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Use of Iterative Linear and Nonlinear Algebraic Methods for Solving Large Stiff Systems of ODEs

Tony F. Chan[1]

September 23, 1984

Abstract

This is the final scientific report for Grant AFOSR-83-0097 titled *Use of linear and nonlinear algebraic methods for solving large stiff systems of ODEs*, which is a continuation of research supported under Grant AFOSR-81-0193 titled *An Investigation of the Use of Iterative Linear Equation Solvers in Codes for Large Stiff Systems of ODEs*. In this report, we summarizes the main results accomplished in this research.

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[1]Computer Science Department, Yale University, Box 2158, Yale Station, New Haven, CT 06520.

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1. Introduction

One of the major uses of the computer in science and engineering is the simulation of physical phenomena. Computer experiments can be carried out on the computer, either to verify the theory or to make predictions, before actual and costly physical experiments are attempted. The resulting savings in cost and increased flexibility greatly extends the kinds of experiments that can be carried out. This technique is heavily used in every area of science and engineering.

The basis of such a simulation is a mathematical model of the physical phenomena. Very often, this takes the form of differential equations. Thus the efficient solution of these equations is critical for the success of the simulation approach. Our research deals with the class of stiff ordinary differential equations, which usually arise in modelling physical systems with many different time scales. They are especially difficult to handle efficiently on a computer because the existence of wiedely varying time scale requires high overall resolution and a consequent high cost. Implicit methods are designed to partially deal with this time scale problem but they in turn give rise to large systems of linear equations which themselves are costly to solve. The purpose of this research is to investigate the use of iterative methods for solving these systems, which should reduce both the computational time and storage requirements over direct methods of solution. The end result is a computer program that can handle very large systems of stiff ODEs which in turn allows simulation of large physcial systems.

We investigated the use of variants of the *preconditioned conjugate gradient* (PCG) method for solving the linear equations, and *truncated Newton-like iterations* for solving the nonlinear equations. Our main objective is to carry out a *systematic* study of the methods involved and to produce a well-documented and well-tested computer code for solving large systems of stiff ODEs that incorporates the results of our study.

A summary of the major results will be described in the next few sections. A list of publications supported by this grant is given in Section 6.

2. Alternating Direction Incomplete Factorizations

The use of a good preconditioning is often essential for the successful application of the conjugate gradient method. One of the most promising class of preconditionings is the so-called Incomplete Factorizations, which can be viewed as factoring the coefficient matrix approximately under the constraint that the factors have to be sparse. For elliptic PDEs, quite a lot of theory has been developed for these preconditionings. Most of these preconditionings have the property that, when applied to the discretization of a self-adjoint elliptic opertor, the number of iterations required to reduce some norm of the error by a factor of ϵ is $O(h^{-1/2}\log(1/\epsilon))$, where h is

the mesh size used in the discretization. By modifying one of these preconditionings, namely, the Dupont-Kendall-Rachford preconditioning (DKR), we have been able to derive some error estimates which suggest that the number of iterations can be reduced to $O(h^{-1/3}\log(1/\epsilon))$. Thus this new preconditioning, which we call ADDKR, is asymptotically faster than DKR. Moreover, numerical experiments on some model elliptic problems indicate that even for problems of moderate size the new preconditioning is competitive with DKR. We feel that this is an important discovery, both theoretically and practically, *since no other known preconditionings in this class have been shown to possess a better asymptotic rate of convergence than DKR.* This work has been published in the SIAM Journal of Numerical Analysis.

3. Nonlinear Preconditionings

One promising idea that some people have noticed in the application of Krylov subspace methods for solving the linear systems $Aw = b$ that arise in the inner loop of a Newton-like iterative method for solving nonlinear systems $F(x) = 0$ (with A being the Jacobian of F at a point x) is the use of the directional differencing (F(x + ϵu) - F(x)) / ϵ for approximating the matrix-vector product Au in the CG algorithm. This avoids explicit evaluations of the Jacobian and only requires function evaluations. However, most of the preconditioning techniques in use now are derived from the matrix elements *explicitly*. It is therefore unclear as to how to apply the preconditionings when the matrix is not explicitly available. This issue does not seem to have been addressed in the literature. We have obtained some results in this direction. We have derived an algorithm for preconditioning the CG iteration with directional differencings that reduces to the SSOR preconditioning in the linear case. It only requires evaluating the *diagonal* elements of the Jacobian which can also be approximated by function evaluations and can be easily incorporated into the CG iteration. We consider it an important discovery because we think the use of directional differencing will prove to be very useful in the stiff ODE context. We have performed some preliminary numerical experiments with the algorithm and they indicate that the new algorithm is as effective as linear preconditioning techniques based on the explicit Jacobian. This work has been published in the SIAM Journal of Scientific and Statistical Computing.

4. Basic CG Variant of LSODE

A program built around the package LSODE by Alan Hindmarsh has been completed. It basically replaces the sparse matrix solver in LSODE with the conjugate gradient solver PCGPACK developed at Yale. The code can now take problems in the sparse format (same as the IA-JA format used in the Yale Sparse Matrix Package (YSMP) and in LSODES) and solves the linear systems that arise at each integration step by variants of the preconditioned conjugate gradient method. It computes the Jacobian *exactly* by rows and uses *absolute* error

control. One of the more subtle issues had been the stopping criterion for the conjugate gradient method, which has to be related to the user supplied error tolerance for the ODEs. No major changes in the ODE strategies have been made in this code.

We have performed a systematic test of the performance of our code on problems in the STIFF DETEST program developed at University of Toronto for testing stiff ODE solvers. Our main objective is to compare it to the sparse option LSODES in the LSODE package. The results confirm the effectiveness of the use of CG-like method in the stiff ODE context. For example, we found that the CG code takes only slightly more steps and function evaluations than LSODE to solve the problems to a comparable accuracy. Frequently, the new code requires only about *one* CG iteration per Newton iteration, which is extremely encouraging considering that no matrix factorizations are needed.

We have performed some tests with the SSOR-preconditioned conjugate gradient method applied to the heat equation in two dimensions. The numerical results agree very well with the theoretical convergence estimates. When h is small, only one or two CG iterations are needed. As h grows, more iterations are needed. As the mesh gets denser, the number of iterations increases at the correct aysmptotic rate. Generally, only very *few* (relative to the size of the linear systems) CG iterations are needed at each integration step and the use of preconditioning *seems to improve the efficiency. These results show that the use of the conjugate gradient* method is very promising, as compared to direct sparse solvers. A technical report has been completed and submitted for publication.

5. Comparison of Krylov subspace methods

A host of algorithms belonging to the same class of Krylov subspace methods have been recently at the focus of several researchers dealing with the solution of large sparse nonsymmetric linear systems. Among them we mention the subclass of the ORTHOMIN(k)(Vinsome), GCR(k) algorithms, (Eisenstat, Elman and Schultz), ORTHORES(k), ORTHODIR(k) developed by Young and Jea, IOM(k) (Saad), Axelsson's method, Lanczos' method and others. Although the literature is rich in methods, few comparisons of the performances have been proposed.

In a recent paper by Saad [3] dealing with the Krylov subspace methods, some comparisons, both theoretical and practical, have been established. In particular it was shown that the ORTHORES(k) method of Jea and Young is in fact equivalent to the IOM(k) method, i.e. that the iterates produced by both algorithms are identical. On the other hand both numerical stability and computational cost are in favor of the IOM(k)

algorithms. A number of comparisons shown in Howard Elman's recent PhD thesis[2] favor the Chebyshev based algorithms, in general, against the Conjugate gradient type methods. A common argument raised against the Chebyshev algorithm is that it requires the knowledge of some of the eigenvalues of A. While there is no doubt that the process of estimating the eigenvalues and obtaining the best ellipse containing the spectrum of A may seem somewhat cumbersome, there are a few important points that can make the process highly competitive:

1. Once the optimal parameters are known the method is extremely fast;

2. There are some hybrid methods under investigations which combine the expensive method (e.g. GCR(k)) and the inexpensive Chebyshev algorithm in an efficient way;

3. In the context of time dependent problems, the problem of estimating the parameters is eased by the fact they are likely to evolve smoothly thus allowing to use a set of parameters for a large number of steps.

In solving stiff ODE's, the choice of a method is rendered difficult because one has to select a method which is sufficiently robust to handle problems of different types and nonetheless able to take advantage of the particular context of ODE's. Many of the methods described above may break down in the same way that the conjugate gradient method breaks down for indefinite systems. Some theoretical results show that for truely stiff problems, almost all the eigenvalues will lie in the right half of the complex plane. However, it is still important to devise algorithms which are more robust. We have developed a stable version of the Krylov subspace method for indefinite and nonsymmetric problems has been developed. It is similar but more economical than the SYMMLQ algorithm for indefinite problems and the same algorithm can handle nonsymmetric problems as well. This work has been published in the Siam Journal of Scientific and Statistical Computing.

6. List of reports and presentations supported by AFOSR-81-0193

1. "Alternating Direction Incomplete Factorizations" by Tony F. Chan, Ken Jackson and Benren Zhu, Yale CS Report #208, 1981. SIAM J. Numer. Anal. 20(1983), pp.239-257. Presentation given at SIAM meeting at Cincinatti, Oct. 1981, and at the Canadian Mathematical Society meeting in Toronto, July, 1982.

2. "Nonlinearly Preconditioned Krylov Subspace Methods for Discrete-Newton Algorithms", by Tony F. Chan and Ken Jackson, Yale CS Report #259. Siam J. Sci. Stat. Comp. 5(1984), pp.533-542. Paper presented at 1982 Sparse Matrix Symposium at Fairfield Glades, Tenn.

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[2]"Iterative methods for large, sparse, nonsymmetric systems of linear equations', Yale University, Computer Science Dpt. Report #229

3. "Practical Use of Some Krylov Subspace Methods for Solving Indefinite and Unsymmetric Linear Systems", by Youcef Saad, SIAM J. Sci. Stat. Comp, 5(1984), pp.203-228. Presented at the SIAM meeting on Linear Algebra and Discrete Mathematics, Raleigh, NC. April 1982.

4. "The Numerical Solution of Large Systems of Stiff ODEs", by Tony F. Chan and Ken Jackson, 1982. Research Report YALEU/DCS/RR-312, April, 1984. Paper presented at SIAM National meeting at Stanford in July, 1982. Submitted for publication in Siam J. Sci. Stat. Comp.

5. "Fourier Methods with Extended Stability Intervals for the Korteweg - de Vries Equation", by Tony F. Chan and Tom Kerkhoven, Research Report YALEU/DCS/RR-295, Dec., 1983. Accepted for publication in the Siam J. Numer. Anal.

7.. Professional Personnel Associated with this Project:

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Unsupported:
    Ken Jackson, Assistant Professor
    Benren Zhu, Research Associate
    Youcef Saad, Research Associate
    Tom Kerkhoven, Graduate Assistant in Research

8. Meetings Attended and Papers Presented

11/6-11/83 SIAM, Norfolk, VA "Parallel Processing for Scientific Computing"
    (No paper given)
11/26-28/83 Math dept., Arizona State University.
    "Dealing with singularities in bifurcation problems."
and, Consultation with Gene Golub, Stanford University, on
    Conjugate Gradient Methods
7/6-10/83 Consultation with Ken Jackson, University of Toronto, on
    Iterative Methods for Stiff ODE codes.

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