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13. ABSTRACT *(Maximum 200 words)*

The objective of this project was to study numerical methods for solving sparse linear systems of equations of the type that arise from discretized partial differential equations. Such systems arise in mathematical models of numerous physical processes including turbulent flow, chemical reactive flow, semiconductor device simulation, and structural mechanics. For many such problems, analytic solutions are not available, so the only way of obtaining insight into the model is through numerical approximation and solution. The solution of sparse linear systems is often the most costly task, in terms of both computer time and storage, required by this process, so that improving the efficiency of such computations is of critical importance for the construction of accurate numerical models. Emphasis has been on sparse iterative methods for solving these systems, and implementation of linear system solvers on parallel computers. Major results are summarized in the final report.

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Iterative Methods for Large Sparse Linear Systems Arising from Partial Differential Equations

Final Report

Howard C. Elman

March 26, 1992

U. S. Army Research Office
Grant Number DAAL0389-K-0016

Computer Science Department
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A. Problem Statement

The objective of this project was to study numerical methods for solving sparse linear systems of equations of the type that arise from discretized partial differential equations. Such systems arise in mathematical models of numerous physical processes including turbulent flow, chemical reactive flow, semiconductor device simulation, and structural mechanics. For many such problems, analytic solutions are not available, so the only way of obtaining insight into the model is through numerical approximation and solution. The solution of sparse linear systems is often the most costly task, in terms of both computer time and storage, required by this process, so that improving the efficiency of such computations is of critical importance for the construction of accurate numerical models. Our emphasis is on sparse iterative methods for solving these systems, and implementation of linear system solvers on parallel computers.

B. Summary of Major Results

Results have been obtained in four general areas:

1. *Iterative methods for non-self-adjoint elliptic problems.* In a series of studies, we have developed, tested and analyzed iterative algorithms for solving the two-dimensional convection-diffusion equation discretized by finite differences. One class of methods that has been demonstrated to be successful for this problem is *line relaxation methods*, combined with a *reduced system* methodology. Here, the discrete problem is first treated by one step of block Gaussian elimination, which reduces the size of the problem by roughly a factor of two. The resulting reduced system is then ordered using a line ordering and solved by block relaxation methods. Analytic bounds on the rate of convergence of these methods show them to be rapidly convergent, with rates that actually improve as the amount of convection in the model increases (i.e. as the problem becomes more non-self-adjoint). Extensive numerical experiments on model problems confirm the fast convergence predicted by the analysis, and they also indicate that the analytic results (which apply only to constant coefficient problems) agree with the behavior of the methods on variable coefficient problems, e.g. with turning points. Moreover, experimental and analytic results show the methods to be be more effective than analogous techniques applied

to the "unreduced" system. Empirical results also identify effective ordering strategies, and they show that acceleration with Krylov subspace methods such as the generalized minimum residual method can be used to improve the convergence properties. This work was done in collaboration with G. H. Golub of Stanford University and G. Starke of the University of Karlsruhe.

In a related study, techniques based on preconditioning by incomplete LU factorization were considered for the discrete convection-diffusion equation. Analytic results were used to derive incomplete factorization preconditioners that avoid the numerical instabilities displayed when more standard incomplete factorization (ILU and MILU) methods are applied to this problem. The new stabilized methods are adaptive in the sense that their definitions are more closely tied to values of the of the underlying differential operator than traditional algebraic methods in this class. The methods were shown to be very robust and much more effective than standard methods for solving a wide collection of benchmark problems, including examples with variable coefficients or locally refined meshes.

2. *Finite element solvers on parallel computers.* We have performed a study of parallel implementation of a finite element solution technique for second order elliptic differential equations on a shared memory parallel computer, the Alliant FX/8. The focus was on the *hp*-version of the finite element method, which achieves accuracy by using both high order basis functions and mesh refinement. The algorithm used includes local elimination of high order basis functions with support internal to elements, combined with preconditioned conjugate gradient solution of unknowns on element interfaces. Results indicate that the fully parallel computations (local assembly and elimination) dominate the computational cost, and that the global (i.e. less highly parallel) operations, such as preconditioners, represent a small percentage of overall costs. New results include a clear picture of the effects of architectural features such as cache memory on performance; a demonstration of the use of efficiently coded kernels from the BLAS3 library to improve performance; a predictive analytic model of the effects of synchronization of local operations; and a demonstration that high order elements are an efficient means of achieving high accuracy. This work was in collaboration with I. Babuška, K. Markley, and D. K. Lee of the University of Maryland.

3. *Multilevel preconditioners and their implementation on large-scale parallel computers.* We have performed several studies of multilevel preconditioners for both two-dimensional and three-dimensional discrete self-adjoint elliptic differential equations. An advantage of such methods is their fast convergence, which depends only logarithmically on the number of mesh points. New results include efficient parallel algorithms for these techniques, grid generation strategies that relate multilevel methods more closely to underlying differential operators, and extensive numerical experiments on a large scale parallel computer, the Connection Machine 2. The enhanced algorithms greatly improve the performance of these methods for solving anisotropic problems and problems with discontinuous coefficients, and experiments on the Connection Machine show that they are effective on parallel machines provided communication costs are not too high. In addition, a new algebraic hierarchical basis multigrid method has been developed that has an optimal rate of convergence (i.e., independent of the number of mesh points), and displays faster experimental convergence than related methods such as the algebraic multilevel method. This project was performed in collaboration with X.-Z. Guo of the University of Maryland.

4. *Parallel sparse direct solvers.* In a study of parallel direct solution of sparse positive-definite linear systems, we compared the performance of two versions of parallel sparse Cholesky factor-

izations, based on two strategies of task assignment, dynamic allocation and static allocation. The first allocation strategy is commonly used on shared-memory machines, where a "pool of tasks" is accessible to all processors; the second type of strategy is needed for distributed memory machines. An advantage of static allocation strategies is that they can be used on either class of machine. Our tests, on a shared-memory 20-processor Encore Multimax computer, indicate that the best dynamic allocation strategy displays parallel efficiencies of roughly 85%, compared with efficiencies of about 50% for the best static strategies (so that the latter are roughly 60% as effective). Enhancements of static algorithms designed to make use of idle processors dramatically improves performance by reducing spin-waiting times. This work was in collaboration of G. Zhang of the University of Maryland.

C. List of Publications and Technical Reports

Refereed Journal Publications

"Relaxed and stabilized incomplete factorizations for non-self-adjoint linear systems," *BIT* 29:890-915, 1989.

"Iterative Methods for cyclically reduced non-self-adjoint linear systems II," with G. H. Golub. *Mathematics of Computation* 56:215-242, 1991.

"Line iterative methods for cyclically reduced discrete convection-diffusion problems," with G. H. Golub. *SIAM Journal on Scientific and Statistical Computing* 13:339-363, 1992.

"Parallel Implementation of the *hp*-version of the Finite Element Method on a Shared-Memory Architecture," with I. Babuška and K. Markley, UMIACS-TR-90-139, 1990. To appear in *SIAM Journal on Scientific and Statistical Computing.*

"Parallel Sparse Cholesky Factorization on a Shared Memory Multiprocessor," with G. Zhang, UMIACS-TR-91-86, 1991. To appear in *Parallel Computing.*

Reports Submitted for Publication

"Performance of the *hp*-Version of the Finite Element Method with Various Elements," with I. Babuška, Institute for Physical Science and Technology Report BN-1128, 1991. Submitted to *International Journal for Numerical Methods in Engineering.*

"Performance Enhancements and Parallel Algorithms for Two Multilevel Preconditioners," with X. Z. Guo, UMIACS-TR-91-143, 1991. Submitted to *SIAM Journal on Scientific and Statistical Computing.*

"On the Convergence of Line Iterative Methods for Cyclically Reduced Non-Symmetrizable Linear Systems", with G. H. Golub and G. S. Starke. Submitted to *Numerische Mathematik.*

"The Algebraic Hierarchical Basis Multigrid Method," by Xian-Zhong Guo, UMIACS-TR-92-8, 1992. Submitted to *SIAM Journal on Numerical Analysis.* (An abridged version of this paper has been awarded first prize in the student paper competition at the Copper Mountain Conference on Iterative Methods, April 1992.)

Conference Proceedings and Book Chapters

"Line Iterative Methods for Cyclically Reduced Non-Self-Adjoint Elliptic Problems," with G. H. Golub, in *Transactions of the Seventh Army Conference on Applied Mathematics and Computing,* 1989, ARO Report 90-1, pp. 457-466.

"Block Iterative Methods for Cyclically Reduced Non-Self-Adjoint Elliptic Problems," with G.

H. Golub, in D. Kincaid and L. Hayes, Editors, *Iterative Methods for Large Linear Systems*, Academic Press, 1990, pp. 91-105.

Theses

"Use of Linear Algebra Kernels to Build an Efficient Finite Element Solver," by Dennis Kah-Yuk Lee, Master's Thesis, 1992.

D. Scientific Personnel

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Graduate Research Assistants:	Xian-Zhong Guo (Ph.D., Applied Mathematics, expected, May 1992) Dennis Lee (M.A., Computer Science, expected, May 1992) Thomas Stone