DOE/ER/25048--4

DE92 014236

PARALLEL SUPERCOMPUTING: ADVANCED METHODS, ALGORITHMS AND SOFTWARE FOR LARGE-SCALE PROBLEMS

Progress Report

April 1991 - April 1992

Graham F. Carey
Aerospace Engineering and
Engineering Mechanics Department

and

David M. Young
Center for Numerical Analysis
The University of Texas at Austin
Austin, TX 78712

April 1992

PREPARED FOR THE U.S. DEPARTMENT OF ENERGY
UNDER GRANT NUMBER DE-FG05-87ER25048

Progress Report

Research has continued with excellent progress and new results on methodology and algorithms. We have also made supporting benchmark application studies on representative parallel computing architectures. Results from these research studies have been reported at scientific meetings, as technical reports and as journal publications. A list of pertinent presentations and publications is attached.

The work on parallel element-by-element techniques and domain decomposition schemes has developed well. In particular, we have focussed on the use of finite element spectral methods (or high p methods) on distributed massively parallel systems. The approach has been implemented in a prototype finite element program for solution of coupled Navier Stokes flow and transport processes. This class of problems is of fundamental interest and basic to many "grand challenge" type problems for which parallel supercomputing is warranted.

The underlying solution scheme is based on biconjugate gradient iteration. Various preconditioning strategies are being studied since these are crucial to efficient iterative solution. We have made performance comparison studies for several preconditioners. The main challenge is to develop an effective preconditioner which does not degrade the parallelism in the computation. We have developed several new preconditioners that appear quite useful. Several of these results are described in some detail in Carey and Barragy (1991). Recently, we have expanded the theoretical work to examine broad questions associated with scalability for parallel domain decomposition techniques. The basic problem was an investigation of domain decomposition for finite element analysis over a network of workstations. The new ideas developed here include the complexity analysis and measures of scalability and insufficiency. This project was conducted jointly with researchers at the Microelectronics and Computer Consortium (MCC). Technical details are given in a forthcoming paper (Carey et al, 1992). We have also carried out scalability studies for the parallel high p schemes and made performance studies on the NCUBE at Sandia (Barragy et al, 1992). This is part of a collaborative research activity with the Parallel Applications Group at Sandia. One of our PhD students (Alan Stagg) is interning at Sandia and working with Doug Cline on parallel parabolized Navier Stokes computations on the NCUBE. We have obtained impressive results.

A new class of GMRES schemes has been developed and their parallel implementation described (Joubert and Carey, 1991). We have also been working intensively on parallel iterative algorithms for nonsymmetric systems. Of particular interest are parallel non-symmetric libraries for the CM2. Performance studies have been carried

out for sparse systems arising from linear elliptic PDE's. We have also extended this treatment to a class of nonlinear PDE's using successive approximation for iterative linearization. Results from this study were presented at the SIAM meeting in fall 1991 and are now being submitted to the Journal of Supercomputing. Several other presentations dealing with new contributions are listed in the attachments.

Work is continuing on the development of improved iterative methods for solving large sparse linear systems where the matrices involved are nonsymmetric and/or indefinite. For such problems, numerical procedures often suffer from some or all of the following: large and irregular oscillations of the residuals; very slow convergence or stagnation; breakdown; excessive computational and memory requirements. Some of our recent work on nonsymmetric systems is described in the reports and papers [JeYo91], [Jo91], [JoCa91], [JoHiCa91], [JoMa91], [JoMaPaWo90], and [JoOp91].

There is currently a considerable amount of interest and activity on nonsymmetric systems. There have been numerous talks given at recent meetings including a Workshop at the University of Minnesota in September 1991 and February 1992 as well as a conference at Copper Mountain, Colorado in April 1992. In January, we organized a Workshop on nonsymmetric systems here in Austin. Among the attendees were Dr. Roland Freund, Dr. Martin Gutknecht and Dr. Bernd Fischer. Also Dr. Gerhard Starke of the University of Karlsruhe, another expert in the field, visited the University of Texas at Austin in April 1992.

Dr. Young and Mr. Vona have continued their work on the development of rapidly convergent iterative methods that are suitable for vector and parallel computers. One class of methods being studied is based on parallel multigrid procedures, which were introduced by Frederickson and McBryan. Substantial progress has been made, as described in [YoVo90] and in Mr. Vona's doctoral dissertation, is nearing completion. (Dr. Paul Frederickson, one of the inventors of parallel multigrid methods is now officially a member of Mr. Vona's Doctoral Committee). Another class of methods being considered involved the use of rational iteration methods that are based on implicit methods for solving time dependent problems. A preliminary report on this work has been completed; see [YoVo92].

Drs. Kincaid and Young have continued to work on stationary second-degree methods for solving large, sparse linear systems. Such methods do not require the calculation of inner products for each iteration and thus have potential advantages for parallel computers, over the more commonly used conjugate gradient methods. The work accomplished to date is described in [KiYo91], [KiYo92], [YoKi90] and [YoKi92].

Dr. Kincaid continued to work on the vectorization and parallelization of ITPACKV 2D. This resulted in a number of publications [KiOp90], [KiRa91], and [RaKi92]. The Cray Y-MP was used for the parallelization studies.

Dr. Kincaid also worked with a Master's student (Santiago) to improve the performance of an underwater sound model on a parallel computer by using cyclic reduction [SaKi91].

Drs. David Kincaid and Ward Cheney published an advanced textbook, Numerical Analysis: Mathematics of Scientific Computing [KiCh90], which presents a scholarly treatment of the subject.

DOE Sponsored Research

Recent Publications and Presentations

(*Reprint or Preprint Enclosed)

G. F. Carey

Journal Publications

*Barragy, E. and G. F. Carey, Parallel-Vector Computation with High-p Element-by-Element Methods, *International Journal of Computer Mathematics*, In Press 1992.

*Bova, S. and G. F. Carey, Parallel Grid Generation/Optimization Using Block Domain Decomposition, *Communications in Applied Numerical Methods*, In Press 1992.

*Barragy, E. and G. F. Carey, Stream Function Vorticity Solution Using High Degrees (p) Finite Elements and Element-by-Element Techniques, *Communications in Applied Numerical Methods*, Submitted 1991.

*Joubert, W. and G. F. Carey, Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems, Part I: Theory and Part II: Parallel Implementation, *International Journal of Computer Mathematics*, In Press, 1992.

Books

Parallel Supercomputing: Methods, Algorithms and Applications, John Wiley and Sons, U.K., 1989.

Presentations

PCG/CM: A Package for the Iterative Solution of Large Sparse Linear Systems on the Connection Machine, Fifth SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25-27, 1991 (with W. Joubert and P. Highnam).

Asynchronous Nonlinear Iteration and Domain Decomposition, Fifth SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25-27, 1991 (with A. Stagg).

Invited Speaker, Supercomputers and Smart Algorithms, SSC Seminar, Superconducting Super Collider Laboratory, Dallas, TX, March 9, 1990.

Parallel Mesh Generation Optimization Using Domain Decomposition, A Parallel Circus at Stanford University, Stanford, CA, March 29, 1990 (with S. Bova).

Seminar, Directions in Finite Element Research, The University of Texas at San Antonio, April 16, 1990.

Element-by-Element Techniques, Texas Finite Element Circus, Rice University, Houston, TX, October 8, 1990.

Gigaflop Performance for Navier Stokes Computations on the YMP, Poster Display, London, England, October 1990 (with A. Lorber).

Seminar, Finite Element Research Involving Vector-Parallel h and p Methods, Northwestern University, Evanston, IL, October 25, 1990.

Parallel Finite Element Computations, MCC Workshop on Parallel Applications in CFD, Austin, TX, February 14, 1991.

Recent Progress in Finite Element Research and Parallel Computing, EG&G Idaho Inc., Idaho Falls, ID, March 15, 1991.

Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems, Fifth SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25-27, 1991 (with W. Joubert).

Supercomputing and Mathematical Modelling, Public lecture to student body and faculty of LBJ High School Science Academy, Austin, TX, April 12, 1991.

Some Research Topics in Computational Fluid Dynamics, Schlumberger, Tulsa, OK, April 25, 1991.

CRAY Lecture, "Vector-Parallel Supercomputing", Computational Techniques and Applications Conference (CTAC) '91, Adelaide, Australia.

Embedded Iterative Solution of Nonlinear PDE's on the Connection Machine, Fourth SIAM Conference on Applied Linear Algebra, University of Minnesota, Minneapolis, MN, September 11-14, 1991 (with W. Joubert).

Some Aspects of Domain Decomposition, Workshop on Iterative Methods for Nonsymmetric Problems, The University of Texas, Austin, TX, January 8, 1992.

Workshops/Shortcourses

Symposium/Workshop on CFD in Environmental and Manufacturing Problems, December 7-8, 1990, The University of Texas, Austin, TX.

Workshop on Methods and Algorithms, January 24, 1991, The University of Texas, Austin, TX.

Workshop on Iterative Methods for Nonsymmetric Problems, January 8, 1992, The University of Texas, Austin, TX, (with D. Young, D. Kincaid and W. Joubert).

D. M. Young and D. Kincaid

Conferences/Workshops

Drs. Young and Kincaid attended the *Fifth SIAM Conference on Parallel Computation* in Houston in March 1991. Dr. Kincaid presented a paper at one of the poster sessions. They also attended a *Workshop on Parallel Multigrid Methods and Domain Decomposition* which was held at the Center for Parallel Computation at Rice University. Dr. Young was the "distinguished speaker" for this meeting and gave the opening talk on "Parallel Multilevel, Rational Iteration and ADI Methods" [YoVo91].

Dr. Young was an invited participant and gave a talk at a conference in numerical linear algebra which was held at the Mathematics Institute in Oberwolfach, Germany, in April 1991.

Dr. Young was an invited speaker at a conference on numerical linear algebra held in DeKalb, Illinois, in June 1991. He gave a talk on "Stationary Second Degree Methods." He also visited Northern Illinois University and gave a talk on "Parallel Multilevel Methods."

Dr. Young attended the *NA-Day Conference* on May 11, 1991, at the University of Illinois and gave a talk on "Stationary Second-Degree Methods."

Dr. Young was a participant and gave a talk at the NSF sponsored *Workshop on Multigrid Methods* which was held at George Washington University in Washington, D.C., in June.

Dr. Young was an invited speaker at a conference on the *Numerical Solution of Partial Differential Equations* held at Harvard University in June in honor of the 80th birthday of Professor Garrett Birkhoff. A paper based on his talk will appear in the conference proceedings.

Dr. Kincaid organized a session on "Parallel/Vector Iterative Methods" at the *13th IMACS World Congress on Computation and Applied Mathematics*, Trinity College, Dublin, Ireland, during July 1991. He gave a talk on "Parallelizing ITPACKV 2D."

Dr. Kincaid visited the USSR Academy of Sciences, Department of Numerical Mathematics, Moscow, for a week during July and August 1991, and gave a talk on the "ITPACK Project."

Dr. Young visited the University of Tennessee, Knoxville in September 1991 and gave the *Robert Todd Gregory Memorial Lecture*. He also participated in a joint mini-conference organized by the University of Tennessee and Oak Ridge National Laboratory.

Dr. Kincaid presented a keynote address on "Stationary Second-Degree Iterative Methods and Recurrences" at the *IMACS International Symposium on Iterative Methods in Linear Algebra* in Brussels, Belgium, in April 1990. He also co-organized a session on "Parallel Methods with Dr. C. Wu of J. Kepler University, Vienna, Austria. Dr. Kincaid presented a talk in this session on "Parallelizing ITPACKV 2D for the Cray Y-MP."

Dr. Kincaid organized a mini-symposium on "Iterative Methods and Algorithms" for the *Second SIAM Conference on Linear Algebra in Signals, Systems and Control* in San Francisco in November 1990.

Drs. Young and Kincaid attended a *Workshop on Computational Fluid Dynamics (CFD)* in Austin in January 1991.

Drs. Young and Kincaid attended a *Parallel CFD Workshop* at the Micro-Computer and Electronic Corp. (MCC) in Austin in January 1991. They also attended a *Parallel Applications in the Oil Industry Workshop* at MCC in February 1991. At this workshop, they presented a joint talk on CNA software such as ITPACK and NSPCG and on their current research related to the topic of the workshop.

Drs. Young and Kincaid attended the *Second International Conference on Industrial and Applied Mathematics* in Washington, DC, in July 1991.

Publications

*[JeYo91]
Jea, Kang C., and Young, David M. [1991] "Commentaries on Three Papers of Cornelius Lanczos," Report CNA-252, Center for Numerical Analysis, University of Texas at Austin.

*[Jo91]
Joubert, Wayne D. [1991]. "Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations," to appear in *SIAM Journal of Matrix Analysis and Applications.*

*[JoCa91]
Joubert, Wayne D., and Carey, Graham F. [1991]. "Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems," (To appear in the Proceedings of the *Fifth SIAM Conference on Parallel Processing for Scientific Computing*, Houston, Texas.)

*[JoCa91]
Joubert, Wayne D., and Carey, Graham F. [1991]. "Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems. Part I: Theory, Part II: Parallel Implementation," May 1991, to appear in *International Journal of Computer Mathematics*, Gordon Breach publ., special issue on preconditioned conjugate gradient methods; also Report CNA-251, Center for Numerical Analysis, The University of Texas at Austin, May 1991.

*[JoHiCa91]
Joubert, Wayne D., Highman, Peter, and Carey, Graham F. [1991]. "PCG/CM: A Package for the Iterative Solution of Large Sparse Linear Systems on the Connection Machine," to appear in the *Proceedings on Parallel Processing for Scientific Computing*, Houston, Texas.

*[JoMa91]
Joubert, Wayne D., and Manteuffel, Thomas A. [1991]. "Iterative Methods for Nonsymmetric Linear Systems," appeared in *Iterative Methods for Linear Systems*, (David R. Kincaid and Linda J. Hayes, eds.), Academic Press, Boston, 149-171.

*[JoMaPaWo90]
Joubert, Wayne D., Manteuffel, Thomas A., Parter, Seymour V., and Wong, Sze-Ping [1990]. "Preconditioning Second-Order Elliptic Operators: Experiment and Theory," Proceedings of Copper Mountain Conference on Iterative Methods, April 1990; *SIAM Journal of Scientific and Statistical Computation.*, 13, 1, 259-288, 1992.

*[JoOp91]
Joubert, Wayne, and Oppe, Thomas C. [1991] "Improved SSOR and Incomplete Cholesky Solution of Linear Equations on Shared Memory and Distributed Memory Parallel Computers," Report CNA-253, Center for Numerical Analysis, University of Texas at Austin.

[KiCh90]
Kincaid, David and Cheney,Ward . Numerical Analysis: Mathematics of Scientific Computing, Brooks/Cole Publishing Co., Pacific Grove, CA 1990, 690 pages.

*[KiOp90]
Kincaid, David R. and Oppe, Thomas C. Recent vectorization and parallelization of {ITPACK}. In O. Axelsson and L.Y. Kolotilina, editors, Preconditioned Conjugate Gradient Methods, pages 58-78. Springer-Verlag, New York, 1990. Lecture Notes in Mathematics 1457.

*[KiRa91]

*Joubert, Wayne, and Graham F. Carey. "Embedded Iterative Solution of Nonlinear PDE's on the Connection Machine," (Submitted February 1992 to *International Journal for High Speed Computing).*

*Joubert, Wayne. "A Robust GMRES-Based Adaptive Polynomial Preconditioning Algorithm for Nonsymmetric Linear Systems," To be Submitted to *SIAM Journal on Matrix Analysis and Applications*, May 1992; Special issue for Second Copper Mountain Conference on Iterative Methods.

All papers removed and cycled separately —

DATE
FILMED
07/8/92