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Numerical Algorithms for Parallel Computers

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Final Technical Report - AFOSR 86-0154

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Table of Contents

Technical Accomplishments

Throughout the duration of this grant 5/86-8/89, progress has been made on five fronts: analysis of parallel iterative methods using Fourier analysis techniques, preconditioners for linear systems on parallel architectures, numerical grid generation algorithms for fighter aircraft configurations, parallel domain decomposition algorithms for symmetric eigenvalue problems, and parallel language design issues from an applications point of view. Two Ph.D. theses have been completed.

Fourier Analysis Techniques

The successful use of the SOR method on parallel machines requires the computations to be ordered so that parallel operations can occur. For the simpliest problem stencil (5-point), David M. Young's famous Red/Black ordering will suffice. For more complicated stencils, more colors are necessary as reported in Adams and Ortega[1982]. However, this multicoloring may lead to different convergence properties of the SOR method than is exhibited by the standard rowwise ordering of unknowns. One step in resolving this dilemma about how to color the unknowns was given in Adams and Jordan[1986]. This paper showed how to find orderings that were equivalent to the rowwise ordering, but did not find the optimal relaxation parameter for any of the orderings.

Collaboration with David M. Young and Randall LeVeque resulted in calculating the optimal relaxation parameter for several four-color orderings of the 9-point Laplacian. The approach in Adams, LeVeque, Young[1988] was to represent each of the grid points of a particular color in a Fourier series and analyze the interaction of the points of different colors. Our results show that for this problem, there are only two equivalence classes of orderings with each class having different convergence properties from the other.

Analysis of this type can be applied to other iterative methods as well. In Adams[1989], it is shown how to apply these ideas to two-level hierarchical basis preconditioners.

Preconditioners

The first type of preconditioner that we investigated is of the polynominal type. In Adams[1985], it was shown that taking m-steps of the SSOR method could be used to efficiently precondition symmetric and positive definite systems of linear equations. This strategy involves a forward pass followed by a backward pass through the problem grid, and these steps must be performed sequentially. A new twist, appropriate to try for parallel machines, is to perform both passes simulaneously and average the results. The question is whether such a preconditioner is effective in reducing the number of iterations required for convergence (as compared to its multiplicative SSOR counterpart) and whether this preconditioner can be efficiently parallelized. In Adams and Ong[1988], we compare these two polynominal preconditioners. Both were programmed in POKER (Larry Snyder's parallel language) and ran on the Blue Chip Emulator (Snyder's emulated for his actual Chip machine). Results show that the additive method can suffer from the step necessary to average the results (this step was absent in the SSOR method) because processors must communicate to do this. In the paper we give conditions for both strategies to be effective on parallel machines. In addition, we analyze the new method theoretically and derive the optimal relaxation factor.

The second type of preconditioner that we investigated is one originally proposed by Yserentant[1986]. This preconditioner is based on the use of a hierarchical basis for the underlying finite element space. For an $n \times n$ system arising from two dimensional elliptic problems, the method is known to require $O(nlogn)$ work on a sequential machine. We have implemented this method for two dimensional problems on the Flexible-32 shared memory parallel machine at NASA Langley Research Center and have shown it to be superior to the Incomplete Cholesky preconditioner. These results were presented at the 1987 ASME Winter meeting held in Boston and are reported in Adams and Ong[1987].

Maria Elizabeth Ong, in her Ph.D. thesis (just completed), has shown how to extend the method to three dimensional problems using tetrahedral elements. She described a refinement strategy for tetrahedrons that gives a preconditioner that is as cheap to implement each iteration as the corresponding one for two dimensions. She proved that an upper bound for the resulting preconditioned system scaled by a diagonal matrix in the number of levels is $O(h^{-1})$ where h is the mesh spacing in each coordinate direction. This is an order of improvement over $O(h^{-2})$ for no preconditioning, but we do not see the logarithmic improvement that is realized in two dimensions. This method with tetrahedral elements was implemented on the Cray XMP and Flexible-32 to verify the theory and test its parallel properties, respectively. Ms. Ong was awarded a student scholarship for this work. She was given an expense paid trip to Tromsoe, Norway to present the results at the Second International Conference on Vector and Parallel Computing.

She also analyzed this preconditioner in the context of non-uniform grid refinement and showed bounds on the nonuniformity so that the theoretical properties of the method still hold. She also gives the conditions for expecting this preconditioner to work in conjunction with finite difference grids (as opposed to finite element ones). This work arose from the collaboration we have had with David P. Young at Boeing. Ms. Ong spent six weeks during the summer of 1988 at Boeing in Seattle investigating the incorporation of these preconditioners in the code TRANAIR and vectorizing the 3D preconditioner on the Cray. After observing that the preconditioner did not work as well when the grid was refined in a nonuniform way, she was then able to prove why this was indeed the case.

Many other questions have arisen from this work. A promising avenue to analyze these methods in more detail is the Fourier analysis techniques used by Adams, LeVeque, and Young[1988] and by Chan, Kuo[1988]. In Adams, et.al., we applied Fourier techniques to find the spectral radius and optimal SOR relaxation parameter for the 9-pt Laplacian. The problem reduced to analyzing the roots of a quartic equation. Chan and Kuo used similar ideas to analyze a two-level multigrid method. Efforts so far have shown that a two level hierarchical preconditioner can be analyzed with similar ideas and the result is again a quartic equation. This work is reported in Adams[1989].

Numerical Grid Generation

Another student (and Boeing employee), Joseph Manke, has recently completed his Ph.D. thesis on a new elliptic grid generation algorithm, suitable for modelling flow around fighter aircraft configurations. The approach is a multi-block one that will eventually lead to an efficient parallel implementation. He investigated the use of cubic spline basis functions in conjunction with the elliptic grid generating equations. The hope is that these two approaches combined will result in a method that is more general (in that it will interface well with existing surface geometry packages that use splines) and less costly than current approaches to grid generation. Experiments confirm this hope. Mr. Manke presented his results at the 2nd International Conference on Numerical Grid Generation in Computational Fluid Dynamics in Miami, Florida, December 1988. Hopefully these ideas will be incorporated into the grid generation software at Boeing.

Parallel Eigenvalue Solvers

Work on efficient parallel eigenvalue solvers is ongoing with another Ph.D. student, Kevin Gates. We are investigating divide and conquer strategies for solving eigenvalue problems on parallel machines. These ideas involve modification of the strategy used by Dongarra and Sorenson[1987]. Preliminary work was done by Mr. Gates while spending the summer of 1988 at the Oak Ridge National Laboratory. While there, he implemented several eigenvalue solvers on the hypercube and Sequent machines for comparison. We are now collaborating with Peter Arbenz at ETH, Switzerland on extensions of the basic theory to multiple rank-one updates, such as those described in Arbenz and Golub[1988], to the nonsymmetric problem. Peter Arbenz will spend the summer of 1990 in Seattle collaborating on these ideas.

Parallel Language Design

We have had ongoing collaboration with the parallel language design effort in the Department of Computer Science at the University of Washington. This effort is headed by Prof. Larry Snyder, Prof. David Notkin, and Prof. Loyce Adams. Our interest is to ensure that the parallel language that is developed will be appropriate for large scale scientific applications problems. To that end, we have programmed many different applications using POKER (Larry Snyder's old parallel language) and have provided feedback to the design group for its improvement and for features it has that are useful to applications programmers. An example project was conducted by my student. Kevin Gates. He investigated the POKER implementation of the famous benchmarking program SIMPLE and reported in his paper, Gates[1989], areas for improvement of POKER.

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Third SIAM Conference on Parallel Processing for Scientific Computing, Los Angeles, CA., December 1987, Maria E.G. Ong and Kevin Gates attended.

Mathematisches Forschungsinstitut Oberwolfach - Numerical Linear Algebra and Parallel Computation Conference, Loyce Adams presented *Implementation of the Hierarchical Basis Preconditioner on a Shared Memory Machine,* Oberwolfach, West Germany, February 1988.

Third SIAM Conference on Applied Linear Algebra, Loyce Adams presented minisymposium talk *Preconditioners on Parallel Computers,* Madison, WI., May 1988.

Third SIAM Conference on Applied Linear Algebra, Maria Elizabeth G. Ong presented minisymposium talk *The 3D Linear Hierarchical Basis Preconditioner*, Madison, WI., May 1988.

The 2nd Intl. Conference on Numerical Grid Generation in Computational Fluid Dynamics, Joseph Manke presented *A Tensor Product B-Spline Method for 3D Multi-Block Elliptic Grid Generation*, Miami Beach, Fla., December 1988.

ASME Winter Annual Meeting, Loyce Adams presented *A Comparison of Preconditioners for GMRES on Parallel Computers,* Boston, December 1987.

Tromsoe Conference on Parallel Computation, M.E.G. Ong presented *The 3D Linear Hierarchical Basis Preconditioner and Its Shared Memory Parallel Implementation,* Tromsoe, Norway, June 1988.

Iterative Methods Conference honoring David Young, Loyce Adams presented *Fourier Analysis of Two-Level Hierarchical Basis Preconditioners,* Austin, TX, October 1988.

SIAM Conference on Sparse Matrices, Glenedon Beach, Oregon, May 1989, M.E.G. Ong and Kevin Gates attended.

Laboratory Interactions

Oak Ridge National Laboratory: Spent several days with Bob Ward's group during the *Special Year for Numerical Analysis.* This visit included discussions with Michael Heath, James Ortega, Charles Romine, Al Geist, and David M. Young.

Oak Ridge National Laboratory: Kevin Gates, a Ph.D. student spent the summer of 1988 at Oak Ridge testing a new eigenvalue solver on the Hypercube and Sequent machines. He was visiting Michael Heath's group. His thesis, to be completed in one and one half years is concerned with divide and conquer ideas for eigenvalue problems.

ICASE, NASA Langley Research Center: Consultant summers 1987, 1988. During the summer 1987, interaction with Randall LeVeque and David M. Young at ICASE resulted in the paper on the 9-pt SOR results for the Laplacian (see Papers). Maria Elizabeth Ong also visited ICASE during the summer of 1987 and consulted with

Anne Greenbaum and David Young concerning preconditioners for conjugate gradient methods. She also interacted with Tom Crockett (of ICASE) concerning the Flexible-32 parallel machine. While there, she completed her parallel implementation of the hierarchical basis preconditioner.

Lawrence Livermore National Laboratory: Maria Elizabeth G. Ong and Loyce Adams visited in August 1988 to consult with Steven Ashby on polynominal preconditioning. Ms. Ong gave a seminar on hierarchical basis preconditioners. Steven Ashby visited the University of Washington in October 1988 to continue the collaboration.

Boeing, Seattle, WA: We have strong collaboration with David P. Young at Boeing. His group is interested in incorporating some of our ideas about preconditioning into their TRANAIR code. Maria Elizabeth G. Ong spent six weeks at Boeing the summer of 1988 working with David P. Young's group. While there, she completed the 3D implementation of her preconditioner on the Boeing Cray and investigated the feasibility of incorporating these ideas into TRANAIR.

Boeing, Seattle, WA: Joseph Manke, a Ph.D student, is also a Boeing engineer working on a numerical grid generation package for use at Boeing. His Ph.D. thesis is concerned with a multi-block approach to grid generation around both commercial and fighter aircraft. He recently completed his Ph.D. The hope is that his ideas will be used in Boeing's grid generation packages.

Other Collaborations

Prof. Adams and her students Maria Elizabeth Ong and Kevin Gates have had ongoing collaboration with the parallel programming research in the Computer Science Department at the University of Washington headed by Prof. Larry Snyder and Prof. David Notkin and Prof. Loyce Adams. Ms. Ong has investigated additive type preconditioners using the Poker system. Mr. Gates has been actively involved in parallel language design issues. He has implemented various codes in the Poker language (of Snyder) and has recommended changes to the language from the viewpoint of an applications programmer. This collaboration has given us an opportunity to use parallel systems developed on campus and to provide input to the next language design to be tackled by the computer science group.

Prof. Adams spent March 1989-July 1989 on leave to the Computer Science Department at ETH, Zürich, Switzerland. While there she taught a graduate class on parallel algorithms and collaborated with Dr. Peter Arbenz and Prof. Walter Gander on eigenvalue solvers for parallel machines.

Dr. Anne Greenbaum visited Seattle to discuss hierarchical basis preconditioners with Prof. Adams and Maria Elizabeth Ong.

Maria Elizabeth Ong visited Prof. Andy Wathen in Bristol, England to discuss finite element type preconditioners.

Maria Elizabeth Ong visited Prof. Nancy Nichols in Reading, England to discuss iterative methods.