MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

T a g u n g s b e r i c h t 29/1981

Numerische Verfahren zum Lösen von steifen Anfangswertaufgaben

28.6. bis 4.7.1981

Die Tagung fand unter der Leitung von Herrn G. Dahlquist (Stockholm) und Herrn R. Jeltsch (Aachen) statt. Da nur das halbe Institut zur Verfügung stand, konnten leider viele Interessenten nicht eingeladen werden. Zwei Drittel der 32 Teilnehmer kamen aus dem Ausland.

Das Ziel der Tagung war es, eine intensive Aussprache zwischen den theorieorientierten und den mehr softwareinteressierten Forschern anzuregen. Daß dies gelang, ist aus den Themen der 27 Vorträge ersichtlich, in denen der neueste Stand der Forschung im ganzen Problemkreis dargestellt wurde. Dieser reichte von der theoretischen Behandlung von Zeitdiskretisationen bis hin zur praktischen Softwareherstellung.

Unter anderem wurden folgende Probleme angesprochen:
nicht exponentiell anwachsende Fehlerschranken bei nichtlinearen steifen Differentialgleichungen; Kontraktivität, algebraische und absolute Stabilität, und zwar sowohl Beziehungen untereinander als auch die Wechselwirkung mit der Genauigkeit der Verfahren; gemischte Systeme von Differentialgleichungen und algebraischen Gleichungen; Randwertaufgaben mit inneren Grenzschichten; Konstruktion neuer Verfahren mit optimalen Eigenschaften; automatisches Erkennen der Steifheit eines Differentialgleichungssystems oder eines steifen Teilsystems; automatische Schrittweiten- und Ordnungssteuerung; Implementierung der Rückwärtsdifferentations-Formeln, Extrapolationsverfahren, Rosenbrocktyp Verfahren und semi-implizite Runge-Kutta Verfahren.

Es entstand zwischen den beiden Gruppen der mehr theoretisch und mehr softwareinteressierten Teilnehmern ein reger Gedankenaustausch. Dieser schlug sich nicht nur in lebhaften Diskussionen während des Vortragsprogramms nieder, sondern wurde durch informelle Sitzungen in kleineren Gruppen und persönliche Gespräche weitergeführt. Die anregende Atmosphäre des Instituts und die vorbildliche Betreuung förderten den harmonischen Verlauf der Tagung. Der Leitung des Instituts und dem Personal des Hauses gilt daher der besondere Dank der Teilnehmer.

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Vortragsauszüge

G. BADER:

On the Stability of the Extrapolation Method based on the Semi-Implicit Mid-Point Rule

The aim of the present investigation is to analyze the stability properties of the semi-implicit mid-point discretization with polynomial extrapolation for general nonlinear initial value problems. As it turns out, part of the discrete approximations are A-stable (while for all approximations $A(\alpha)$ - and stiff - stability holds). This result also carries over from scalar case to dissipative *systems* of the kind $y' = Ay$. Finally conditions for contractivity in the non-linear case are given. The techniques used apply to general semi-implicit discretizations (e. g. W-methods). The presented results will appear in a more general context as part of a joint paper together with E. Hairer and Ch. Lubich.

J. C. BUTCHER:

General Linear Methods: Prospects as Stiff Solvers

General linear methods were proposed as a class worthy of study because they generalized in a natural way the two main classes of numerical methods (Runge-Kutta and linear multistep) for ordinary differential equations. In this lecture, some of the properties of general linear methods will be reviewed and, in particular, they will be considered from the point of view of suitability for the treatment of stiff problems. The hope is to retain many of the desirable properties of Runge-Kutta methods such as good stability regions, ease of starting and ease of step size changing but at the same time to achieve something like the efficiency of linear multistep methods together with their convenient and reliable local error estimating facility.

J. R. CASH:

Advanced Steppoint Methods for ODE's

An advanced steppoint method for the numerical integration of the initial value problem $y' = f(x,y)$, $y(x_0) = y_0$ has the general form $g_1(y_{n+k}) = g_2(x, y_{n+k-1}, y_{n+k-2}, \dots , y_n, \bar{y}_{n+k+1})$. This k-step formula computes an approximate solution at $n + k$ in terms of the solution at back points x_{n+i}, $0 \leq i \leq k-1$, and in terms of an approximation $\bar{y}_{n+k+1}$ at the advanced steppoint x_{n+k+1} . An implicit predictor formula is used to generate approximations $\bar{y}_{n+k}$, $\bar{y}_{n+k+1}$ and then a higher order corrector, normally with better stability properties, is used to compute y_{n+k} . Such formulae have recently been proposed by Cash and by Cash and Bond. In this talk we examine various extensions to these approaches. Connections with more familiar integration-formulae are established and some new algorithms are proposed.

G. DAHLQUIST:

On the Local and Global Errors of One-Leg Methods

A one-leg method for numerical integration of a differential system $dy/dt = f(y,t)$ is defined by a difference equation of the form

$$h_n^{-1} \rho y_n = f(\sigma y_n, \sigma t_n) \quad , \qquad (*)$$

where ρ , σ are the difference operators,

$$\rho y_n = \sum_{j=0}^{k} \alpha_j y_{n-j} \quad , \quad \sigma y_n = \sum_{j=0}^{k} \beta_j y_{n-j} \quad .$$

Let $(L_d\varphi)(t_n) \triangleq h_n^{-1} (\rho\varphi)(t_n) - (D\varphi)(\sigma t_n)$, (differentiation error operator) ,

$(L_i\varphi)(t_n) \triangleq \sigma\varphi(t_n) - \varphi(\sigma t_n)$, (interpolation error operator) .

The formula for the local error given previously, contained the Jacobian in the right hand side and gives therefore a wrong impression of how the methods work on stiff problems. The following new expression is given for the local truncation error, $(L_d - DL_i)\, y(\sigma t_n)$, which is valid also for variable step size. Its asymptotic form is analysed, and it is used for obtaining equations for the global error, here defined as $\sigma y_n - y(\sigma t_n)$, (instead of $y_n - y(t_n)$) . The dominant part of the global error satisfies a variational differential equation. The contractivity analysis for difference equations of the form (*) is used to show that the remaining part of the error is negligible (for a suitable choice of step size), e. g. if the differential system can be partitioned into a stiff and a non-stiff part, each of which satisfies monotonicity conditions, related to different circle-bounded subsets of the stability region of the method. (The form of such methods was given in the speaker's article "G-Stability is Equivalent to A-Stability", BIT 1978.)

P. DEUFLHARD:

Order and Stepsize Control in Extrapolation Methods

The talk presents a new theory for joint order and stepsize control in extrapolation methods. This theory defines a locally optimal order that can be determined along any trajectory to be computed. In addition, Shannon's information theory is applied to derive some ideal convergence model that is expected to describe the behaviour of an extrapolation method over a large set of test problems. Extensive numerical comparisons document a drastic acceleration in stiff integration and a mild acceleration in non-stiff integration by the new device. Moreover, a significant increase in reliability, robustness and portability of the extrapolation codes is achieved.

W. H. ENRIGHT:

The Use of Partitioning in Stiff Solvers

There are several effective numerical methods available today for solving stiff systems. These methods are usually implicit and require at least the solution of a linear system of equations on each time step. As a result the computing time for these methods is frequently dominated by the cost of the associated linear algebra. Significant improvement in performance is possible if one adopts techniques that can exploit any structure that is inherent in certain classes of stiff problems. If a stiff system is structured in such a way that only a few transient components are present then we should use methods that are able to exploit the structure. Enright and Kamel (1979) have investigated ways to exploit this structure by modifying the linear algebra modules while others have suggested the use of different formulas for different components. Various aspects of these approaches will be analysed.

R. FRANK:

B-Convergence of Runge-Kutta Methods

Global error bounds of the type $\|\eta_\nu - y(t_\nu)\| \leq C(t_\nu, m, M_i, i \in I)h^n$ are derived for certain implicit Runge-Kutta methods, applied to nonlinear stiff initial value problems $y' = f(t,y)$, $y(0) = y_0$, $t \in [0,T]$, $f: \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$. There m denotes the onesided Lipschitz-constant of the right hand side f , and M_i are bounds for certain derivatives of the exact (smooth) solution. For Gauss and Radau II A formulas we have the order $p = s$ (s = number of stages of the method) and for Radau I A formulas the order is $p = s - 1$. The well known test equation $y' = \lambda(y - g(t)) + y'(t)$, $y(0) = g(0)$, demonstrates that improvements of the order results (i. e. increasing values of p) are essentially impossible.

C. W. GEAR:

Differential-Algebraic Equations Revisited

The implicit equation $F(y, y', t) = 0$, $y(0)$ specified, has a well-behaved solution if F is smooth and $[\partial F/\partial y']^{-1}$ is bounded, and it can easily be solved numerically. When $\partial F/\partial y'$ is singular, consistency conditions must be satisfied by the initial values. Even when a unique solution exists, the numerical problem can be arbitrarily difficult. For the linear case we examine the nilpotency of the Matrix pencil $[\partial F/\partial y , \partial F/\partial y']$. If the nilpotency does not exceed 2, the linear case presents no great difficulties, but higher nilpotencies cause serious numerical problems and non convergence of methods. Even a simple non-constant coefficient linear problem appears to be insolvable numerically in the nilpotency 2 case, but nilpotency one problems can be solved easily.

I. GLADWELL:

Stability and Other Properties of Direct Integration Methods for Second Order Systems

We will discuss a stability analysis of direct integration methods for second order systems of ordinary differential equation initial value problems. The discussion will include the choice of test equation and examples will be given analysing some widely used engineering methods. We will also discuss other properties of these numerical methods including algorithmic damping, phase lag and phase error.

R. D. GRIGORIEFF:

Zur Stabilität von Mehrschrittverfahren auf nichtäquidistantem Gitter

Es wird die asymptotische Stabilität von Mehrschrittverfahren auf nicht äquidistantem Gitter betrachtet. Die Koeffizienten des linearen Teils des Verfahrens dürfen variabel sein.

Der Hauptsatz lautet wie folgt: Es bezeichne ρ_j das charakteristische Polynom m-ten Grades des linearen Teils des Verfahrens an der Stelle x_j des Gitters. Sei dann $\rho_j^*(z) := \rho_j(z)(z-1)$ und A_j^* die zu ρ_j^* gehörige Begleitmatrix. Bei Lipschitzstetiger Nichtlinearität liegt Stabilität genau dann vor, wenn die Folge von Matrizen bzw. Zeilenvektoren

$$\prod_{j=k}^{l} A_j^* \quad \text{bzw.} \quad e'_{m-1} \sum_{j=k}^{l} \prod_{r=k}^{j-1} A_r^* \quad , \quad e'_{m-1} := (0,\dots,0,1) \in \mathbb{C}^{m-1} \quad ,$$

gleichmäßig in k, l und der Schrittweite beschränkt sind. Aus diesem Kriterium leitet man in einfacher Weise bekannte Bedingungen von Gear et. al. und Zlatev her. Für die BDF-Formeln erhält man Stabilität für Gitter mit $h_{j+1}/h_j < 1 + \sqrt{2}$ bzw. $12/11$ für $m = 2$ bzw. 3.

E. HAIRER:

Constructive Characterization of A-Stable Approximations to EXP(Z)

Relations between the concepts of A-stability and algebraic stability (for implicit Runge-Kutta methods) are investigated. We prove: Let $R(z) = P(z)/Q(z)$ be an A-stable rational approximation to EXP(Z) of order $p \geq 2m - 6$ $(m = \deg Q(z))$, then there exist algebraically stable Runge-Kutta methods of order p with $R(z)$ as stability function. It is conjectured that the statement remains true without the assumption $p \geq 2m - 6$. The proof is based on a characterization of A-stable approximations to EXP(Z), which is the content of the talk.

R. JELTSCH:

Stability and Accuracy of Time Discretizations of Initial Value Problems

Three techniques to relate the size of stability regions to the accuracy of "linear" methods for solving ODE's are discussed:

1. The stability regions of two multistage multistep methods are compared.
2. Low order linear multistep methods are approximated by high order ones without changing the stability region very much.
3. The asymptotic behaviour of the scaled stability region of the explicit Taylor expansion method is studied as the number of stages goes to infinity.

P. KAPS:

Rosenbrock-Type Methods

In the first part, Rosenbrock methods for nonautonomous ODE's are investigated. It is shown that additional order conditions must be considered. A simple rule to obtain the order conditions is given. It exists such a method with order 4 and 4 stages. In the second part, a joint work with S. Poon and T. D. Bui, we give a comparison of two kinds of stepsize control: Richardson extrapolation and embedding techniques. It is shown that the usual assumption that Richardson extrapolation is much worse is not true.

H.-O. KREISS:

Numerical Methods for Singular Perturbation Problems

Consider a system of ordinary differential equations $y' + A(x)y = f(x)$ for $0 \leq x \leq 1$ with boundary conditions $B_0\, y(0) + B_1\, y(1) = g$. We solve this problem with variable gridsize h_ν and assume that the problem is stiff i. e.

$|hA| >> 1$, $h = \max_{\nu} h_{\nu}$. The behaviour of solutions are discussed, in particular the difficulties connected with turningpoints. Extension to nonlinear problems are also indicated.

F. T. KROGH:

Implementation of Variable Step BDF Methods for Stiff ODE's

A variable order method for integrating ordinary differential equations requires a basic algorithm, and algorithms for changing stepsize and estimating errors. In addition, algorithms for selecting stepsize and integration order are required. In the case of stiff equations one requires in addition decisions on when to factor the iteration matrix and when to recompute the Jacobian matrix. We examine these kinds of questions for the case of the backward differentiation formulas and give algorithms which attempt to unterstand the local characteristic of the problem in order to minimize the number of Jacobian evaluations, matrix factorizations, function evaluations and backsolvers.

W. LINIGER:

A-Contractivity of k-Step Methods with Variable Steps

The theory of A-contractivity identifies families of multistep-formulas which, if implemented as one-leg methods, produce bounded solutions for dissipative (monotone negative) nonlinear systems of differential equations and/or for the variable coefficient test equation $\dot{x} = \lambda(t)x$, for any $\lambda(t)$ with $\mathrm{Re}\,\lambda(t) \leq 0$ and arbitrary variable step sequences. The popular A-stable two-step backward differentiation method does not belong to this family and, in fact, becomes unstable for certain problems of the latter type.

M. MÄKELÄ:

On some Rational Methods

The implicit term is removed from the conventional backward differentiation methods using a rational approximation $(\nabla^k y_{n+1}/\nabla^k y_n)\ \nabla^k f_n$ instead of $\nabla^k f_{n+1}$. The behaviour of the modification is compared to the conventional methods numerically using different constant steps and constant orders solving a variety of problems. In nonstiff problems the modification is fully competitive in accuracy using fewer function evaluations. In stiff problems the behaviour of the modification is difficult to predict. Sometimes the modification is superior but in some near by problems it turns out to be unstable.

H. N. MOLTHEI:

A-stable Collocation Methods with Multiple Nodes

The collocation methods treated by the author in the last years produce spline approximations for the solutions of initial value problems for ordinary differential equations. Some general results on A-stability given by Wanner, Hairer and Nørsett in 1978 are formulated for these methods in the case where they are equivalent to certain implicit Runge-Kutta methods. Hereby the dependence on the nodes and their multiplicities becomes apparent. The applicability of a characterization of all A-stable methods of order $2m - 4$ given by Wanner is regarded too.

O. NEVANLINNA:

Linear Multistep Methods and Anglebounded Nonlinearities

Three closely related problems were discussed:

1) Can a linear multistep method be truly accurate if a lot of stability is required?

2) How can we obtain reliable stability results for A(α)-stable schemes when we apply them to nonlinear problems?

3) Are there highly accurate linear multistep methods at all?

Answers provided: 1) no, 2) a technique was provided, 3) questionable.

P. RENTROP:

Partitioned Runge-Kutta Methods with Stepsize Control and Stiffness Detection

For the numerical solution of the autonomous initial value problem $y'(t) = f(y(t))$, $y(t_0) = y_0$, $t > t_0$, $y \in \mathbb{R}^n$, partitioned Runge-Kutta methods are studied, consisting of an A-stable Rosenbrock-Wanner method for the treatment of the stiff components and a customary Runge-Kutta method for the nonstiff components. The problems connected with an automatic stiffness detection and implementation of a stepsize control are discussed. Two algorithms are presented. The first algorithm PRK4 of order (3)4 possesses an automatic componentwise stiffness detection. The second algorithm RKF4RW treats the system of differential equations as nonstiff or as stiff. RKF4RW includes the well-known Runge-Kutta-Fehlberg method of order 4(5). It is possible to embed into the RKF4 algorithm a ROW-method of order (3)4, where the fourth order approximation is A-stable. Usually RKF4RW is the faster algorithm and the system stiffness detection works more reliable than the componentwise stiffness detection in PRK4.

R. SCHERER:

Zusammenhänge zwischen verschiedenen Klassen impliziter Runge-Kutta-Verfahren

Implizite Runge-Kutta-Verfahren spielen eine wichtige Rolle bei der numerischen Behandlung steifer DGl-Systeme. In den letzten Jahren sind verschiedene Klassen und Typen impliziter Runge-Kutta-Verfahren hergeleitet und untersucht worden (z. B. G , I , I_A , II , II_A , Butcher-Familie, Ehle-Familie). Mit Hilfe einer "Spiegelung" φ und einer "Transposition" ψ werden Zusammenhänge zwischen diesen Klassen aufgezeigt (z. B. $I\text{-}\varphi\rightarrow II_A\text{-}\psi\rightarrow I_A\text{-}\varphi\rightarrow II\text{-}\psi\rightarrow I$). Bei Anwendung des Transpositionsprinzips bleiben die Stabilitätseigenschaften erhalten, bei Anwendung des Spiegelungsprinzips werden sie ins Gegenteil verkehrt (z. B. I_A , II_A B-stabil, I , II nicht A-stabil). Diese Beziehungen sind sehr interessant im Hinblick auf Stabilitätsuntersuchungen und im Hinblick auf die Konstruktion impliziter Runge-Kutta-Verfahren.

L. F. SHAMPINE:

Type-Insensitive ODE Codes Based on Implicit A(α)-stable Formulas

Traditionally ODE codes are intended for stiff problems, or for non-stiff problems, but not for both types. Codes based on A(α)-stable formulas can be made insensitive to the type by adapting the scheme for evaluating the formula to the changing type of the problem as the integration proceeds. A way to do this will be described and some numerical results from a research-grade code will be given.

M. N. SPIJKER:

Contractivity of Runge-Kutta Methods

Let $V(t)$ denote the solution of a given initial value problem for a system of ordinary differential equations. Consider a k-step method producing approximations u_n to $V(nh)$ (for $h > 0$ and $n \geq k$) when starting values $u_0, u_1, \ldots, u_{k-1}$ are given. Such a method is called contractive if $|\tilde{u}_n - u_n| \leq |\tilde{u}_{n-j} - u_{n-j}|$ $(1 \leq j \leq k\ ,\ n \geq k)$ for any two sequences $\{\tilde{u}_n\}$, $\{u_n\}$ produced by the method using any $h > 0$. In this lecture it is shown that any Runge-Kutta method that is generally contractive, has an order $p \leq 1$. Further the concept of a contractivity threshold is introduced which makes it possible to include also methods with $p > 1$.

P. THOMSEN:

Implementation of SDIRK-Methods

The amount of computational work used by codes that implement SDIRK-methods is highly influenced by how the solution of the systems of nonlinear equations are monitored. The tolerance used in the stepping critirion for the iterative process is discussed and a strategy for bounding the errors introduced is proposed. The rate of convergence of the iterative processing is estimated from the residual norms directly and is used for stepsize control and guidance in the choice of iteration method. An interpolation formula based on calculated derivatives has been derived and this is used for getting starting values. Two third order SDIRK-methods with embedded formula for error estimation giving AN-stability are found to have good properties with respect to implementation.

P. J. VAN DER HOUWEN:

A-stable Runge-Kutta Methods for Volterra Integral Equations of the Second Kind

In this contribution Volterra integral equations are solved by using ODE techniques. Splitting the integral in a forward and backward part, the forward part is evaluated by an RK method, the backward part either by again using the RK formula or by using an LM method. With respect to the test equation $\dot{y} = \lambda y$ the first class of methods (extended RK methods) possess the same stability region as the RK method used but is computationally expensive, whereas the second class (mixed methods) is much cheaper at the cost of a reduced stability region. To overcome this disadvantage, modified mixed methods are proposed which retain the stability region of the generating RK formula but now at the cost of a possible reduction of the order of convergence.

G. WANNER:

The Number of Positive Weights of a Quadrature Formula

The following Theorem is discussed:

Consider an interpolatory quadrature formula with nodes c_i and weights b_i $(i = 1,\ldots,m)$ of order $2m - (2k + 1)$.

If $M(t) = (t - c_1)\ldots(t - c_m)$ and two polynomials f , g of degree k are defined by the relation $M(t) = P_{m-k}(t)f(t) - P_{m-k-1}(t)g(t)$, and if D is defined as the Cauchy index of the path $(f(t), g(t))$, then $2n_- = k - D$, where n_- denotes the number of b_i's which are negative. Therefore, the quadrature formula is positive iff $D = k$.

Positive quadrature formulas are interesting in the stability analysis for non-linear stiff differential equations. This is a joint work with G. Sottas, Genève.

H. A. WATTS:

Initial and Subsequent Step Size Selection in ODE Codes

One of the more critical issues in solving ordinary differential equations by a step-by-step process occurs in the starting phase. Somehow the procedure must be supplied with an initial step size that is on scale for the problem at hand. It must be small enough to yield a reliable solution by the process, but not so small as to significantly affect the efficiency of solution. For general purpose computing, an automatic step size adjustment procedure for choosing steps is essential to produce an accurate solution efficiently. This step size control is usually based on estimates of the local errors incurred by the numerical method. Because most codes also employ algorithmic devices which restrict the step size control to be moderately varying (for reliability) subsequent steps usually tend to stay on scale of the problem. This is not always so, as sometimes happens when working with crude tolerances on problems having rapidly varying components. In this talk, we shall discuss an algorithm for obtaining a good starting step size and some improvements in dealing with subsequent steps.

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