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13. ABSTRACT (*Maximum 200 words*)

Research was directed toward developing robust and efficient iterative methods for large-scale systems of nonlinear algebraic equations, especially discretizations of continuous problems such as partical differential and integral equations. The specific goal was to develop effective Newton iterative methods (implementations of Newton's method using iterative linear algebra methods) and improved iterative linear solvers for use in them. A theoretically sound abstract framework was formulated. Significant progress was made toward a well-developed software implementation. Useful advances were made in the development and understanding of iterative linear solvers.

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1. Objectives.

The broad objective of this research was to provide robust and efficient iterative methods for large scale systems of nonlinear and linear algebraic equations, especially those arising from discretizations of partial differential equations, integral equations, and other continuous problems. The methods of interest for nonlinear systems were mainly Newton iterative (truncated Newton) methods, i.e., implementations of Newton's method in which an iterative linear solver is used to solve approximately the linear systems that characterize Newton steps. Also of interest were quasi-Newton methods, in which Newton steps are determined using an approximate Jacobian maintained by updating. The methods of interest for linear systems were mainly Krylov subspace methods for general nonsymmetric linear systems, together with "residual smoothing" techniques applied to them.

Specific research objectives for Newton iterative methods were to develop (1) theoretically sound and practically effective "globalization" techniques (for enhancing convergence from poor initial guesses) and strategies for terminating the linear iterations at each Newton step, (2) implementations of iterative linear solvers that are particularly well suited for use in Newton iterative methods, and (3) high-level experimental software that will provide a prototype for codes suitable for public distribution. Concomitant objectives for iterative linear solvers were (1) to develop more efficient and robust implementations of the generalized minimal residual (GMRES) method and (2) to explore theoretical and practical applications of "residual smoothing" techniques to short-recurrence Lanczos-based methods,

2. Summary of the research effort.

2.1. Newton iterative methods.

Newton iterative methods are currently used in many important scientific applications, including many with considerable industrial importance, e.g., aircraft dynamics modeling at Boeing and semiconductor modeling at Bell Labs. In addition to their effectiveness on important problems, these methods also offer a nonlinear "framework" within which to transfer to the nonlinear setting any advances in linear system solving, e.g., new algorithms for nonsymmetric linear systems or algorithms that exploit advanced machine architectures. In spite of their conceptual simplicity, these methods involve complex issues, principally the following:

1. *How accurate should each approximate Newton step be, i.e., when should the linear iterations be stopped?* While some accuracy is clearly necessary, obtaining more accuracy requires more linear iterations, which entails greater expense, and away from a solution, there is a point beyond which it may be unnecessary and even counterproductive.
2. *How should the method be "globalized"?* All Newton-like methods require "globalization" procedures that test steps for adequate progress and, if necessary, modify them to obtain steps that provide it. The issue here is how to construct globalizations that are compatible with the strategy for stopping the linear iterations and other algorithmic features.
3. *Which iterative linear solver should be used?* This is a very important issue that has become more difficult to address with the proliferation of iterative linear solvers in the last few years; see §2.2 below. The best choice may depend very much on the application, but there are some general considerations relating to compatibility with the globalization and the strategy for stopping the linear iterations.

It is assumed below that the problem is to find a zero of a nonlinear function $F : \mathbf{R}^n \rightarrow \mathbf{R}^n$.

General, theoretically sound frameworks for Newton iterative methods have been notably absent from the literature, and a preliminary goal of this research was to develop such frameworks. The first two issues outlined above can be addressed very effectively in the more general context of an inexact Newton method [SR5][1], formulated as follows:

INEXACT NEWTON METHOD [SR5]:

LET x_0 BE GIVEN.

FOR $k = 0$ STEP 1 UNTIL ∞ DO:

FIND **some** $\eta_k \in [0, 1)$ AND s_k THAT SATISFY THE INEXACT NEWTON CONDITION $\|F(x_k) + F'(x_k)\, s_k\| \leq \eta_k \|F(x_k)\|$.

SET $x_{k+1} = x_k + s_k$.

A Newton iterative method can naturally be regarded as a special case of an inexact Newton method: At the kth step, one first chooses η_k and then applies the iterative linear solver to the Newton equation $F'(x_k)\, s = -F(x_k)$ until the inexact Newton condition holds. Note that the issue of when to stop the linear iterations is now the issue of choosing η_k.

In §2.1.1, research relating to general inexact Newton methods is described; this provided the desired general frameworks for Newton iterative methods. In §2.1.2, work is outlined relating to a Newton iterative implementation of a particular inexact Newton method formulated in [P1]. Research on iterative linear solvers that relates to the third issue above is discussed in §2.2.

2.1.1. Inexact Newton methods. It is shown in [SR5] that the local convergence of an inexact Newton method is controlled by the choices of the η_k's, and simple choices are outlined in [SR5] that result in desirable convergence rates. However, that paper does not address either global convergence or deeper issues associated with choices of the η_k's.

Beginning in 1989, the PI began a collaboration with S. Eisenstat that resulted in inexact Newton methods with very strong global convergence properties. The results are written up in [P1], the original version of which appeared as a research report in February, 1991. During the 1991-94 period of this grant, there were significant revisions of [P1], including considerable extension of the original results. This paper appeared in *SIAM Journal on Optimization* in May, 1994.

[1] Referencing conventions are as follows: Publications acknowledging support from this grant are referenced by [P...] and listed in §3. Supplementary references are referenced by [SR...] and listed in §4. Talks on research supported by this grant are referenced as [T...] and listed in §6.1.

In follow-up work to [P1], the PI worked with Eisenstat on the issue of making refined choices of the η_k's. Choices that had previously been proposed result in desirably fast asymptotic convergence near a solution but do not adequately address efficiency and robustness away from a solution. The central issue is that of *oversolving* the Newton equation, i.e., going to the expense of reducing the linear residual norm, which is also the local linear model norm, beyond the point at which the local linear model begins to depart significantly from the nonlinear function. Several very promising choices of the η_k's were arrived at which minimize oversolving on a number of realistic test problems while retaining desirably fast asymptotic convergence near a solution. Furthermore, our testing indicates that, by maintaining good agreement between the nonlinear function and its local linear models, these choices relieve the globalization of much of its burden and consequently enhance the robustness of the method. This work is written up in [P6].

2.1.2. Newton iterative backtracking implementations. A general inexact Newton backtracking method is formulated in [P1] that, although simple, has strong global convergence properties and allows for choices of the η_k's that result in desirably fast asymptotic convergence to a solution. Code was developed for a Newton iterative implementation of this method that uses restarted GMRES [SR11, SR15] as the iterative linear solver. GMRES is a natural first choice for the iterative linear solver because it is robust, generally applicable, and well understood; other solvers will be implemented in future work. This code was very useful in experiments concerning the choices of the η_k's in the work with Eisenstat described above; these experiments in turn allowed us to determine a preferred choice for general use in the code.

At present, the code can be considered a high-level experimental code. This code and its performance on an initial set of test problems (PDE's and integral equations) have been described in the proceedings of the 1992 Copper Mountain Conference on Iterative Methods [P3], and it has received mention in the notes for a short course on optimization software given in conjunction with the 1992 SIAM Meeting on Optimization in Chicago [SR17]. It is planned to expand [P3] into a paper suitable for journal publication and to further develop the code into a robust, efficient, portable code that is suitable for public distribution.

Consideration of extensions or alternatives to basic features of the code has been undertaken. In collaboration with M. Pernice of the scientific staff of the Utah Supercomputing Institute at the University of Utah and L. Zhou, a postdoctoral associate there, the PI has begun investigation of globalization alternatives to backtracking and has made initial experiments with iterative linear solvers other than GMRES. Also, jointly with Pernice and Zhou, the PI has initiated research on domain decomposition-based parallel implementations of the code, with applications to reactive flow modeling problems. In other applications, the PI has begun work with M. Wheeler and her associates at Rice University to adapt the code to nonlinear reservoir engineering problems using a domain decomposition approach.

2.2. Iterative linear solvers.

As noted in §2.1, a very important issue in implementing a Newton iterative method is the choice of an iterative linear solver. Of course, iterative linear solvers are also of great interest in their own right. Accordingly, considerable effort has been directed toward the development and understanding of iterative linear solvers.

In recent years, there has been a remarkable proliferation of conjugate gradient–type methods for general nonsymmetric linear systems, especially *Krylov subspace methods.* For solving a system $Ax = b$, these methods begin with an initial x_0 and, at the kth iteration, determine $x_k = x_0 + z_k$ for some correction z_k in the kth Krylov subspace $\mathcal{K}_k \equiv \text{span}\,\{r_0, Ar_0, \ldots, A^{k-1}r_0\}$, where $r_0 \equiv b - Ax_0$. See [SR8] for a general discussion of these methods and a description of specific methods referred to here. This proliferation shows no signs of abating and offers both challenges and opportunities. During the 1991-94 period of this grant, work centered around GMRES [SR11, SR15] and "residual smoothing" techniques for general iterative linear solvers.

2.2.1. GMRES work. GMRES is perhaps the most widely used and best understood iterative method for general nonsymmetric linear systems. Research was directed toward developing more robust and efficient implementations of GMRES.

The PI collaborated with A. Skjellum, P. Brown, and others in the Computing and Mathematics Research Division (CMRD) at Lawrence Livermore National Laboratory (LLNL) to develop a number of different GMRES implementations based on previous [SR15] and current [P2] work of the PI. These implementations differ in the amount and level of BLAS used in them and consequently have differing potentials for exploiting different vector and parallel architectures. One of them was chosen to be the implementation of GMRES in the *Multicomputer Toolbox*, a parallel computing software toolbox developed by the CMRD group. Fortran versions of all of these implementations were made publicly available by the PI through Netlib. This work influenced the GMRES subroutine used in the GMRES–backtracking Newton iterative code described above in §2.1.2.

The PI collaborated with with K. Turner [P4] in determining efficient ways of obtaining high-accuracy solutions with GMRES. A technique outlined in [P4] for efficiently using higher-order finite-differencing in evaluating products of the form $F'(x_k)v$ in GMRES has helped to eliminate inaccuracy without loss of efficiency in the GMRES–backtracking Newton iterative code described above in §2.1.2.

The PI and L. Zhou, then a Utah State graduate student, developed Gram–Schmidt and Householder implementations of GMRES that are simpler than the standard implementations. The simplicity is achieved by starting the Arnoldi basis generation process with Ar_0 instead of r_0 as in the standard implementations. As a result, the GMRES least-squares problem emerges in upper-triangular form, rather than upper-Hessenberg form, and so the usual QR factorization using Givens rotations is unnecessary. These results have been written up in [P2], which will appear as an invited paper in the *Journal of Numerical Linear Algebra and Applications* Special Issue on Iterative Methods and Preconditioners for Nonsymmetric Linear Systems.

The PI also collaborated with P. Brown of the CMRD at LLNL to investigate the performance of GMRES on singular or ill-conditioned systems. This resulted in implementations of GMRES with improved capabilities for detecting and handling ill-conditioning when it threatens to degrade the performance of the method. This work is written up in [P7].

2.2.2. Residual smoothing techniques. The PI and L. Zhou also collaborated on residual smoothing techniques for general iterative linear solvers. At least two methods that have recently received considerable attention, BCG [SR6, SR10] and CGS [SR13], have the undesirable property of often producing wildly varying residual norms, in contrast to the monotone decreasing GMRES residual norms. This has motivated the development of other methods, notably Bi-CGSTAB [SR14] and QMR [SR9]. In recent work in [SR12] and [SR16], it was shown that, given a sequence of iterates produced by any method, one can easily generate an auxiliary sequence with monotone decreasing residual norms. Zhou independently rediscovered this simple technique and developed an equivalent formulation with much better numerical properties. He then extended it to a broad class of residual smoothing techniques and showed that the QMR method is included in this class. He and the PI then worked together to refine these results and carry out a number of numerical experiments. This research showed that residual smoothing techniques are very useful both as practical tools and for the theoretical insights they give into QMR and other QMR-type methods [SR2], [SR7]. This work is written up in [P5]. In other work on residual smoothing, the PI recently wrote an expository note

[P8] in which residual smoothing techniques are used to extend results of Brown [SR1] and Cullum and Greenbaum [SR3], [SR4] correlating "peaks" and "plateaus" of residual norms produced by some well-known pairs of Krylov subspace methods.

2.2.3. Other work. It was noted in §2.1.2 that the PI has begun work with M. Pernice and L. Zhou of the Utah Supercomputing Institute on applications of Newton iterative methods to reactive flow problems. This work also includes applications of GMRES and other iterative linear solvers, with and without residual smoothing, to appropriate linearized test problems. The objectives are to determine effective parallel implementations and preconditioners, especially in conjunction with domain decomposition techniques.

3. Publications.

Publications supported through this grant and acknowledging its support are the following, listed in chronological order:

[P1] S. C. Eisenstat and H. F. Walker, *Globally convergent inexact Newton methods*, SIAM J. Optimization, 4 (1994), pp. 393–422.

[P2] H. F. Walker and L. Zhou, *A simpler GMRES*, Utah State University Math. Stat. Dept. Res. Report 1/92/54, January, 1992, (revised October, 1992), to appear by invitation in the Special Issue on Iterative Methods and Preconditioners for Nonsymmetric Linear Systems, J. Numer. Lin. Alg. Appl., 1994.

[P3] H. F. Walker, *A GMRES–backtracking Newton iterative method*, Proceedings of the Conference on Iterative Methods, Copper Mountain, Colorado, April, 1992; Utah State University Math. Stat. Dept. Res. Report 3/94/74, March, 1994.

[P4] K. Turner and H. F. Walker, *Efficient high accuracy solutions with GMRES(m)*, SIAM J. Sci. Stat. Comput., 13 (1992), pp. 815–825.

[P5] L. Zhou and H. F. Walker, *Residual smoothing techniques for iterative methods*, Special Section on Iterative Methods in Numerical Linear Algebra, SIAM J. Sci. Comput., 15 (1994), pp. 297–312.

[P6] S. C. Eisenstat and H. F. Walker, *Choosing the forcing terms in an inexact Newton method*, Rice University Computational and Applied Math. Dept. Tech. Report TR94-25, Center for Research on Parallel Computation Tech. Report CRPC-TR-94463, and Utah State University Math. Stat. Dept. Res. Report 6/94/75, June, 1994; submitted to SIAM J. Sci. Comput.

[P7] P. N. Brown and H. F. Walker, *GMRES on (nearly) singular systems*, Rice University Computational and Applied Math. Dept. Tech. Report TR94-06, Center for Research on Parallel Computation Tech. Report CRPC-TR-94387, Lawrence Livermore National Laboratory Report UCRL-JC-115882, and Utah State University Math. Stat. Dept. Res. Report 2/94/73, February, 1994; submitted to SIAM J. Matrix Anal. Appl.

[P8] H. F. Walker, *Residual smoothing and peak/plateau behavior in Krylov subspace methods*, Utah State University Math. Stat. Dept. Res. Report 12/94/79, December, 1994; submitted by invitation to the Special Issue on Iterative Methods for Linear Equations, Applied Numerical Mathematics.

4. Supplementary references.

[SR1] P. N. Brown, *A theoretical comparison of the Arnoldi and* GMRES *algorithms*, SIAM J. Sci. Stat. Comput., 20 (1992), pp. 58-78.

[SR2] T. F. Chan, E. Gallopoulos, V. Simoncini, T. Szeto, and C. H. Tong, *A quasi-minimal residual variant of the* Bi-CGSTAB *algorithm for nonsymmetric systems*, SIAM J. Sci. Comput., 15 (1994), pp. 338-347.

[SR3] J. K. Cullum and A. Greenbaum, *Residual relationships within three pairs of iterative algorithms for solving $Ax = b$*, Tech. Report RC 18672, IBM T. J. Watson Research Center, Yorktown Heights, New York, January, 1993; to appear in SIAM J. Matrix Anal. Appl.

[SR4] J. K. Cullum and A. Greenbaum, *Peaks, plateaus, numerical instabilities in Galerkin and minimal residual pairs of methods for solving $Ax = b$*, preprint, 1994.

[SR5] R. Dembo, S. C. Eisenstat, and T. Steihaug, *Inexact Newton methods*, SIAM J. Numer. Anal., 19 (1982), pp. 400–408.

[SR6] R. Fletcher, *Conjugate gradient methods for indefinite systems*, in *Numerical Analysis Dundee 1975*, G. A. Watson, ed., Lecture Notes in Mathematics 506, Springer-Verlag, Berlin, Heidelberg, New York, 1976.

[SR7] R. W. Freund, *A transpose-free quasi-minimal residual algorithm for non-Hermitian linear systems*, RIACS Tech. Rep. 91.18, September, 1991, submitted to SIAM J. Sci. Stat. Comput.

[SR8] R. W. Freund, G. H. Golub, and N. M. Nachtigal, *Recent advances in Lanczos-based iterative methods for nonsymmetric linear systems*, Acta Numerica 1992, Cambridge University Press, 1992, pp. 57–100.

[SR9] R. W. Freund and N. M. Nachtigal, *QMR: a quasi-minimal residual method for non-Hermitian linear systems*, RIACS Tech. Rep. 90.51, December, 1990, to appear in Numer. Math.

[SR10] C. Lanczos, *Solution of systems of linear equations by minimized iterations*, J. Res. Nat. Bur. Stand., 49 (1952), pp. 33–53.

[SR11] Y. Saad and M. H. Schultz, *GMRES: a generalized minimal residual method for solving nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 7 (1986), pp. 856–869.

[SR12] W. Schönauer, *Scientific Computing on Vector Computers*, North–Holland, Amsterdam, 1987.

[SR13] P. Sonneveld, *CGS, a fast Lanczos–type solver for nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 10 (1989), pp. 36–52.

[SR14] H. A. van der Vorst, *Bi-CGSTAB: a fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 13(1992), pp. 631–644.

[SR15] H. F. Walker, *Implementations of the GMRES method*, Computer Physics Communications, 53 (1989), pp. 311–320.

[SR16] R. Weiss, *Convergence Behavior of Generalized Conjugate Gradient Methods*, Ph.D. dissertation, University of Karlsruhe, 1990.

[SR17] S. Wright and J. J. Moré, *Numerical Optimization: Algorithms and Software*, course notes and software guide, Mathematics and Computer Science Division, Argonne National Laboratory, May, 1992; published as *Optimization Software Guide*, Frontiers in Applied Mathematics, Vol. 14, SIAM, Philadelphia, PA, 1993.

5. Professional personnel associated with this research.

Only the PI has received financial support from this grant; however, other personnel have been involved with the research during the 1991-94 grant period as collaborators, as follows:

P. N. Brown, CMRD, LLNL.

S. C. Eisenstat, Computer Science Department, Yale University.

H. Klie, Ph.D. student under the direction of M. Wheeler, Computational and Applied Mathematics Department, Rice University.

M. Pernice, Utah Supercomputing Institute.

C. San Soucie, Ph.D. student under the direction of M. Wheeler, Computational and Applied Mathematics Department, Rice University.

A. Skjellum, CMRD, LLNL (now with the Computer Science Department, Mississippi State University).

K. Turner, Mathematics and Statistics Department, Utah State University.

K. Vang, Ph.D. student under the direction of K. Turner, Mathematics and Statistics Department, Utah State University.

M. Wheeler, Computational and Applied Mathematics Department, Rice University.

L. Zhou, Ph.D. student under the direction of the PI (1993-94 degree), Mathematics and Statistics Department, Utah State University, and postdoctoral associate, Utah Supercomputing Institute (1995-95).

6. Interactions.

6.1. Invited talks.

Invited talks on research supported by this grant during and immediately after the 1991-94 period are as follows:

[T1] *Inexact Newton and Newton iterative methods*, Minisymposium on Nonlinear Equations and Optimization in Infinite-Dimensional Spaces, ICIAM 91: Second International Conference on Industrial and Applied Mathematics, Washington, DC, July, 1991.

[T2] *Choosing the forcing terms in an inexact Newton method*, Conference on Numerical Optimization Methods in Differential Equations and Control, North Carolina State University, July, 1991.

[T3] *Inexact Newton and Newton iterative methods*, Lawrence Livermore National Laboratory, August, 1991.

[T4] *Newton iterative methods*, 6th IIMAS Workshop on Numerical Analysis, Oaxaca, México, January, 1992.

[T5] *A GMRES-backtracking Newton iterative method*, Conference on Iterative Methods, Copper Mountain, Colorado, April, 1992.

[T6] *Residual smoothing methods for iterative linear system solvers*, Lawrence Livermore National Laboratory, August, 1992.

[T7] *Iterative methods for large scale linear and nonlinear systems*, Frontiers Lectures program (three lectures), Mathematics Department, Texas A&M University, October-November, 1992.

[T8] *Inexact Newton and Newton iterative methods*, Mathematics Department, University of Houston, November, 1992.

[T9] *Residual smoothing techniques for iterative linear solvers*, poster presentation, DOE/OSC Applied Mathematics Workshop, Albuquerque, New Mexico, February, 1993.

[T10] *A GMRES-backtracking Newton iterative method*, Special Session on Numerical Optimization, AMS 879th Meeting, Knoxville, Tennessee, March, 1993.

[T11] *Newton iterative and inexact Newton methods*, International Meeting on Linear/Nonlinear Iterative Methods and Verification of Solution, Matsuyama, Japan, July, 1993.

[T12] *Newton iterative methods for large-scale nonlinear systems*, Sandia National Laboratory (Albuquerque), October, 1993.

[T13] *Newton iterative and inexact Newton methods*, Computational and Applied Mathematics Department, Rice University, December, 1993.

[T14] *Choosing the forcing terms in an inexact Newton method*, Colorado Conference on Iterative Methods, Breckenridge, Colorado, April, 1994.

[T15] *Krylov subspace methods and residual smoothing techniques*, Center for Numerical Analysis, University of Texas at Austin, April, 1994.

[T16] *Residual smoothing techniques for iterative methods*, Session on Iterative Solution of Linear Equations, Generalized Conjugate Gradient methods, Preconditioners and Beyond, 14th IMACS World Congress on Computation and Applied Mathematics, Atlanta, Georgia, July, 1994.

[T17] *A GMRES-backtracking Newton-iterative method*, Session on Algorithms and Applications, 15th International Symposium on Mathematical Programming, Ann Arbor, Michigan, August, 1994.

[T18] *Krylov subspace methods and residual smoothing techniques*, Sandia National Laboratory (Albuquerque), August, 1994.

6.2. Consultative and advisory functions.

Several research collaborations were noted in §2 above, and these were often associated with more general consultative and advisory functions, particularly in the case of collaborations with members of the CRMD at LLNL. The PI also visited Texas A&M University for two weeks in October-November, 1992. The first week was spent giving three one-hour talks in the Frontiers Lectures program in the Mathematics Department [T7]. The second week was spent visiting the Institute for Scientific Computation and discussing iterative methods for linear and nonlinear problems in reservoir engineering and seismic data interpretation. Also, in 1993-94, the PI spent a sabbatical visiting the Computational and Applied Mathematics Department and the Center for Research on Parallel Computation at Rice University; he began work with M. Wheeler and her associates there.

Other notable interactions have been with researchers at Boeing. Newton iterative methods with GMRES as the iterative linear solver have been very successfully used at Boeing in electromagnetic, acoustic, and aerodynamic modeling codes. A particularly successful application has been modeling transonic flow by solving the steady state full potential equation for shock locations and strengths on complex 3D aircraft configurations. During the 1991-94 grant period, the PI exchanged ideas and papers with R. Burkhart and D. P. Young on a number of occasions. He also invited Young to speak at a special session at the Copper Mountain Conference on Iterative

Methods in April, 1992, and invited Burkhart to speak in a Minisymposium on Iterative Methods for Large Scale Nonlinear Systems at the SIAM National Meeting in Los Angeles, July, 1992. In November and December of 1992, the PI had a lengthy exchange with L. Wigton, then visiting NASA Langley Research Center, over matters relating to GMRES. These mainly had to do with the accuracy of different implementations and techniques and with the suitability of different implementations for large scale applications. In the summer of 1994, the PI discussed with Wigton various matters having to do with Newton iterative methods, GMRES, and preconditioners.