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1986-1990 FINAL REPORT

Project Titles: Numerical Solution of Nonlinear Algebraic Equations in Stiff ODE Solving (1986-89)
Quasi-Newton Updating for Large Scale Nonlinear Systems (1989-90)

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During the 1986-1989 project period, two major areas of research developed into which most of the work fell: (1) "matrix-free" methods for solving linear systems, by which we mean iterative methods that require only the action of the coefficient matrix on vectors and not the coefficient matrix itself, and (2) Newton-like methods for underdetermined nonlinear systems.

In the 1990 project period of the renewal grant, a third major area of research developed: inexact Newton and Newton iterative methods and their applications to large-scale nonlinear systems, especially those arising in discretized problems. An inexact Newton method is any method in which each step reduces the norm of the local linear model of the function of interest. A Newton iterative method (sometimes called a truncated Newton method) is any implementation of Newton's method in which the linear systems that characterize Newton steps (the "Newton equations") are solved only approximately using an iterative linear solver. Newton iterative methods are properly considered special cases of inexact Newton methods.

We describe the work in these three areas and in other areas below.

1. Matrix-free methods for solving linear systems.

A. C. Hindmarsh and P. N. Brown of the Computation and Mathematics Research Division at Lawrence Livermore National Laboratory have very successfully used the matrix-free GMRES and Arnoldi (IOM) methods in the numerical solution of very large stiff ODE initial-value problems. In this application, iterative linear solvers are used in Newton iterative methods to determine steps of an implicit stiff ODE method. Much of our work in this area, especially as it applies to stiff ODE solving, was carried out in close communication with Brown and Hindmarsh.

Matrix-free methods such as the GMRES and Arnoldi methods have special advantages in the Newton-iterative context, in that they can be used to obtain approximate solutions of the linear Newton equations without necessarily forming or storing Jacobian matrices. Indeed, the action of Jacobian matrices on vectors can be approximated by finite-differences of function values, and so no direct knowledge of Jacobian matrices is necessary.

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Work in this area focussed on the GMRES method but also applies by and large to the Arnoldi method as well. The standard implementations of these methods involve (modified) Gram-Schmidt orthogonalization, which may be a source of significant numerical error. Much of our research was directed toward the development and testing of alternative implementations in which Gram-Schmidt orthogonalization is replaced by more stable orthogonalization using Householder transformations.

Earlier Householder implementations of the GMRES and Arnoldi methods (H. F. Walker, *Implementation of the GMRES and Arnoldi methods using Householder transformations*, Lawrence Livermore Nat. Lab. Rep. UCRL-93589, 1985) have been shown to be potentially unstable and, in particular, to be numerically unsound in stiff ODE applications (A. C. Hindmarsh and H. F. Walker, *A note on a Householder transformation implementation of the GMRES method*, Lawrence Livermore Nat. Lab. Rep. UCID-20899, 1986).

During the 1986-1989 project period, we developed new Householder implementations of the GMRES and Arnoldi methods that are stable and that may offer advantages on very large problems in vector and, in particular, parallel environments. These implementations and their performance on general linear systems are described in [9]. It is shown in [9] that these implementations are indeed numerically superior to the standard Gram-Schmidt implementations, especially as the limits of residual reduction are neared.

The first stable Householder GMRES implementation in [9] was tested on stiff ODE problems by incorporating it in a matrix-free version of LSODE, the stiff ODE solver developed by Hindmarsh at Livermore. This matrix-free version of LSODE was developed by Brown and Hindmarsh using the standard Gram-Schmidt implementations of the GMRES and Arnoldi methods. Several tests did not indicate any numerical superiority of the stable Householder GMRES implementation over the standard Gram-Schmidt implementation; however, for one test problem arising from the discretization of a reaction-diffusion equation, in which the Jacobian became very ill-conditioned for large time, the stable Householder implementation proved more effective in several instances than the Gram-Schmidt implementation, with which the code failed before reaching the desired time values. Results are reported in H. F. Walker, *Experiments with the stable Householder implementation of the GMRES method in stiff ODE solving*, Lawrence Livermore Nat. Lab. Rep. UCID-21343, 1988.

We have also discussed in [10] general and specific implementations and implementational considerations for GMRES and have made new observations about the amounts of arithmetic required by various implementations. The paper [10] grew out of an invited presentation at a Workshop on Practical Iterative Methods for Large-Scale Computations held at the Minnesota Supercomputer Center (October, 1988). We also gave an invited talk on this work at a Miniconference on Linear and Numerical Linear Algebra and Applications held at Northern Illinois University (April, 1989).

We also worked with K. Turner to explore sources and effects of inaccuracy in GMRES. This resulted in versions of GMRES that achieve high accuracy at relatively low cost by making judicious use of a few well placed high accuracy computations [7]. We gave invited talks on this work at Stanford University (July, 1990) and in a minisymposium at the 2nd SIAM Conference on Linear Algebra in Signals, Systems, and Control (November, 1990).

2. Newton-like methods for underdetermined nonlinear systems.

Underdetermined nonlinear systems arise in a variety of contexts, sometimes naturally and sometimes as artifacts of mathematical methods or problem formulations. A particularly important source is parameter-dependent problems, which occur both naturally in physical modeling, e. g., modeling of snap-through buckling of a shallow elastic arch as a load parameter is increased, and through the solution of (perhaps non-parametric) problems using continuation or homotopy methods. Parameter-dependent nonlinear systems arise in solving stiff ODE initial-value problems through the use of implicit methods, which give rise at each time step to a nonlinear system that depends parametrically on the time variable. Since the time variable is fixed during each set of corrector iterations, one might think of these systems as a sequence of non-parametric systems. However, because efficient methods typically carry Jacobian information along through a number of time steps, it is more realistic to regard them as parameter-dependent systems.

The work in this area has been directed toward the development, analysis, and application of Newton and quasi-Newton methods for general underdetermined nonlinear systems.

With S. K. Bourji, we gave in [2] a general treatment of least-change secant updating for nonsquare matrices. In [2], the notion of a least-change secant update is extended to apply to nonsquare matrices and formulas for extensions of the most popular square-matrix updates are given, including the good and bad Broyden updates, the PSB and Greenstadt updates, the sparse Broyden (Schubert) update, and the DFP and BFGS updates. The use of these updates is supported in [2] by a local convergence analysis of certain quasi-Newton methods using them, shows roughly that these methods enjoy local convergence that is q -superlinear if possible and otherwise optimal q -linear, depending on the speed at which parameter values approach limiting values and on whether or not the Jacobian at the solution lies in the set of allowable approximants.

With L. T. Watson, we gave in [12] a study of certain Newton-like methods for underdetermined nonlinear systems, viz., the normal flow and augmented Jacobian methods that are widely used in homotopy or continuation methods, together with quasi-Newton variations of them that use the nonsquare-matrix updates developed in [2]. A local convergence analysis for these methods is given in [12]. This analysis is necessarily a Kantorovich-type analysis because one cannot expect solutions to be isolated in the underdetermined case and therefore no solution can be singled out a priori as a possible limit of an iteration sequence. Our analysis is distinct from traditional Kantorovich-type analyses in that it does not use the traditional "method of majorization" but rather achieves the same results in a more straightforward way. It provides the first local q -quadratic convergence results for the normal flow and augmented Jacobian algorithms and the first local q -superlinear and optimal q -linear convergence results for quasi-Newton variations of these methods that use least-change secant updates. Because this analysis also applies to the well-determined case of an equal number of equations and unknowns, it also provides both an alternative to the traditional Kantorovich analysis of Newton's method and the first Kantorovich-type analysis for general least-change secant update methods.

Experiments with quasi-Newton variations of the normal flow and augmented Jacobian methods (using nonsquare extensions of the good and bad Broyden updates) are also outlined in [12]. These methods were first tested on simple, two-variable problems to show some of their basic properties. They were then used as corrector iterations in predictor-corrector homotopy methods through implementation in HOMPACK, a suite of homotopy method codes developed by Watson. Results are reported in [12].

Invited talks relating to the work in [2] and [12] were given at Arizona State University (October, 1987), Virginia Polytechnic Institute and State University (April, 1988), Colorado State University (April, 1988), the AMS-SIAM Summer Seminar on Computational Solution of Nonlinear Systems of Equations (July, 1988; this talk was published in [11]), Argonne National Laboratory (April, 1989), and the University of Connecticut (December, 1989).

We also worked with Watson and others to experiment with GMRES and a variety of other iterative linear solvers in Newton-iterative formulations of homotopy methods for parameter-dependent nonlinear systems. The results of this work have been published in [3] and [6].

3. Inexact Newton and Newton iterative methods.

In a major collaboration with S. C. Eisenstat, we investigated globally convergent inexact Newton methods. The immediate result was the paper [4], which we expect to lay the groundwork for a great deal of useful research over the next several years. In [4], we formulated a number of general and somewhat specific inexact Newton algorithms that have very strong global convergence properties. As noted in [4], these can be used to provide a global convergence analysis for well-known globalizations of (exact) Newton's method, such as backtracking and model trust region globalizations. Their main purpose, however, is to provide new, theoretically sound algorithmic frameworks for the practical implementation of methods that are inherently inexact Newton methods, in particular Newton iterative methods.

This research has begun to bear fruit in recent work in developing software implementations of Newton iterative methods. We have at this time a prototype Newton iterative code based on the ideas in [4] that uses GMRES as the iterative linear solver and backtracking as the globalization. This prototype code has proved very successful on a number of PDE and integral equation problems. Our intention is to develop it further with the consideration of other iterative linear solvers and globalizations, to test it on a broader set of more difficult problems, and ultimately to produce and make publicly available high-quality software that incorporates the features that are found to be most effective.

We have given invited talks on the work in [4] at the SIAM 1990 Annual Meeting (July, 1990), the Utah Supercomputing Institute Fall Workshop on Numerical Algorithms (November, 1990), North Carolina State University (March, 1991), the Second International Conference on Industrial and Applied Mathematics (July, 1991), the Conference on Numerical Optimization Methods in Differential Equations and Control (July, 1991), and Lawrence Livermore National Laboratory (August, 1991).

4. Research in other areas.

A research project in theoretical fluid dynamics grew out of the work on matrix-free iterative methods for linear systems. Vijay K. Gupta, a theoretical hydrologist visiting the Utah Water Resources Laboratory in 1985-1986, proposed a series of numerical experiments aimed at determining the asymptotic behavior (as a parameter approaches infinity) of certain integrals associated with solutions of a convection-diffusion equation. The purpose was to gain insight into the asymptotic dispersion of contaminants in fluids moving in porous media. A necessary part of the experiments was solving very large non-symmetric linear systems from the discretized PDE, and so this seemed an excellent opportunity for testing the matrix-free methods on realistic problems. The numerical experiments were inconclusive. However, the underlying problem turned out to be amenable

to analytical treatment using eigenfunction expansions of compact operators. General tools for attacking the problem were developed, and interesting insights into the problem were gained in important special cases. The results were written up in [8] and were included in the joint paper [1] with Gupta and R. Bhattacharya of the Department of Mathematics at Indiana University.

An invited talk on joint work with J. D. Gonglewski was given at the 5th IIMAS Workshop on Numerical Analysis, Mérida, México, in January, 1989. This was related to Gonglewski's dissertation work, which was supported through this grant, and concerned certain quasi-Newton methods for general maximum-likelihood estimation that are analogous to well-known special methods for nonlinear least-squares problems. A particular application of interest was maximum-likelihood estimation of parameters in (finite) statistical mixture densities. This work was published in [5].

We also worked with L. T. Watson and M. P. Windham in applying homotopy methods, as implemented in HOMPACK, to maximum-likelihood estimation for statistical mixture densities. An invited talk on this work was given at the 2nd Conference of the International Federation of Classification Societies (June, 1989), but the results have not yet been published.

Finally, we worked with P. N. Brown and Y. Saad to explore uses of quasi-Newton updating in developing preconditioners for iterative linear solvers. Several attractive formulas were developed and a number of experiments with linear and nonlinear problems were carried out. The results were promising, but we have not yet found an application in which our quasi-Newton preconditioners were clearly the methods of choice. Consequently, the results have not yet been published. Invited talks on this work were given at Cornell University and North Carolina State University (both in December, 1989).

Graduate students supported through this grant:

1. John D. Gonglewski, University of Houston, supported 7/86–9/86, Ph.D. awarded 8/86, dissertation: *On Quasi-Newton Methods for Maximum-Likelihood Estimation with Applications to the Mixture Density Problem*.
2. Samih K. Bourji, Utah State University, supported 9/86–8/87, Ph.D. awarded 8/87, dissertation: *Least-Change Secant Updates of Non-Square Matrices*.
3. Eric T. McQueen, Utah State University, supported 9/87–6/88, no degree awarded.
4. Yi Qian, Utah State University, supported 1/90–9/90, M.S. awarded 10/90, thesis: *Inexact Newton and Newton iterative methods*.

Invited presentations by H. F. Walker relating to research supported through this grant, 1986 – present:

1. *Least-change secant updates for parameter-dependent nonlinear systems*, Conference on Nonlinear Parameter-Dependent PDE's and Their Effective Solution, Arizona State University, Nov., 1987.
2. *Least-change secant update methods*, colloquium talk, Mathematics and Computer Science Departments, Virginia Polytechnic Institute and State University, April, 1988.
3. *Least-change secant update methods*, colloquium talk, Mathematics Department and SIAM Rocky Mountain Regional Group, Colorado State University, April, 1988.
4. *Newton-like methods for underdetermined systems*, 19th AMS-SIAM Summer Seminar on Computational Solution of Nonlinear Systems of Equations, Fort Collins, Colorado, July, 1988.

5. *Implementations of the GMRES method*, Workshop on Practical Iterative Methods for Large Scale Computations, held at the Minnesota Supercomputer Center, Oct., 1988.
6. *Quasi-Newton methods for maximum-likelihood estimation*, 5th IIMAS Workshop on Numerical Analysis, Mérida, México, Jan., 1989.
7. *Quasi-Newton methods for underdetermined systems and path following*, Argonne National Laboratory, April, 1989.
8. *The GMRES method*, Miniconference on Linear Algebra, Numerical Linear Algebra, and Applications, Northern Illinois University, April, 1989.
9. *Homotopy methods for mixture estimation problems*, 2nd Conference of the International Federation of Classification Societies, Charlottesville, VA, June, 1989.
10. *Preconditioning with low-rank updates*, Center for Applied Mathematics, Cornell University, December, 1989.
11. *Preconditioning with low-rank updates*, Mathematics Department, North Carolina State University, December, 1989.
12. *Newton and quasi-Newton methods for well-determined and underdetermined systems*, Mathematics Department, University of Connecticut, December, 1989.
13. *Globally convergent inexact Newton methods*, Minisymposium on Nonlinear Optimization, SIAM 1990 Annual Meeting, Chicago, IL, July, 1990.
14. *Efficient high accuracy solutions with GMRES(m)*, Computer Science Department, Stanford University, July, 1990.
15. *Newton-like methods for large-scale nonlinear systems*, USI Fall Workshop on Numerical Algorithms, Utah Supercomputing Institute, Salt Lake City, UT, November, 1990.
16. *Efficient high accuracy solutions with GMRES(m)*, Minisymposium on Large-Scale and Parallel Matrix Computations, 2nd SIAM Conference on Linear Algebra in Signals, Systems, and Control, San Francisco, CA, November, 1990.
17. *Inexact Newton and Newton iterative methods*, Mathematics Department, North Carolina State University, March, 1991.
18. *Inexact Newton and Newton iterative methods*, Minisymposium on Nonlinear Equations and Optimization in Infinite-Dimensional Spaces, ICLAM 91: Second International Conference on Industrial and Applied Mathematics, Washington, DC, July, 1991.
19. *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.
20. *Inexact Newton and Newton iterative methods*, Lawrence Livermore National Laboratory, August, 1991.

Publications and reports acknowledging support of this grant:

- [1] R. Bhattacharya, V. K. Gupta, and H. F. Walker, *Asymptotics of solute dispersion in periodic porous media*, SIAM J. Appl. Math., 49 (1989), pp. 86–98.
- [2] S. K. Bourji and H. F. Walker, *Least-change secant updates of nonsquare matrices*, SIAM J. Numer. Anal., 27 (1990), pp. 1263–1294.
- [3] C. Desa, K. M. Irani, C. J. Ribbens, H. F. Walker, and L. T. Watson, *Preconditioned iterative methods for homotopy curve tracking*, SIAM J. Sci. Stat. Comput. (to appear).
- [4] S. C. Eisenstat and H. F. Walker, *Globally convergent inexact Newton methods*, Utah State University Math. Stat. Dept. Res. Report February/91/51; submitted to SIAM J. Optimization.
- [5] J. D. Gonglewski and H. F. Walker, *Quasi-Newton methods for maximum-likelihood estimation*, in *Advances in Numerical Partial Differential Equations and Optimization: Proceedings of the Fifth México–United States Workshop*, S. Gómez, J.-P. Hennart, and R. A. Tapia, eds., SIAM Proceedings in Applied Mathematics, Vol. 47, Society for Industrial and Applied Mathematics, Philadelphia, PA, 1991, pp. 332–345.
- [6] K. M. Irani, M. P. Kamat, C. J. Ribbens, H. F. Walker and L. T. Watson, *Experiments with conjugate gradient algorithms for homotopy curve tracking*, SIAM J. Optimization, 1 (1991), pp. 222–251.
- [7] K. Turner and H. F. Walker, *Efficient high accuracy solutions with GMRES(m)*, SIAM J. Sci. Stat. Comput. (to appear).
- [8] H. F. Walker, *On integrals associated with a certain partial differential equation*, Utah State University Math. Dept. Report 1986/36, July, 1986.
- [9] H. F. Walker, *Implementation of the GMRES method using Householder transformations*, SIAM J. Sci. Stat. Comput., 9 (1988), pp. 152–163.
- [10] H. F. Walker, *Implementations of the GMRES method*, in *Proceedings of the Workshop on Practical Iterative Methods for Large Scale Computations*, D. L. Boley, D. G. Truhlar, Y. Saad, R. E. Wyatt, and L. E. Collins, eds., published in Computer Physics Communications, 53 (1989), pp. 311–320.
- [11] H. F. Walker, *Newton-like methods for underdetermined systems*, in *Computational Solution of Nonlinear Systems of Equations*, E. L. Allgower and K. Georg, eds., Lectures in Applied Mathematics Vol. 26, American Mathematical Society, Providence, RI, 1990, pp. 679–699.
- [12] H. F. Walker and L. T. Watson, *Least-change secant update methods for underdetermined systems*, SIAM J. Numer. Anal., 27 (1990), pp. 1227–1262.

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