MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

T a g u n g s b e r i c h t 29/1983

Error Asymptotic and Defect Corrections

July 3 to July 9, 1983

The organizers of this meeting were Klaus Böhmer (Marburg), Victor Pereyra (Caracas, Venezuela), and Hans Stetter (Vienna).

The defect (or residual) of a given approximation may be used for the construction of corrections to this approximation. This basic principle - for which the term "defect correction" is now widely used - underlies many iterative processes in Numerical Mathematics; often asymptotic expansions play a role in this context.

It was the aim of this conference to bring together specialists from different fields in Numerical Mathematics applying defect corrctions to a variety of problems, e.g., stiff initial problems, ordinary boundary value problems, partial differential equations, integral equations, eigenvalue problems and high-accuracy calculations. Many interesting talks and numerous discussions established a strong interaction.

As always in Oberwolfach, the personnel staff coddled the guests, and the atmosphere in the institute was the optimal prerequisite for private and scientific contacts.

F. CHATELIN:

Newton methods for iterative refinement of eigenelements of linear operators

Let A be an $n \times n$ matrix in $\mathbb{C}^n$. To deal with close or multiple eigenvalues of total algebraic multiplicity m, we consider the nonlinear equation

(*) $F(U) = AU - U(Y^H AU) = 0$,

where the unknowns are the m columns of the $n \times m$ matrix U normalized by $Y^H U = I$, where Y is a given $n \times n$ matrix. The columns of U span the invariant subspace M for A associated with the m eigenvalues of the $m \times m$ matrix $B = Y^H AU$. B represents $A_{|M}$ in the adjoint bases (U,Y).

Starting from an approximate invariant subspace X for A such that $Y^H X = I$, and applying Newton and modified Newton methods on (*) yield several iterative schemes to refine on X. This is used in two ways:

(i) as a computational scheme,

(ii) as a means to derive a posteriori error bounds in terms of the $n \times m$ residual $R = AX - X(Y^H AX)$.

The same method applies to a closed linear operator in a Banach space (integral or differential).

R. FRANK:

Defect correction and stiff ordinary differential equations

The B-convergence properties of certain Defect-Correction methods, based on the implicit Euler scheme and on the implicit midpoint rule are discussed. It turned out, that full B-convergence results do not hold in this case; nevertheless it was possible to prove " Restricted B-convergence" for these methods i.e. satisfactory global error bounds could be derived under the following assumption: The eigenvalues of the Jacobian $f_y(0,y_0)$ at the starting point are either "moderately sized" or satisfy the relation $h \cdot \mathrm{Re}(\lambda_i) << 0$.

W. GROSS:

Hartree-Fock methods

This talk is thought as an introductory one to give the framework for the talks of B. Schmitt and R. Schwarz. It describes the way how one comes from the Schrödinger equation in wavemechanics via the variational principle to the socalled Hartree-Fock equations (HFE) for the radial parts of the electron wavefunctions.

Abstracts

K. BÖHMER:

Discrete Newton methods for the Bader-Deuflhard method in stiff initial value problems

Discrete Newton methods are defined as follows: compute a discrete approximation ζ to the original (nonlinear) problem with exact solution z. Linearize the discrete problem at the solution $\zeta^0 := \zeta$ and compute the iterations ζ^l from $(F^h)'(\zeta^0)(\zeta^l - \zeta^{l-1})$ = -(modified defect for ζ^{l-1}). Under certain, easily verifiable conditions, one finds the asymptotic expansion $\zeta^l(t) - z(t) = \sum_{j=(l+1)p}^{q} h^j e_{j,l}(t) + O(h^{q+\alpha})$ in grid points t and for p, the order of the basic method. This approach is applied to the Bader-Deuflhard method for stiff initial value problems. The relations to other known results are discussed and experiments are reported.

M. BRAKHAGE:

A quadrature formula method for integral equations with a logarithmic singularity

The integral equations treated are of the form $\int_0^1 k(x,x')u(x')dx' = f(x),\ x \in [0,1]$ with $k(x,x') = \frac{c}{\pi}\ln(2\sin|\pi(x-x')|) + \bar{k}(x,x')$, with $\bar{k}$, f, u being 1-periodic and smooth (C^∞) or some variants. A "primitive approximation" is given by solving the system of linear equations

$$\sum_{\nu=0}^{N-1} h\, k(\lambda h,(\nu-\tfrac{1}{2})h)\, u_\nu = f(\lambda h),\ \lambda = 0, \ldots, N-1,\ h = \frac{1}{N},\ N = 2M+1$$

and defining u_h by trigonometrical interpolation. For this rough approximation method an "nonstandard" asymptotic error expansion can be derived, which - for each given order $O(h^l)$ - gives rise to a refined discretization method of this order. The properties of numerical stability are discussed and the theoretical results are tested by numerical experiments. It is indicated, that this method is a special case of a more general concept, which allows a unified treatment of discretization for differential operators and a certain class of integral operators.

The (HFE) are a coupled system of second order differential equations on a semi-infinite interval with a singularity in the coefficients at $r = 0$, boundary conditions and orthogonality constraints. It is an eigenvalue problem as well.

A short outline is given of methods recently used to solve this problem and some points are mentioned where improvements can be gained especially using defect corrections.

W. HACKBUSCH:

Domain decomposition techniques

The usual defect correction methods for elliptic problems work with discretizations in the whole domain. We describe a "local defect correction", where a second discretization is defined only locally. One multi-grid version of this method is a well-known local mesh-refinement. If there are several separated refined regions, they are coupled by coarse grids. On the other hand we can formulate the elliptic problem as a set of two equations in two overlapping subdomains with additional boundary conditions for the new interior boundaries.

We discuss the solution of the corresponding discrete system of equations by a multi-grid process, in which the major part of the computations can be performed simultaneously in every subdomain.

G. HEDSTRØM:

Extrapolation in a convection-diffusion equation with a boundary layer†

The equation

$$(*) \qquad u_x = \nu(u_{xx} + u_{yy}) , \qquad x > 0, \quad y > 0 ,$$

provides a linear model of the equations of fluid flow with the direction parallel to the x-axis. If the viscosity ν is small and positive and if the boundary conditions for (*) are that $u(x,0) = 0$, $x > 0$, and $u(0,y) = 1$, $y > 0$, then the solution to (*) has a boundary layer near the x-axis. We are frequently interested in computing only the drag u_y at $y = 0$. Suppose that (*) is approximated using central differences with $\Delta x \geq \Delta y$. We show that in the boundary layer ($x/(2\nu)$ large), the error in the drag may be written as a power series in the square of the half cell Reynolds number $\beta_y = \Delta y/(2\nu)$. This finding is consistent with the empirical observation that one may use grids in the boundary layer with a large aspect ratio. We also find, however, that errors are introduced in the outer flow if $\Delta x/\Delta y$ is too large in the region near the origin, the birth of the boundary layer.

† This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

P.W. HEMKER:

Mixed defect correction iteration for the solution of a singular perturbation problem

We describe a numerical (mixed defect correction) method for the solution of a two-dimensional elliptic singular perturbation problem. The method is an iterative process in which two discretizations are used: one with and one without additional artificial diffusion. The method works well for problems with interior- or boundary layers. The resulting discretization is stable and yields a 2nd order accurate approximation in the smooth parts of the solution, without using any special directional bias in the discretization method.

E. KAUCHER:

Residueniteration zur E-Verifikation der Lösung von Gleichungen mit beliebig gewünschter und garantierter Genauigkeit

Eine Lösung eines Problems heißt E-verifizierbar, wenn ein Algorithmus angegeben werden kann, der bei möglichst geringem Speicher-Zeitaufwand

- die Existenz,
- eine Einschließung auf gewünschte Genauigkeit und gegebenenfalls
- die lokale Eindeutigkeit

verifiziert.

Z.B. die Gewaltmethode numerisch mit höheren Genauigkeiten (doppelter, vielfacher, etc. Mantissenlänge) zu rechnen, erfordert zuviel Speicher- und Zeitaufwand gegenüber Methoden, die nur Residuen mit der erforderlichen Genauigkeit berechnen.

Neuere Ergebnisse, die mit E-Algorithmen erzielt wurden, zeigen, daß robuste Algorithmen dahin tendieren, Mehraufwand in Richtung mehr Zeit (durch echte Residueniteration) und weniger in Richtung Speicherplatz erfordern (Schein-Residueniteration).

Es werden einige charakteristische E-Algorithmen mit Residueniteration skizziert und ein Ausblick gegeben auf algorithmische Residueniteration in Funktionenräumen zur Lösung von Differential- und Integralgleichungen.

B. LINDBERG:

Error estimation by defect calculation in finite element discretization

Some ideas on computable pointwise estimates of the errors in finite element discretizations are presented. For the equation $a(u,v) = (f,v)$ where $a(,)$ is a bilinear form and $(,)$ an inner-product a finite element discretization can be written

$$a(\sum c_i q_i, q_j) = (f, q_j) \qquad j = 1,2,\dots N$$

with q_i, $i = 1,2,\dots N$ the basis of a finite element subspace in which we seek the solution (approximate). The defect for equation j is defined as $R_j = a(w,q_j) - (f,q_j)$ where w is properly defined from the solution data $c_1, c_2, \dots c_n$ e.g. $w = \sum c_j Q_j$ with Q_j, $j = 1,2,\dots N$ the basis of another finite-element subspace. The talk concerns practical ways of computing R_j for some one- and two-dimensional problems.

J. MANDEL:

On multilevel iterative methods for integral equations of the second kind and related problems

We discribe a unifying framework for multigrid methods and projection-iterative methods for the solution of integral equations of the second kind, and for the iterative aggregation method for solving input-output relations. The methods are formulated as iterations combined with a defect correction in a subspace. Convergence proofs use contraction arguments and thus involve the nonlinear case automatically.

First a general two-level iterative scheme is defined and its convergence properties are formulated via local Lipschitz constants. The use of secondary iterations is analysed as well. Particular cases displayed in further sections include the methods of Brakhage, Atkinson, and Hackbusch for the solution of systems of equations arising from integral equations.

S. McCORMICK:

The role of defect correction in adaptive discretization

Defect correction ideas can be used in adaptive methods as a basis for a process that has the attributes of both uniform and nonuniform grid discretization. Basically, defect correction can be used to correct the uniform coarser grids in the regions where the (nonextensive) finer grids are placed. This gives the adaptive grid accuracy to the coarser grids in regions outside higher resolution as well as those corresponding to the finer grids. This talk will present the results of such adaptive methods as they apply to oil reservoir simulation.

W. MIRANKER:

Iterative refinement as an ultra-arithmetic process

We describe iterative residue correction for model problems set in function space from an ultra-arithmetic viewpoint. That is, as a flow of information between basis elements of the function space analogous to the propogation of arithmetic information (in either direction) between the digits of floating point numbers during the execution of operations of floating point arithmetic. Such processes are shown to be isomorphic to block relaxation with steering. Numerical examples will be given.

H. MUNZ:

Asymptotic expansions for semilinear elliptic systems

A class of finite difference scheme, due to H.-O. Kreiss, for weakly coupled mildly nonlinear elliptic systems of the type

$$\Delta u_j(x) = f_j(x,u_1(x),\dots,u_m(x)), \quad 1 \leq j \leq m, \quad x \in \Omega$$
$$u_j(x) = g_j(x), \quad 1 \leq j \leq m \quad x \in \partial\Omega,$$

where Ω is a bound region in $\mathbb{R}^n$ is considered.

The schemes use the standard $(2n+1)$-point-approximation of the Laplacian combined with polynomical extrapolation of degreee k near the boundary. The FD-scheme thus obtained is neither of monotone type nor symmetric. No conditions regarding the definitness or the sign-pattern of $\partial_u(f_1,\dots,f_m)^T$ are imposed. The convergence of the FD-solutions to isolated solutions of the original problem and the existence of asymptotic error expansions are stated for $k=4$. Finally we report on numerical tests in which the asymptotic expansions are exploited by a modified deferred correction method.

V. PEREYRA:

Implementation of deferred corrections

We shall discuss the implementation of deferred corrections and related global error estimation on various areas, like, two-point boundary value problems, elliptic partial differential equations, and so on. We will survey available software and mention selected applications.

H.-J. REINHARDT:

On a combination of defect corrections with adaptive finite element methods applied to singularly perturbed differential equations

First, a simple idea will be presented having the aim to improve numerical solutions of linear problems. This approach is based on a-posteriori error estimates which, in a certain sense, monitor the error improvement. On the other hand, realistic a-posteriori error estimates allow an adaptive computation of the numerical approximations, so that a combination of both aspects leads to adaptive defect correction methods. For an example of a linear, singularly perturbed o.d.e., the a-posteriori error estimates associated with a finite element method will be given and numerical results will be presented. This approach can be extended to nonlinear problems, provided that initial approximations (numerical or asymptotic ones) are available. For a rather general class of nonlinear singularly perturbed o.d.e.'s, the (linear) equations of the defect corrections and the corresponding a-posteriori error estimates will be given. Again, the latter allow an adaptive computation of the defect correction terms.

S. RUMP:

Inclusion of the solution of linear and nonlinear equations

A synopsis have been given of new methods for solving algebraic problems with high accuracy. Examples of such problems are solving of linear systems, eigenvalue/eigenvector determination, computing zeros of polynomials, sparse matrix problems, computation of the value of an arbitrary arithmetic expression (in particular the value of a polynomial at a point), nonlinear systems, linear, quadratic and convex programming, over- and underdetermined linear systems etc. over the field of real or complex numbers as well as over the corresponding interval spaces.

The fundamentals of our new methods are developed. The appropriate computer arithmetic (developed by Kulisch and Miranker) is shortly described. The new methods are given by means of a set of mathematical theorems and the corresponding algorithms which do verify the assumptions of the theorems on a computer. All these algorithms based on our new methods have some key properties in common:

- every result is verified to be correct by the new algorithms
- the results are of high accuracy; the error of every component of the result is of the magnitude of the relative rounding error
- the solution of the given problem is verified to exist and to be unique within the computed error bounds
- the computing time of one of the new algorithms is of the same order of magnitude as a comparable (pure) floating-point algorithm (the latter, of course, with none of the above features).

The key property of the new algorithms is that error control is performed automatically by the computer without any effort required on the part of the user. The efficiency of the algorithms has been, for instance, demonstrated by inverting a Hilbert 21 x 21 matrix on a 14 hex (= 17 decimal) computer. This is, after multiplying by a proper factor, the largest Hilbert matrix exactly storable on this computer. After automatically verifying, that this matrix is not singular, the inverse is included with least significant bit accuracy. That means, that the left and right bound of all components of the inclusion are consecutive in the floating-point screen. Our experience shows, that our algorithms very often have the "least significant bit accuracy" property.

B. SCHMITT:

Defect corrections on infinite intervals

If the infinite interval is truncated to a finite one for the solution of a boundary value problem on $\mathbb{R}$, new boundary conditions are needed. The boundary conditions given in the literature for general problems make the use of very large intervals necessary.

For the simple differential equation $-u'' + k^2u = g$ we give the exact discrete boundary conditions for the discrete Newton method with equidistant grid. Also an algorithm is presented which computes these boundary conditions along with the discrete Newton iteration from some basic "data". If these data are known the algorithm computes the discrete Newton iterates on the infinite grid exactly.

W. SCHÖNAUER:

Numerical Engineering: Experiences in designing PDE software with selfadaptive variable step size/variable order difference methods

We want to develop robust and efficient general purpose software for the solution of arbitrary nonlinear systems of elliptic and parabolic PDE's in a rectangular domain. The relative accuracy is prescribed and the method must choose itself the optimal grid and order independently in all coordinates t,x,y,z. There must be selected also the optimal solution method, within a given scale of methods, for the solution of the resulting linear system for the computation of the Newton-Raphson correction. The key to the solution method is the use of families of difference formulae. The discretization error is determined by the difference of difference formulae of these families. The error equation tells us how to choose the grids and orders and how to stop the Newton-Raphson iteration. The Newton-Raphson correction and the discretization error define the stopping criterion for the iterative solution of the linear equations. A polyalgorithm selects the solution method for the linear equations by the comparison of normalized convergence factors. An essential condition is that the resulting program must be fully vectorizable for Vectorcomputers (Supercomputers). The whole solution process is a continuous compromise between robustness and efficiency which quite naturally contradict each other. There will be discussed the sequence "method, algorithm, program" from the point of view of numerical engineering.

R. SCHWARZ:

On the numerical solution of boundary value problems on infinite intervals

The error by truncating the infinite interval and the construction of asymptotic boundary conditions is discussed exemplary for the problem $-y'' + k^2y = g$, where the inhomogenity has special properties as occuring in Hartree-Fock theory. The construction of asymptotic boundary conditions is generalized to the problem $-y'' + f(x)\,y = g$, where f has an asymptotic expansion at infinity and $f(\infty) \neq 0$.

R.D. SKEEL:

Deferred/defect correction for stiff ordinary differential equations

A simple example is given illustrating that defect correction is a nontrivial generalization of deferred correction. The role of global error asymptotics and the meaning of stiffness are discussed, and then the existence of asymptotic expansions for stiff equations is considered. For purposes of deferred/defect correction it is necessary to consider variable stepsize. Error per step and error per unit step are compared. In particular, it is shown that local extrapolation, which is a generalized error per unit step, does not quite increase the order by one.

H.J. STETTER:

Sequential defect correction for high accuracy algorithms

As was shown in the presentation of S. Rump, there exist algorithms in floating point arithmetic which compute the solution of algebraic problems to full floating point accuracy, almost irrespective of the condition of the problem. However, if the result intervals of such algorithms are fed into another such algorithm, a loss of accuracy occurs. It is shown that the principles underlying these algorithms, viz. the representation of the approximations in staggered correction format and the exact computation of defects, may also be used for the coupling of such algorithms into one global high-accuracy algorithm. The strategy by which the required accuracy in the individual algorithms is achieved dynamically and automatically, comprises 3 passes: In a first pass, the individual results are corrected to a preset accuracy, at the same time estimates of the relative condition numbers are determined. With the aid of these, the necessary accuracy is obtained in the second pass. The third pass generates the required interval inclusions. These ideas apply equally to the analytic defect correction algorithms described in the contributions of R. Kaucher and W.L. Miranker.

M. VAN VELDHUIZEN:

Asymptotic expansions of the global error for the implicit midpoint rule (stiff case)

In this contribution a new stability result for the implicit midpoint rule is given. This new result gives estimates independent of the stiffness of the (scalar) differential equation. By means of this stability result one is able to obtain an asymptotic expansion in powers of the average step size for a stiff scalar linear problem. In discretizing this problem by the implicit mid-point rule we use a fine mesh in the boundary-layer region, a coarse mesh far away from the boundary-layer region, and a gradual increase of the step size in between. In this way an asymptotic expansion for the global error can be proved, under the condition that the number of gridpoints multiplied by the logarithm of the "stiffness" is small. This expansion is valid uniformly on the domain of integration.

J.G. VERWER:

Step-by-step stability in the numerical solution of shallow water equations

Shallow water equations - a nonlinear system of hyperbolic partial differential equations - describe flow problems in fluid dynamics. Applications are found in e.g. oceanography (water elevations due to storms) and meteorology (weather prediction). Numerical computations with these equations are often hampered by nonlinear instabilities, the so-called exponential blow ups. We will provide insight in the origin of these instabilities. Next we will show how to overcome the difficulties by an energy method stability analysis. Finally we will present some approximation schemes, derived along the lines of these energy method, for which stability is warranted, despite the nonlinearities. Among others, an LOD-scheme which can be implemented such that only linear tridiagonal systems of algebraic equations need to be solved.

Report by: B. Schmitt, W. Gross

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