coefficients of the method. We show the advantages of the new code in perturbed problems, and its interesting behavior in mode PEC.

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Postprocessing the linear finite element method

Julia Novo & Javier de Frutos
(University of Valladolid, Spain)

In [1] a postprocessing technique, developed earlier for spectral methods [2], is extended to the finite-element methods for dissipative partial differential equations. In that paper the authors claim that the postprocessing technique does not improve the order of convergence of the finite-element method when using piecewise-linear polynomials. Obviously, this a drawback that limits seriously the range of applicability of the method. However, the new method has been proven to have a superior rate of convergence than the standard finite-element method when other than linear elements are used (say, quadratic, cubic ...)

In this talk we present a modification of the analysis technique that allows us to prove an optimal rate of convergence, in the H^1 norm, of postprocessed linear finite element methods. A superior rate of convergence over standard methods is then obtained also in the case of linear finite element methods.

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Quantum motion numerical calculation for axial channeling

Sergey Nurmagambetov
(Karaganda State University, Kazakhstan)

Wave function that describe the quatum motion of channeling particles in solids usually are determined by numerical methods applying in solid state physics like APW, OPW and so on. But because of two-dimensional case it can be used more direct solving numerical methods. Based on one-dimensional numerical analysis of plane channeling that is used the symmetric form of linearly independed solutions we are applied this method for two-dimensional case. First, various linearly independed solution of given symmetry are determined at edges of elementary cell. Then using random walking Monte-Carlo calculations the wave function is determined for inner space of elementary cell. In paper we discuss various types of wave functions and energy sufface for diamond like structure crystals.

Stability of W-methods with applications to operator splitting
Alexander Ostermann
(Université de Genéve, Switzerland)

We analyze the stability properties of linearly implicit Runge-Kutta discretizations of the parabolic initial value problem $u' + Au = Bu$. We work in an abstract Banach space setting, assuming that A is the generator of an analytic semigroup and that B is relatively bounded with respect to A. The numerical method treats A implicitly, whereas the right-hand side involving B is discretized in an explicit way. Therefore the method can be seen as a splitting method. As an application of our stability results, the convergence of such splitting methods is shown. Moreover, the layout of a geometric theory for discretizations of semilinear parabolic problems $u' + Au = f(u)$ by W-methods is presented.

Coupled High Order Boundaries in Numerical Solution of Hyperbolic Equations
Manouchehr Parsaei
(Tehran University, Iran)

When approximating hyperbolic conservation laws numerically any groups of S-equations (resulting from the difference equations) can be assumed to define a coupling between S independent waves. This coupling determines the inter-relationship between the amplitude of the solution waves at S consecutive nodes. This relationship is presented in the form of S eigen-pairs or in a way S component waves each having a distinct phase and group velocity. At the out flow boundaries the boundary conditions participate in defining these inter-relationships and new sets of eigen-pairs are produced. When the first group of solution waves approaches the boundaries each of the above wave components is decomposed in to the second set of waves (e-vectors) and depending on the sign of the group velocity of those waves parts of them move on and pass through the boundaries and the other parts are reflected back in to the system. The later waves are now converted back to the first form, this results in a deformation in the shape of the reflected waves together with a change in their speeds. In this talk we present this coupled method of analyzing boundary conditions and compare it with the time Fourier transformation method in which the order of the difference equations are used to determine the behavior of the discretization at the boundaries. Some numerical results are presented to support the points made.

Numerical modeling forest fire spread initiation
Valeri A. Perminov
(Belovo Branch of Kemerovo State University, Russia)

In this paper the theoretical investigation of the problem of forest fire spread in windy was carried out. The research was made by means of the mathematical modeling methods of physical processes. It was based on numerical solution of two dimensional Reynolds equations for the description of turbulent flow taking into account for diffusion equations chemical components and equations of energy conservation for gaseous and condensed phases. In this context, a study - mathematical modeling - of the conditions of forest fire spreading that would make it possible to obtain a detailed picture of the change in the velocity, temperature and component concentration fields with time. The paper suggested in the context of the general mathematical model of for-

est fires gives a new mathematical setting and method of numerical solution of a problem of a radioactive spread above the forest region.

Let us examine a plane problem of radiation-convection heat and mass exchange of forest fuels in all forest strata with gaseous combustion products and radiation. The surface fire source is modeled as a plane layer of burning forest fuels with known temperature as a function of time and turned off after the forest fire initiation. It is assumed that the forest during a forest fire can be modeled as a two-temperature multiphase non-deformable porous reactive medium. Let there be a so-called ”ventilated” forest massif, in which the volume of fractions of condensed forest fuel phases, consisting of dry organic matter, water in liquid state, solid pyrolysis products, and ash, can be neglected compared to the volume fraction of gas phase (components of air and gaseous pyrolysis products). 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.

Because of the horizontal sizes of forest massif more than height of forest - h, system of equations of general mathematical model of forest fire was integrated between the limits from height of the roughness level - 0 to h. The three dimensional problem formulated above is reduced to a solution of the two dimensional system of equations. The thermodynamic, thermophysical and structural characteristics correspond to the forest fuels in the canopy of a pine forest. The solution of the system of equations with initial and boundary conditions may result in defining the fields of velocity, temperature, component concentrations and radiation density. To close the system, the components of the tensor of turbulent stresses, and the turbulent heat and mass fluxes are determined using the local-equilibrium model of turbulence.

The boundary-value problem was solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions was calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting was then integrated. A discrete analog for system of equations was obtained by means of the control volume method using the SIMPLE algorithm.

The accuracy of the program was checked by the method of inserted analytical solutions. Analytical expressions for the unknown functions were substituted in system of differential equations and the closure of the equations were calculated. This was then treated as the source in each equation. Next, with the aid of the algorithm described above, the values of the functions used were inferred with an accuracy of not less than 1dimensions of the control volumes on the solution was studied by diminishing them. The time interval was selected automatically.

Fields of temperature, velocity, component mass fractions, volume fractions of phases and concentration components were obtained numerically. It allows to investigate dynamics of forest fire spread under influence of various external conditions: a) meteorology conditions (air temperature, wind velocity etc.), b) type (various kinds of forest combustible materials) and their state(load, moisture etc.). A great deal of final and intermediate gaseous and dispersed combustion products of forest fuels is known to be exhausted into the atmosphere during forest fires: carbon monoxide, carbon dioxide, nitrogen oxide, water, soot, smoke, methane, other hydrocarbons and etc. The knowledge of these kinds of ejection enables a full estimate of the damage from forest fires to be made. The results obtained agree with the laws of physics and experimental data.

The research has been carried out due to the financial support of RFBR (Project code 98-01-03013).

Approximations of coupled differential and difference equations by ordinary differential equations

Larisa Piddubna & Igor Cherevko
(The State University of Chernivtsy, Ukraine)

There has been a great development of the theory of functional-differential equations (FDE) due to the increasing number of applications of FDE in various fields of science and technology. Of special interest are the coupled differential and difference equations. The approximation algorithm of FDE by a sequence of ordinary differential equations (ODE) has been considered [1-3] in the researches of control and stability problems in systems with delay. The aim of the present talk is to obtain approximation results for new classes of time lag systems and use them for modeling in electrodynamic. As straightforward application of the above result we shall consider the particular circuit described in [4] by means of system partial differential equations. These equations are reduced to a difference-differential equation of neutral type that may be written inform the coupled differential and difference equations.

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A method of characteristics for solving multirate partial differential equations in radio frequency application

Roland Pulch
(Universität Karlsruhe (TH), Germany)

A multirate behaviour with widely separated time scales arises often in circuit simulation. This is especially given in radio frequency circuits, which are used in communication electronics. Their behaviour in time makes the analysis of such circuits more difficult. By means of a new approach, which bases on a PDE model, these problems can be avoided.
In the talk, we introduce this model and discuss the arising system of PDEs. Furthermore, a new numerical method to solve the system with periodic boundary conditions is presented. This technique differs from other approaches by using the special structure of the underlying PDE.

Numerical Solution of a Nonlinear Model of Urea Hydrolysis Reactor

Mohammad R. Rahimpour & A. Azrapour
(Shiraz University, School of Engineering, Iran)

Numerical Solution of a Nonlinear Model of Urea Hydrolysis Reactor
Abstract
In this paper a mathematical model used for simulation of an urea hydrolysis reactor. This model is able to obtain the temperature and concentration profiles along the reactor. The Newton-Raphson

method used to solve the nonlinear algebraic equations to calculate the equilibrium and non-equilibrium concentration amounts. Also the half-method used to satisfy the activity coefficients of the reaction components. In this reactor a plug-flow model is considered and the partial differential equations of the model was solved by the explicit numerical method. The mathematical model results compared with the data of an industrial-scale plant. The numerical results were in a good agreement with the data of the industrial-scale plant.

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On Implicit Euler for High-Order High-Index DAEs

Jürgen Sand

(Dept. of Computer Science, Univ. of Copenhagen, Denmark)

The Implicit Euler method is seldom used for solving differential-algebraic equations (DAEs) of differential index $r \geq 3$, since the method in general fails to converge in the first $r - 2$ steps after a change of stepsize and after the initial point.

However, if the differential equation is of order $d = r - 1 \geq 1$, an alternative variable-step version of the Euler method can be shown uniformly convergent. This variable-step method is equivalent to the Implicit Euler except for the first $r - 2$ steps after a change of stepsize and after the initial point.

Generalization to DAEs with differential equations of order $d > r - 1 \geq 1$, and to variable-order Backward Differentiation Formulas is discussed.

Strategies for the Numerical Solution of the Navier-Stokes Equations

Joerg Sautter

(University of Düsseldorf, Germany)

Expensive or dangerous experiments are being more and more frequently replaced by numerical simulations. In addition, a simulation produces the possibility to analyze processes which can not be tested in an experiment. Weather forecasts, for example, depend strongly on efficient numerical simulations in fluid dynamics. I will show some general ideas for time integration and their

limitations, capabilities and advantages. Then I will present a numerical comparison of some time stepping schemes and different approaches for the discretization and solution of the Navier-Stokes equations for incompressible homogeneous fluids.

Implicit Taylor series methods and stiff semi-linear initial value problems
Hans-Eberhard Scholz
(Martin-Luther-Universität Halle-Wittenberg, Germany)

In this talk we discuss results concerning the solvability of the algebraic equations, stability, and convergence properties of the implicit Taylor series method applied to two classes of stiff semi-linear systems of differential equations. All these results are independent of the stiffness of the systems.

Qualitative Properties of Discretizations for Index 2 DAE's
Johannes Schropp
(Universität Konstanz, Germany)

We analyze numerical discretizations applied to index 2 DAE's and compare the asymptotic and geometric features of the numerical and the exact solution. For a class of discrete schemes satisfying the first order constraint exactly it is shown that the geometric and asymptotic properties of the DAE are reproduced correctly. The proof combines reduction techniques of discretized index 2 DAE's to ODE's with some invariant manifold results of Nipp and Stoffer.

Numerical Approximation of Nonlinear BVPs by means of BVMs
Ivonne Sgura & Francesca Mazzia
(Department of Mathematics E. De Giorgi - University of Lecce, Italy)

Let us consider the following nonlinear Boundary Value Problem (BVP)

$$\begin{aligned} y' &= f(t,y), \;\; t_0 \le t \le T, \\ g(y(t_0), y(T)) &= \eta \end{aligned}$$

where $f, g : [t_0, T] \times \mathbb{R}^m \to \mathbb{R}^m$, $y, \eta \in \mathbb{R}^m$, f and g are differentiable functions.
The numerical solution of the nonlinear BVPs can be found using two different approaches. The basic one is to use a numerical method to form a discrete algebraic system which can be solved with a Newton iteration to obtain a discrete solution. The other approach consists in applying the Newton method to the nonlinear differential equation. Each iteration requires the solution of a linear BVP. In practice the solutions of the continuous linear subproblems can only be discrete approximations. Therefore the theory of inexact Newton method must be used to determine how accurately we must solve these subproblems to ensure the convergence to the solution of the continuous non linear problem. The two approaches are equivalent if the grid is not changed during the iterative process.
In this paper we apply the quasi-linearization technique together with an improvement of the mesh selection strategy presented in [1] and we use Boundary Value Methods to discretize the continuous linear BVPs. Stopping criteria on the residual of each linear BVPs and on its approximate solution are given to guarantee the local convergence to the nonlinear solution. Numerical experiments on

stiff problems show the behavior of this technique, giving rather satisfactory results compared with well known solvers for BVPs.

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Adaptive Collocation and Least-Squares Method for Navier-Stokes Equations

Vasily P. Shapeev & Leonid G. Semin

(Institute of Theoretical and Applied Mechanics SB RAS, Russia)

In the present study the method of collocation together with least-squares (CLS) for solving boundary-value problems for stationary Navier-Stokes equations in two dimensions is proposed. The approximate solution is found as piecewise polynomial function: $\begin{pmatrix} \vec{v} \\ p \end{pmatrix} = \sum_j a_{jm}\varphi_j,$ where φ_j are the basic functions, m is cell number. The velocity components are thought as second order polynomials, pressure - as linear function. Moreover, basic functions are taken in such manner that the approximate solution satisfies continuity equation. Coefficients a_{jm} will be determined from collocation equations and matching or boundary conditions. Number of these equations is greater than number of unknown coefficients a_{jm}. Solution of this system of equations is thought in terms of least-squares method [L.G. Semin, V.P. Shapeev. Computational Technologies, 1998, Vol.3, No. 3, p. 72-84]. The order of convergence not worse than second was observed in numerical experiments in problems with smooth solutions at moderate Reynolds numbers. Algorithm of grid adaptation to solution singularities is implemented. Grid is adapted on the base of a-posteriory error estimation. As numerical experiments have shown, grid refines first of all in those subdomains where solution of initial differential problem has large gradients. This study was performed under financial support of RFBR, grants 99-01-00515 and 00-01-00370.

Multistage algorithms for numerical solution of ODEs

Yauheni Sonets & V. V. Bobkov

(Belarusian State University, Belarus)

For numerical solution of initial value problems for a system of nonlinear ordinary differential equations (ODEs) in the form

$$u'(t) = f(t, u(t))$$

one-step multistage algorithms of variable order are proposed. These algorithms are based on approximation of the original problem by initial value problems for systems of linear ODEs with constant coefficients. In the general case for arbitrary function f one does not have enough information on structure of the exact solution. In the case of a system of linear ODEs such information is available and can be used for construction of more efficient specialized methods.

Multistage linearization of the original problem is performed on the basis of technique of successive corrections. The essence of this technique is successive improvement of an initial approximation to the exact solution of the system of nonlinear ODEs within the integration step. Calculation of the improved approximation is based on information on defect of the preceding one. Thus, the proposed algorithms have a feedback with the systems they are applied to. This feedback affects their structure and choice of their parameters.
Different variants of the algorithms and results of numerical experiments are discussed.

Are the Stability Estimates, in the Kreiss Matrix Theorem, Sharp ?
Marc Spijker
(Leiden University, The Netherlands)

In the stability analysis of numerical processes for solving initial value problems, one is often faced with the task of estimating the spectral norm of the n-th power of given matrices. Stable processes are distinguished by the property that moderate upper bounds for these norms exist.
The Kreiss matrix theorem gives conditions under which such moderate bounds are valid. One of the conditions in the theorem involves the resolvent of the matrices under consideration. This so-called resolvent condition is known to imply upper bounds which grow linearly with the order of the matrices as well as with the exponent n.
It is a long standing problem whether these upper bounds can be sharpened to bounds which grow much slower than linearly with the order or with n. The solution to this problem will be given in this talk. The underlying research was carried out jointly with S. Tracogna and B.D. Welfert.

Path Following-Collocation Method for Solving Burger's Equation
Muhammed I. Syam
(United Arab Emirates University, UAE)

Anew numerical technique is presented for solving the Burger's equation. It is pased on the theory of the Collocation and path following methods. Theoretical and numerical results are presented.

The dynamical behaviour of Runge-Kutta time discretizations for nonlinear parabolic problems near an equilibrium point
Mechthild M. F. Thalhammer & C. Gonzalez & A. Ostermann & C. Palencia
(University of Innsbruck, Austria)

Runge-Kutta time discretizations of nonlinear evolution equations are studied in an abstract Banach space setting of analytic semigroups that includes fully nonlinear parabolic initial-boundary value problems.
We give smooth and nonsmooth-data error estimates for the backward Euler method and a convergence result for strongly $A(\theta)$-stable Runge-Kutta methods. We further show that the geometric properties near a hyperbolic equilibrium are well captured by the discretization.
Numerical examples illustrating the theoretical results are presented.

DAE Structure and Index in Dependence on MOSFET Modelling in Circuit Simulation
Caren Tischendorf
(Humboldt-University of Berlin, Germany)

The simulation of MOS integrated circuits requires the inclusion of special models describing the voltage-current or charge-current characteristics of the MOS elements. These models arise from the solution of the Poisson equation describing the statical behaviour coupled with the continuation equations describing the charge carrier transport in the semiconductor.
Different levels of the models may change the qualitative solution behaviour of the resulting DAE equations. Beside conventional explicit models we analyze new semi-implicit MOSFET models used in circuit simulation. We show the influence on the structure and the index of the resulting DAEs.

Solving Partial Differential Equations with Using Power Polynomials
Zdzislaw W. Trzaska
(Warsaw University of Technology, Poland)

The paper presents new approach to explicit solutions for two linear simulataneous partial differential equations with damping terms

$$u_x = Ri + Li_t, \quad i_x = Gu + Cu_t \tag{4}$$

where $x \in (0, l)$ and $t \in (0, \infty)$, with $u = u(x, t)$ and $i = i(x, t)$ denoting the transversal variables (e.g. voltage in an electrical transmission line or pressure in a hydraulic system) and longitudinal variable (e.g. current or flow), respectively. The subscripts stay for derivatives with respect to independent variables x and t. Longitudinal and transversal parameters per unit length of the system are denoted by R, L and G, C, respectively. Corresponding initial $u(x, 0)$ and $i(x, 0)$ as well as boundary $u(l, t)$ and $u(0, t) = \mathcal{A}_{(t)} i(0, t)$ conditions are specified. It is shown that solutions for (1) can be based on particular forms of power polynomials

$$P_n(y) = \sum_{k=0}^{n} a_{n,k} y^k, \qquad T_m(y) = \sum_{r=0}^{m-1} b_{m,r} y^r \tag{5}$$

in indeterminate $y = y(s)$ depending on the equations coefficients and the complex frequency s. Some basic properties of the power polynomials (2) are investigated and links between them are established. In result the solution for (1) are given by

$$\begin{aligned} U_n(y) &= P_n(y) U_0(s) + bT_n(y) I_0(s), \\ I_n(y) &= aT_n(y) U_0(s) + P_{n-1}(y) I_0(s) \end{aligned} \tag{6}$$

Problems involving equalities and limits are also solved. For $N \to \infty$ we can write

$$\frac{U_{N+1}}{I_{N+1}}_{|N\to\infty} = \frac{U_N}{I_N}_{|N\to\infty} = Q_\infty \tag{7}$$

Substituting (2) into (3) and solving (4) for Q_∞ yields

$$Q_\infty = \frac{y \pm \sqrt{y^2 + 4y}}{2a} \tag{8}$$

which remains valid if the condition $Q_{N+1} = Q_N$ for $N \to \infty$ is replaced by $Q_n(y) = Q_0(s)$ for $n = 1, 2, ..., N < \infty$.

A new method to solve first order Systems of nonlinear two-point boundary value problems
Marnix Van Daele & J.R. Cash
(Universiteit Gent, Belgium)

Deferred correction, which looks like,

$$\phi(\eta) = 0 \tag{9}$$
$$\phi(\bar{\eta}) = \psi(\eta) \tag{10}$$

is a widely used technique for the solution of first order systems of nonlinear two-point boundary value problems

$$\frac{dy}{dx} = f(x, y), \quad a \leq x \leq b, \quad g(y(a), y(b)) = 0. \tag{11}$$

In an influential paper, Skeel has proven the following result. Consider the approximate numerical solution of (11) on a mesh $\pi : a = x_1 < x_2 < \ldots < x_{N+1} = b$. Denote by Δy the restriction of the continuous solution $y(x)$ to the finite grid π. Let ϕ be a stable numerical method and assume that the following conditions hold for the deferred correction scheme (9), (10) : (i) $\|\eta - \Delta y\| = O(h^p)$, (ii) $\|\psi(\Delta y) - \phi(\Delta y)\| = O(h^{r+p})$ and (iii) $\psi(\Delta w) = O(h^r)$ for arbitrary functions w having at least r continuous derivatives. If $\phi(\bar{\eta}) = \psi(\eta)$ then $\|\bar{\eta} - \Delta y\| = O(h^{r+p})$.
In the context of two-point BVPs, ϕ can be chosen to be a Runge-Kutta methods of order p while $\psi = \phi - \phi^*$ where ϕ^* is a Runge-Kutta method of order $p + r$. For most of the schemes derived so far $r = 2$. Recently however, we have established the conditions to obtain higher values of r and in this talk we will consider a particular scheme based on Lobatto methods of overall order 8 for which $p = 4$ and $r = 4$. Special attention will be paid to construction of interpolants and the problem of error estimation.

Accuracy improvement with RKN methods
Tanja Van Hecke & Marnix Van Daele
(Universiteit Gent, Belgium)

Deferred correction is one of the acceleration techniques to improve the accuracy of a basic, simple method to solve ODEs with boundary conditions. We applied this technique on second order boundary value problems of the type $y'' = f(x, y)$ and found a way to increase the order of the basic numerical method by using a suited error estimator. The basic method as well as the error estimator are based on mono-implicit Runge-Kutta-Nyström methods which have the advantage that the dimension of the system to be solved when applying the numerical method on a BVP can be strongly reduced. A maximization of the increase of order of accuracy will be discussed as well as the stability of the scheme. Within this deferred correction scheme mono-implicit methods will be compared with Lobatto IIIA methods especially in case of stiff problems.

Exponentially-fitted Runge-Kutta methods: construction and implementation
Guido Vanden Berghe & L. Ixaru & H. De Meyer
(Universiteit Gent, Belgium)

Exponentially-fitted Runge-Kutta (EFRK) methods with s stages are constructed, which exactly integrate differential initial-value problems whose solutions are linear combinations of functions of the form $\{x^j \exp(\omega x), x^j \exp(-\omega x)\}$, ($\omega \in \mathbb{R}$ or $i\mathbb{R}, j = 0, 1, \ldots, jmax$), where $0 \leq jmax \leq \lfloor s/2 - 1 \rfloor$, the lower bound being related to explicit methods, the upper bound applicable for collocation methods. Explicit methods with $s \in \{2, 3, 4\}$ belonging to that class are constructed. For these methods a study of the local truncation error is made, out of which follows a simple heuristic to estimate the ω-value. By combining a fourth-order explicit EFRK method with an equivalent classical embedded (4,5) Runge-Kutta method a more sophistacted technique is developed for the estimation of the occurring ω-values. Error and step-length control is carried out by using the Richardson extrapolation procedure. Some numerical experiments show the efficiency of the introduced methods. Some preliminary results for implicit EFRK methods will be presented.

Extrapolation methods in Lie groups
Jörg Wensch
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Considered are differential equations on Lie groups given by $y' = v(t, y)|_{y(t)}$. Here $y : \mathbb{R} \to G$ is a curve on a Lie group and v is a map into the corresponding Lie algebra. This Lie algebra is to be interpreted as the set of right invariant vector fields.
The generalisation of Runge-Kutta methods of order 3 and higher on this class of problems makes the introduction of correction functions necessary. Here we consider the application of extrapolation methods on this class of problems. An asymptotic expansion of the global error in quadratic terms for symmetric methods is proved. The explicit midpoint rule is used as the basic method for an extrapolation algorithm.
The new methods of order 4 and 6 are compared with standard extrapolation procedures of the same order.

Structural analysis for stochastic DAEs in circuit simulation
Renate Winkler
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Modeling electrical networks influenced by thermal noise leads to specially structured differential-algebraic equations (DAEs) disturbed by white noise. To understand these systems it is necessary to use the theory of (explicit) stochastic differential equations (SDEs). We show that this is only possible if the noise sources do not disturb the constraints of the DAE. We then derive existence and uniqueness results for the solutions of stochastic DAEs of index 1 or 2. Similarly, we obtain convergence results for a semi-implicit Euler-method for specially structured stochastic DAEs of index 1 or 2.
We express the necessary conditions in terms of the topology of the electrical network. Alternatively, we discuss a model with colored noise sources.

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