MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 27/1993

Differential-Algebraic Equations:
Theory and Applications in Technical Simulation

June 13 - June 19 1993

The meeting was organized by H.G. BOCK (Heidelberg), P. RENTROP (München), and W.C. RHEINBOLDT (Pittsburgh).

The meeting's 37 talks showed the growing importance of differential-algebraic equations in many areas of application like multibody system dynamics, chemical engineering, biomechanics, civil engineering, or ecology, where DAE models are often a more natural, if not the only way of describing a system. This has also prompted much theoretical work especially in the fields of differential geometry and numerical analysis. The former leads to an understanding of DAEs as differential equations on manifolds (or: with invariants), and the latter contributes a number of new discretization schemes for DAEs together with ways to preserve the invariants. All in all, the results presented at the meeting clearly demonstrated that DAEs are a lively field of active research fostered by theory and application alike, from which many exciting results are still to be expected in the future.

Some of the topics taken up during the meeting are: Numerical Solution of DAEs with Ill-Conditioned Constraints, Multistep Methods for Constrained Multibody Systems (MBS), Optimization Problems for DAEs with Invariants, Stability Investigations for Discretization Schemes for DAEs, Symplectic Integration of Constrained MBS, Regularization of DAEs, DAEs versus ODEs in MBS Dynamics, A New Reduction of the EULER-LAGRANGE Equations, Stabilization of Invariant Manifolds, DAEs in River Models, Event-Controlled Simulation, DAEs in Chemical Engineering, Numerical Solution of General Higher Index DAEs, and many more.

The meeting brought together researchers from universities and industry, many of whom are just starting their careers. These young scientists in particular profited from the participation of many renowned researchers and the opportunity for discussions with them in the unique atmosphere of the institute.

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Abstracts

Numerical Solution of Differential-Algebraic Equations with Ill-Conditioned Constraints

L. PETZOLD
University of Minnesota
(Joint work with Y. RES & T. MALY)

We consider the numerical solution of higher-index differential-algebraic equations with ill-conditioned or rank-deficient constraints. These types of problems arise for example in the solution of constrained mechanical systems, when a mechanism's trajectory passes through or near a kinematic singularity. We derive a class of methods for these problems which are based on minimization of the norm of the constraints. The new methods are analogous to trust region methods of numerical optimization. We give error estimates and convergence and stability results for the new methods, and present some numerical experiments which illustrate their effectiveness.

Multistep and One-Leg Discretizations of Structured DAES

GUSTAF SÖDERLIND
Lund University, Sweden
(Joint work with CARMEN AREVALO, Univ. Simon Bolivar, Venezuela)

We consider various possibilities of discretizing semi-explicit index 1 and 2 DAEs in HESSENBERG form, with special emphasis on order and convergence. The equations are discretized by multistep and one-leg methods adapted to the structure of the problem - the system is partitioned equation-wise or variable-wise. It is shown how these discretizations are related, and that they cover a broad class of possible techniques, including BAUMGARTE stabilization and the so-called indirect approach. In addition, we show that it is possible to solve index 2 problems with explicit methods, resembling the "half-explicit" methods due to HAIRER, BRASEY and LUBICH. Full order conditions are given, thus constructing a comprehensive theory for the order of compound discretizations. For one-leg methods, "order reduction" may occur; it is briefly discussed and demonstrated that this is a resonance effect, if difference operators with unimodular roots are applied to the system. An important conclusion is that the system must not be "overdiscretized", and an example is given showing that it is feasible to consider treating problems with Lagrangian multipliers, without discretizing the multiplier variables.

A Multistage Approach to Optimization Problems for DAEs with Invariants

VOLKER SCHULZ
IWR, Universität Heidelberg

Typical boundary value problems for DAEs with invariants are initial value problems (e.g. index reduced descriptor-form for multibody systems), two point boundary value systems (e.g. discretizations of PDEs), overdetermined BVP (from parameter identification) or optimization BVP (e.g. optimal design, direct optimal control problems). A fifth type brings additional invariants into the game, which are not an outcome of the system dynamics: BVPs derived from optimal control problems by the necessary Pontrjagin conditions. These BVPs really need to be stabilized by invariants. In a multiple shooting method this can be done by projection of the trajectory and its Wronskian to their invariant manifolds after each integration step. A second approach is applicable to multiple shooting and collocation, which are both standard methods for the numerical solution of BVPs. The idea is first of to satisfy the considered invariant and solve the arising continuity conditions on the remaining space of degrees of freedom as good as possible. This is equivalent to orthogonal projection of the solution at the gridpoints and can be shown to have "very good" linear convergence behavior (generalized GAUSS-NEWTON method). This approach leads to a natural frame work not only to treat ordinary boundary value problems for DAEs with invariants, but also BVP with an objective function to be minimized.

β-Blockers for Multistep Methods for Constrained Multibody Systems

CLAUS FÜHRER & GUSTAF SÖDERLIND
Lund University, Sweden & DLR, Oberpfaffenhofen

For classification of various approaches to numerically solve Constrained Multibody Problems by means of multistep methods the dead beat control approach is studied, when applied to the discretized form. It could be shown that by shifting certain eigenvalues related to the σ-generating polynomial into the origin the class of so-called half explicit methods are obtained.

Shifting other σ-related eigenvalues in the index-3 case results in the well-known GEAR-GUPTA-LEIMKUHLER approach. The index-reduced index-2 formulation introduces invariants to the problem. These can be associated with the roots of the ρ-generating polynomial. These can be turned into constraints (0-eigenvalues) by applying the same technique as above resulting in coordinate projection methods.

By this technique the relation between coordinate projection and derivative projection methods, the discrete state space form and others could be shown for the linear case.

Stability Investigations for Semi-Explicit Index-2-Systems

RÜDIGER WEINER
University of Halle
(with JÖRG WENSCH & KARL STREHMEL)

We consider linear, time dependent DAEs of index 2

$$\begin{aligned} y' &= B(t)y + C(t)z + q(t) \\ 0 &= D(t)y + r(t) \end{aligned}$$

We assume the essential underlying ODE (in the form introduced by ASCHER and PETZOLD)

$$V' = (\lambda_1 + \lambda_2)V + g(t)$$

to be dissipative. Our aim is to derive conditions for the numerical solution to be contractive for the essential underlying ODE. Under additional assumptions we obtain for projected RUNGE-KUTTA methods for the difference of numerical solutions a relation of the form

$$W_{n+1} = R(h\lambda_1, h\lambda_2)W_n,$$

R the "extended stabilty function". The components determined by λ_2 are integrated by the underlying RK-method, the components determined by λ_2 are integrated in a different way, for DIRK-methods explicitly. Stability regions for common RK-methods are plotted, numerical tests confirm the theoretical results.

Small Perturbations in Differential-Algebraic Systems of Index 2 and 3

MARTIN ARNOLD
Universität Rostock

The perturbation index of a differential-algebraic system gives an intuitive measure of the difficulties that have to be expected during the numerical solution. For systems in HESSENBERG form, upper bounds for the influence of perturbations on the analytical solution are known from the definition of the perturbation index. These can be improved substantially for the differential components of the solution. For systems that are linear in the algebraic components the bounds can be further decreased. If systems in HESSENBERG form are discretized by suitable methods then similar bounds can be obtained for the influence of small errors that arise in the implementation on the computer (e.g. errors in the iteretive solution of systems of nonlinear equations and round-off errors). Several modifications of the discretized schemes for higher index systems have been discussed in the literature. The error bounds can be used to prove that some of these modifications yield numerical methods that are more robust against small errors in the numerical solution.

State-Estimation within Multibody Simulation Software

WILLI KORTÜM
DLR - Oberpfaffenhofen

State-estimators (KALMAN filters, LUENBERGER state-observers) are required for controlled mechanical systems such as advanced "mechatronic" vehicles. On the other hand, vehicle system dynamics is modelled as multibody systems leading to DAEs. In this presentation, first the technological problem was stretched. It leads to the request to implement nonlinear state-estimators within a descriptor (DAE)-formulation of the multibody equations of motion. In the following a brief survey of the state-of-the-art of MBS software and its suitability for implementing state-estimators was given. Then, the different versions of observers and KALMAN filters and their computational efforts were pointed out. This included state-observers for descriptor formulations as well as the so-called EKF (= extended KALMAN filter). Finally, the implementation of such estimators within a specific MBS-code was sketched and (a) rather large lists of open problems both theoretical and computational were presented with the intent to create appetite in the audience to attack some of them ...

Differential-Algebraic Equations for Hominoid Models and Insulator Chains

PETER KAPS
Universität Innsbruck

We give the equations of motion in descriptor form for three applications:

1. Simultaneous determination of the coefficient of kinetic friction and drag area in straight running on a slope with variable inclination.

2. Determination of the reaction forces for an Alpine skier running over moguls.

3. Load transposition caused by insulator failure on a double tension set of high voltage lines. For an insulator string with 33 elements the equations of motion are numerically integrated on state space form as ODE and on descriptor form using generalized cartesian coordinates as DAE. The DAE formulation is easier and leads to shorter computing times.

Symplectic Integration of Constrained Multibody Systems

ERNST HAIRER & LAURENT JAY
Université de Genève

The equations of motion for constrained multibody systems are written in the Hamiltonian formalism. For their numerical solution we search for methods which are

a) symplectic

b) stiffly accurate.

It is shown that no RUNGE-KUTTA methods can satisfy these requirements. Within the class of partitioned RUNGE-KUTTA methods the combination of LOBATTO IIIA and LOBATTO IIIB methods is proposed. It is symplectic, stiffly accurate, super-convergent, and the numerical solution satisfies the same constraints as the analytical solution does. The main results with proofs are presented in the thesis of LAURENT JAY.

BDF Methods for Stiff DAEs: On Stability and Convergence

CHRISTIAN LUBICH
Universität Würzburg

Backward differentiation formulae (BDF) are widely used in the numerical solution of differential-algebraic equations. This talk is concerned with stability and convergence results for such methods. Stiff DAEs of index 1 and 2 are considered, taking the equations of motion of strongly damped constrained mechanical systems as an example. The basic assumption is uniform well-posedness in $\mathcal{L}^2$ of the frozen-coefficient linearized problems. By combining FOURIER and perturbation techniques, it is shown that BDF methods produce numerical solutions that are l^2-stable in the algebraic variables, and l^∞-stable in the differential variables. Convergence of optimal order then follows.

Half-Explicit Methods for Index 3 DAEs: Pros and Cons

ALEXANDER OSTERMANN
Universität Innsbruck

This talk is concerned with the numerical integration of semi-explicit index 3 DAEs by half-explicit RUNGE-KUTTA methods. These methods only treat the algebraic variables (and equations) implicitly, hence have computational advantages compared to fully implicit schemes. A short overview, concerning the convergence properties of such methods is given. It turns out that there exist half-explicit methods of arbitrarily high order. The implementation can be done in a way very similar to half-explicit index 2 methods. Due to the fairly high index, the resulting codes are of course more sensitive with respect to perturbations.

Regularization for DAEs

ROBERT O'MALLEY
University of Washington

The $\varepsilon = 0$ problem for the index-one DAE

$$\begin{aligned} \dot{u} &= A(t)u + B(t)v + f(t) && (m \text{ eqns}) \\ 0 &= C(t)u + \varepsilon D(t)v + g(t) && (n < m \text{ eqns}) \end{aligned}$$

($\varepsilon > 0$) is an index-two DAE when CB is invertible. It is equivalent to the singular perturbation problem

$$\varepsilon\dot{u} = -BD^{-1}(Cu + g) + \varepsilon(Au + f)$$

when D^{-1} exists. Setting

$$u = \binom{y}{z} \quad \text{and} \quad D^{-1} = B'(BB')^{-1}\begin{bmatrix} \Lambda(t) & 0 \\ 0 & 0 \end{bmatrix}(C'C)^{-1}C$$

yields the decoupled fast-slow system

$$\begin{cases} \varepsilon\dot{y} = -\Lambda(t)\left(y + [I_n 0](C'C)^{-1}C'g + \varepsilon\left(A\binom{y}{z} + f\right)_1\right) \\ \dot{z} = \left(A\binom{y}{z} + f\right)_2 \end{cases}$$

whose solution is clear when $\Lambda(t)$ has a hyperbolic splitting.

Attention to the boundary value problem with

$$R_0u(0) + R_1u(1) = S$$

prescribed is given.

On Index-2 Differential Algebraic Equations

Roswitha März
Humboldt-Universität Berlin

Linear continuous coefficient index-2 DAEs $A(t)x'(t) + B(t)x(t) = q(t)$ as well as quasilinear equations $A(t)x'(t) + g(x(t),t) = 0$ are discussed, where g is supposed to have a continuous Jacobian $g'_x(x,t)$ and certain part of $g'_t(x,t)$. The nullspace $\ker A(t) =: N$ is assumed to be constant. Let Q denote a projector into N, $P := I - Q$. Forming $A_1(t) := A(t) + B(t)Q, N_1(t) := \ker A_1(t), S(t) := \{z \in \mathbb{R}^m : B(t)z \in \operatorname{im} A(t)\}, S_1(t) := \{z \in \mathbb{R}^m : B(t)Pz \in \operatorname{im} A_1(t)\}$, we may characterize index-2 DAEs by the conditions

$$\dim(N \cap S(t)) = \text{const.} > 0, N_1(t) \oplus S_1(t) = \mathbb{R}^m.$$

Denote by $Q_1(t)$ the projector onto $N_1(t)$ along $S_1(t), P_1(t) := I - Q_1(t)$. Now the decomposition $\mathbb{R}^m = N \oplus PS_1(t) \oplus PN_1(t)$ becomes true, and we may decouple the linear DAE in its characteristic parts. An analogous decoupling of integration methods (BDF, IRK) makes their behaviour transparent. In particular it comes out that the same methods are produced for the inherent regular ODE iff the projector $P_1(t)$ is constant.

For nonlinear DAEs assume the nullspace component Qx to be involved in the derivative free part linearly. In that case, linearization makes sense. Given a solution $x_* \in C^1_N$, the initial value problems $A(t)x'(t) + g(x(t),t) = 0, PP_1(S)(x(S) - z) = 0$ are proved to have C^1_N solutions for sufficiently small $| PP_1(S)(z - x_*(S)) |$ via linearization and decoupling. Following these lines, the BDF is shown to be feasible and weakly unstable but convergent with the expected order. However, while for linear DAEs the weak instability is related to the nullspace components Qx_l only, even in nonlinear Hessenberg form DAEs the state components $PP_{1,l}x_l$ are also affected by that instability.

On Stability of Dynamical Systems Described by Differential-Algebraic Equations

PETER C. MÜLLER
Bergische Universität Wuppertal

Singular systems (descriptor systems, differential-algebraic equations) are a recent topic of research in numerical mathematics, mechanics and control theory as well. But compared with common methods available for investigating regular systems many problems still have to be solved making also available a complete set of tools to analyze, to design and to simulate singular systems. In this contribution the aspect of stability of motion is considered. Some new results for linear singular systems are presented based on a generalized Lyapunov matrix equation. Particularly, for mechanical systems with holonomic constraints the well-known stability theorem of THOMSON and TAIT is generalized. Some additional results are given for nonlinear mechanical systems with holonomic constraints based on the LYAPUNOV theory with respect to a part of variables using the Hamiltonian as a LYAPUNOV function.

Differential-Algebraical versus Ordinary Differential Equations in Multibody System Dynamics

WERNER SCHIEHLEN
University of Stuttgart

DAEs are popular in multibody system dynamics. The reasons are as follows:
1. standard modeling techniques can be applied,
2. singularities don't occur and as a consequence
3. multistep integration works continuously without any restart.

In principle, DAEs may replace the expert in multibody dynamics simulation by the computer. However, DAEs are far away from real time simulations and, therefore, ODEs are still of interest in multibody system dynamics.

Complex multibody systems are analysed by cutting the loop resulting in tree topology and kinematic closing constraints, i.e. DAEs, which means a standard modeling technique. For tree topology systems nonrecursive and recursive formalisms like NEWEUL and SIMPACK, respectively, are generating the open loop equations of motion automatically. The constraints are given by implicit equations which can be inverted to explicit equations between dependent and conserved independent coordinates using results from kinematics (WOERNLE, 1988). Then, coordinate partitioning is introduced where two different sets of conserved independent coordinates are controlled by the projection criterion to overcome singularitites (BLAJER 1991, SCHIRM 1993). The motion coupling or the reaction coupling, respectively, closes finally the loop, i.e. the DAEs are reduced to ODEs. Further, the multistep integration code is modified resulting in an efficient restart after changing the set of independent coordinates. As example, a torus chain is considered and simulation results are discussed.

Geometric Index and Tractability Index

Michael Hanke
Humboldt-Universität zu Berlin

For fully implicit DAEs $F(x, x') = 0$ Reich proposed a reduction process using geometric considerations. Via this process, a geometric index can be defined. Rabier and Rheinboldt gave sufficient conditions for this approach to work. At the end of the reduction process we arrive at an ODE on a certain manifold. This is more than actually needed. Indeed, it would be sufficient to construct a state space form which demands less smoothness properties. One can modify the geometric reduction process in this respect if one has the additional assumption fulfilled that the kernel of $F_y(x, y)$ is independent of (x, y).

Moreover, it is possible to translate the geometric conditions into conditions in terms of F for the index 2 case. Going this way we arrive at the matrix chain approach by Griepentrog and März. The latter turns out to be an (easily computable in practice) analytical counterpart of the geometry behind the scenes.

On the Existence, Uniqueness of Solutions and the Convergence of Wave Relaxation Methods for DAEs

Marian Kwapisz
University of Gdansk, Poland

The DAE system

$$\begin{aligned} x'(t) &= f(x, x, x', x', y, y)(t)\,, \quad x(0) = \bar{x}_0 \\ y(t) &= g(x, x, x', x', y, y)(t) \end{aligned}$$

with the Volterra operators f, g was considered.

The existence and uniqueness results for this system were established under the assumption that f and g are Lipschitz continuous with Lipschitz coefficients a_i and $b_i, i = 1, 2, \ldots, 6$, respectively, and that the spectral radius of the matrix

$$\begin{pmatrix} a_3 + a_4 & a_5 + a_6 \\ b_3 + b_4 & b_5 + b_6 \end{pmatrix}$$

is less than one.

It was also shown that under the same conditions the waveform relaxation method (WRM)

$$\begin{aligned} x'_{k+1}(t) &= f(x_{k+1}, x_k, x'_{k+1}, x'_k, y_{k+1}, y_k)(t), \quad x_{k+1}(0) = \bar{x}_0 \\ y_{k+1}(t) &= g(x_{k+1}, x_k, x'_{k+1}, x'_k, y_{k+1}, y_k)(t), \end{aligned}$$

x_0, y_0 arbitrarily chosen, converges uniformly. It was shown also that for this method one can get better error evaluation than for the standard PICARD iteration (all indexes on the right hand side are k). It was mentioned that WRM is suitable for parallel techniques.

A New Reduction of the EULER-LAGRANGE Equations

WERNER C. RHEINBOLDT
University of Pittsburgh

A new approach is presented for the numerical solution of the EULER-LAGRANGE equations based upon the reduction of the problem to a second order ODE on the constraint manifold. This procedure differs from the standard index-three DAE-approach and allows to bypass some of the difficulties encountered with higher index problems. The algorithm guarantees that the constraints are automatically satisfied and requires a minimal number of evaluations of second order derivative terms. In fact, second order derivatives are shown to enter only through the second fundamental tensor of the constraint manifold. This tensor may be computed either explicitly when second derivatives are available or via an approximation procedure. Examples show that the method compares well with other available software.

Stabilization of Invariant Manifolds, DAEs and Mechanical Systems

URI ASCHER
University of British Columbia, Vancouver

BAUMGARTE's method for stabilizing index-reduced mechanical systems is probably still the most popular stabilization technique. However, the choice of the parameters of this method is unclear. We argue why the choice of these parameters is bound to remain elusive. We then proceed to consider a sequence of improvements. First, consider the stabilization of ODE invariants. Then, discretize the stabilizing term in a special way. The obtained method is related to coordinate projection. Its effectiveness is demonstrated by examples.

In the second part of the talk DAEs with singularities but smooth solutions are considered. A new Sequential Regularization Method is proposed to solve such problems.

Numerical Integration of Constrained Hamiltonian Systems

S. REICH
Institut für Angewandte Analysis and Stochastik, Berlin

Different generalizations of symplectic and/or energy preserving integration schemes for Hamiltonian systems were considered. These include constrained Hamiltonian systems and the generalized EULER equations on n-dimensional LIE groups. Especially we looked at techniques that decompose the given differential equations into sub problems that can be integrated exactly. Those splitting schemes can be analysed conveniently by the BALSER - CAMPBELL - HAUSDORFF formula and result in symplectic and/or energy preserving schemes.

On the Transient Behavior of Sinusiodal Electrical Oscillators

W. MATHIS
Lehrstuhl für Theoretische Elektrotechnik (RSE), Wuppertal

The description equations of electrical networks for oscillator circuits are of the type of algebro-differential equations. Where the associated solution manifold contains at least a limit cycle. The steady-state behavior can be described by averaging or harmonic balance type methods. In the literature several variants of these methods and their implementations will be discussed. On the other hand for designers of oscillators its transient behavior to the steady-state is of some interest. Especially for the case of crystal oscillators no robust methods are available till now. In this paper the usefulness of LMS methods (e.g. BDF) as well as linear methods based on trigonometric polynomials will be discussed and illustrated with realistic electrical oscillator networks. Another approach for considering the transient of oscillatory behavior based on the calculation of its envelop of a solution. We present some ideas and results for extending L. PETZOLD's method to calculate the envelop of an oscillatory solution.

Numerical Properties of Circuit Models in Industrial Applications

U. FELDMANN
(Siemens, München)
coauthor: M. GÜNTHER (Technical University München)

Models of electric circuits are often discussed in mathematical literature about numerical integration of differential algebraic equations. Unfortunately many results cannot be transferred directly to real life applications, because the underlying assumptions either cannot be checked easily or even are not fulfilled.

The purpose of the talk is to demonstrate on simple practical examples, how important numerical characteristics like index, stiffness and smoothness are affected by the scheme for setting up the equations and by the accuracy level of modeling.

Application of ROW Methods for DAEs and PDEs in River Models

GERD STEINEBACH
Bundesanstalt für Gewässerkunde, Koblenz

The blaze at the Sandoz chemical factory in Basel in 1986 resulted in large amounts of chemically polluted water with catastrophic consequences in the river Rhine. This was the starting-point to develop a Rhine alarm model for the prediction of the transport and dispersion of a pollution plume.

The model is based on an analytical approximation to the solution of the underlying convection-diffusion equation. A more detailed modelling of river processes is possible if numerical methods are taken into account. The method of lines in connection with ROW methods for the time-integration of the semi-discretized PDEs is used in various applications. To avoid well known order-reduction phenomena, the index-1 DAE code RODAS (HAIRER, WANNER, 1991) was slightly modified to fulfil the additional order-conditions according to SCHOLZ (1989) and OSTERMANN, ROCHE (1991).

Simulation Levels for Gasflow Networks

GABRIELE ENGL & PETER RENTROP
Technische Universität München

A network formulation is introduced for the simulation of gas transmission systems like a multi-cylinder internal combustion engine. The components of a gas flow network (chambers, pipes, connections) and the mathematical model depend on the simulation level.

Chamber-states are described by ODE systems in time t. Unsteady gas oscillations in pipes are not taken into account on a simple simulation level. A more complex model includes pipes and the modelling of the pipe flow by the one-dimensional EULER equations of gas dynamics, a hyperbolic system of PDEs. Algebraic equations are introduced by boundary conditions for the pipe flow. Semi-discretization of the resulting system of equations leads to a DAE-system.

The numerical solution is based on a TVD method for the pipe equations and a predictor-corrector method for the remaining DAE system. Numerical simulation results are presented for an internal combustion engine: A higher simulation level provides more information for an improved charge cycle.

Descriptor Forms and Numerical Integration Methods for Constrained Mechanical Systems

BERND SIMEON
Technische Universität München

The equations of constrained mechanical motion form a system of index 3. This descriptor form exhibits various difficulties for the numerical integration. The first part of the talk concentrates on a new formulation of the equations of motion as projecting descriptor form of index 1. The basic idea is a redundant second order formulation of the equations of motion. It turns out that this second order formulation can be transformed into an index 1 system where certain projections guarantee that the solution satisfies all constraints. In case of the index 2 formulation, the transformation leads to an ODE-formulation where standard methods can be applied. In the second part, implementation aspects are discussed and practical examples from multibody system dynamics illustrate the properties of this approach.

Numerical Methods for Constrained Hamiltonian Dynamics

BEN LEIMKUHLER
University of Kansas

Molecules are multibody systems with tiny bodies. We looked at the various approaches used to handle constraints in the multibody dynamics world and developed these for particle dynamics with one additional requirement: symplecticness. In this way, we get Hamiltonian state space forms, Hamiltonian underlying ODEs (courtesy P. DIRAC) and then, finally and most practically we found direct symplectic discretizations for constrained systems. We are applying the latter techniques in macromolecular modelling where the constraints arise through the removal of the highest frequency modes (corresponding to X-H chemical bonds).

Event-Controlled Simulation

PER GROVE THOMSEN
Technical University of Denmark

In many technical applications the dynamic model may change state. The changes of state are controlled by functions that change sign. The control of state transition is very important for the simulation process. In the presentation a strategy of using continuous extensions to the numerical solution is suggested for this process. In the case of ODE systems this is a known strategy, in the case of DAEs the problem of finding consistent initial values for the restart in the new state leads to a constrained optimization problem. New GERK-methods are used for index 1 and 2. The ideas are illustrated by a Reactor Vessel problem.

Differential-Algebraic Equations in Chemical Engineering

EDDA EICH
Linde AG, Höllriegelskreuth und München

The dynamic simulation of chemical plants leads to differential-algebraic equations with discontinuities in the right hand side and in the variables themselves. It is shown for various models of unit operations that the index is in most cases 2. Higher index problems occur depending on the specifications and may result from control specifications. Discontinuities arise due to the presence of controllers and valves and the change of physical property equations (e.g. phase changes). Numerical problems as well as solution approaches are given. These include the solution of the large nonlinear systems and the treatment of discontinuities.

Software Tools for Sensitivity Analysis of Numerical Solutions of Multibody System Dynamics

JENG YEN
Computer Aided Design Software, Inc., Iowa, USA

Modeling parameters of multibody systems are used to describe geometry of the constraints, characteristics of applied forces mass-inertia properties of bodies, etc. The sensitivity of numerical solution with respect to the modeling parameters is often the key to design improvements, moreover, the sensitivity information can be also used for some numerical treatments of the equations and for selecting appropriate numerical integration methods. The parameters in CAD and CAE are usually determined by either tedious calculation or some ad hoc measurements. However, the effectiveness of numerical methods for multibody systems is subject to the modeling parameters. The goal of this sensitivity analysis of multibody system dynamics is to obtain computational efficiency of simulation within the required accuracy of numerical solutions. Applying automatic differentiation software tools to multibody system code, a computer-oriented model is proposed to perform the sensitivity analysis of numerical solutions of constrained mechanical systems.

Efficient Integrators for Constrained Motion Equations

FLORIAN A. POTRA
University of Iowa

By local parametrization of the differentiable manifold defined by the position and velocity constraints the equations of constrained motion are reduced to a system of (unconstrained) equations in a minimal number of coordinates. In turn the latter system can be integrated by standard ODE solvers. However, it is more efficient not to perform this reduction explicitly but to work with the constrained variables of the original problem. We show different ways for implementing efficiently this idea for implicit and especially for explicit multistep and RUNGE-KUTTA methods.

An Inverse Dynamics ADAMS-STÖRMER Method for the Simulation of Multibody Systems in Technical Applications

REINHOLD VON SCHWERIN
IWR, Universität Heidelberg

The method is a result of an attempt at an optimal dovetailing of multibody formalisms and numerical solution methods, which is only possible to arrive at through close interdisciplinary cooperation. The basic approach is to treat the equations of motion of multibody systems as delivered by multibody formalisms in their inverse dynamics (or residual) form and, in the DAE case, to operate on the Index 1 system. The solution of the arising linear systems is performed by a structure exploiting linear algebra method which also leads to a cheap way to perform coordinate projection to the invariant manifolds. Furthermore, the method takes advantage of the fact that the dynamic equations are of second order thus avoiding a substantial amount of overhead.

Automatic Evaluation of Taylor Coefficient Vectors and their Jacobian Matrices

ANDREAS GRIEWANK
Argonne National Laboratory

The numerical integration of ordinary differential equations and differential algebraic equations requires the evaluation or approximation of time-derivatives and Jacobians w.r.t. the state-vector. It is shown here that these quantities can be evaluated with high accuracy and at an a priori bounded complexity when the right hand side and constraints are defined by computer programs. Sparsity can be exploited and discontinuities can be detected.

Computation of Initial Values for Differential-Algebraic Equations on Supercomputers

W. SCHMIDT
Technische Universität München

The computation of initial values for DAEs leads in general to a system of nonlinear equations. A new method for systems of nonlinear equations is introduced. It is based on the extension of KRYLOV-subspace to the nonlinear case and on the strategy of minimizing residuals. In the difference to linear problems the determination of a correction vector in the nonlinear KRYLOV subspace leads to a nonlinear least squares problem. With information from the hierarchical structure of the method, these problems can be solved very efficiently.

The Numerical Solution of General Higher Index DAEs by a Constraint Preserving Integrator

STEPHEN L. CAMPBELL
North Carolina State University

Many numerical methods exist for solving DAEs. However all of these approaches require some assumptions on index and structure. Most methods require the index to be 1 or 2 and sometimes 3. A general approach had been presented before, however, it did not preserve constraints. This talk presents the first general integrator for higher index DAEs which preserves all constraints, including the implicit ones. No assumptions are made on the structure. Preliminary results from an integrator under development are presented.

DAEs Arising in the Simulation of Chemically Reacting Flows

ULRICH MAAS
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Numerical simulation of reacting flows is a challenging task due to the strong interaction of flow field, chemistry and molecular transport. Mathematical modelling is performed by solving the set of NAVIER-STOKES equations (i.e. conservation of mass, momentum, energy and species mass) which involves an enormous numerical and computational effort due to the large number of equations, the strong coupling, the non-linearity and the stiffness introduced by the chemical kinetics. A numerical model is presented which is based on the method of lines. Spatial discretization of the partial differential equation system on adaptive grids leads to a large number of ordinary differential and algebraic equations. It is shown that this approach allows the detailed simulation of reacting flows in up to 2 D geometries. However, for practical applications there is a need of simplifying the governing equation system. An approach is presented which allows to decouple the fast time scales of the chemical reactions and thus enables a reduction of the number of governing equations. The method is based on an eigenvector analysis of the chemical rate equations. It can be applied quite generally to reacting flows.

Solution Properties of Differential-Algebraic Systems Espacially in the Presence of Singularities

P. J. Rabier
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A recently developed differential-geometric existence theory for general implicit differential-algebraic systems (DAEs) has led to new results about certain classes of singularities of the solutions of these equations. These singularities include, for instance, the so called impasse points for RLC circuits and they occur also rather frequently in many other applications. The general theory will be reviewed and, where applicable, new results will be presented.

Numerical Treatment of DAEs with Impasse Points

Renate Winkler
Humboldt-Universität zu Berlin

We consider mainly semi explicit autonomous DAEs

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

with $x(t) \in \mathbb{R}^n, y(t) \in \mathbb{R}^m$ and sufficiently smooth functions f and g. Under certain degeneracy conditions a local singularity of g'_y causes impasse points, where no continuation of the solution exists. Standard codes for DAEs fail in the neighborhood of such points. To overcome this, we applied an idea of P. Rabier and W. C. Rheinboldt (1992) for ODEs with certain singular points directly to the DAE. We changed the independent variable t, took a suitable normalizing condition and obtained an augmented quasilinear DAE with geometrical or differential index 1.

The last part of the talk was devoted to the numerical simulation of the 'jump' to the stable part of M for systems with singularly perturbed background. Our aim is to find the 'drop' point. For this we propose simply to increase (or decrease) the values of some component y_i together with a homotopy-method for the computation of the other components of y in dependence on y_i so long as we find a new solution of $g(x,y) = 0$.

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