

DOE/ER/25048--79

FINAL REPORT

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

DOE NO. DE-FG05-87ER25048  
Period 8/1/87-7/31/94

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The focus of the subject DOE sponsored research concerns parallel methods, algorithms, and software for complex applications such as those in coupled fluid flow and heat transfer. The research has been directed principally toward the solution of large-scale PDE problems using iterative solvers for finite differences and finite elements on advanced computer architectures. This work embraces parallel domain decomposition, element-by-element, spectral, and multilevel schemes with adaptive parameter determination, rational iteration and related issues.

In addition to the fundamental questions related to developing new methods and mapping these to parallel computers, there are important software issues. Our group has played a significant role in the development of software both for iterative solvers and also for finite element codes. In particular, the ITPACK Project (Drs. Young and Kincaid) led to the development of several packages of iterative schemes and accelerators that are widely used in the scientific community. Recent vectorized versions of ITPACK and a derivative for nonsymmetric systems, NSPCG, have been used successfully by industry for device modeling, reservoir simulation, computational fluid dynamics and many other applications. We are extending the algorithms and software to parallel systems using the concept of iterative "kernels." This algorithm/software development was incorporated with "intelligent" finite difference and finite element schemes with adaptive refinement capabilities that permit the grid and solution to evolve concurrently.

Our research in computational fluid dynamics (CFD) led to sustained multi-Gigaflop performance rates for parallel-vector computations of realistic large scale applications (not computational kernels alone). The main application areas for these performance studies have been two-dimensional problems in CFD. In particular, we focused on Navier-Stokes problems (Dr. Carey) and on chemical-recovery-reservoir simulation (Dr. Sepehrnoori). The chemical flood simulator is based on our software UTCHEM, which now is being used extensively in the Petroleum industry and is being extended to a parallel distributed environment. In our prototype Navier-Stokes program NSFLO on the CRAY Y-MP, an artificial timestep scheme is developed for integration to a steady state using domain decomposition. This program is being extended to the C-90, KSQ and TERA architecture families. It will also be developed for our INTEL hypercube and similar configurations.

Over the course of this DOE sponsored research significant progress has been made. A report of the progression of the research follows and at the end of the report is a list of related publications and presentations over the entire grant period.

### *Phase 1*

This research project concerned finite element methods for partial differential equations and the solution of the discrete systems using iterative methods on advanced vector and parallel processors. This study embraced several aspects of the subject including: theoretical analysis and development of new methods, investigation of associated algorithms, strategies for mapping algorithms to vector and parallel architectures, and finally, applications to large scale partial differential equation problems such as those encountered in Navier-Stokes theory for viscous flow and in multi-phase multi-component flows for reservoir simulation.

### Finite Element Research

Finite element methods have evolved to become one of the dominant techniques for approximate solution of boundary and initial value problems in engineering and science. There has been a significant effort in developing associated finite element software for scientific computers. To date most of the effort has been directed towards scalar processors and in more recent years to vector computing. Part of the focus of the research concerned the development of finite element methods both for parallel and vector-parallel solution. Our studies were not limited to classical finite element methods alone but also included work on boundary element techniques. This particular aspect of the work was quite new.

Certain classes of problems permit a mathematical formulation as a boundary integral or surface integral equation, common examples being potential problems where the Green-Gauss identities can be applied to determine the governing integral equation. When such an integral formulation can be constructed, it is natural to develop a finite element formulation in this setting and this leads, in fact, to the boundary element method. The boundary of the domain is discretized as a union of finite elements and a piecewise polynomial approximation basis introduced on the boundary discretization. However, the test functions in the new boundary integral formulation correspond to the Green's function for the operator in question and hence the resulting system of equations is no longer sparse. That is, the boundary element method involves the discretization of only the boundary of the domain but leads to a full system of equations rather than the sparse systems that are normally encountered in finite element methods.

The boundary element system is then solved, usually by means of Gaussian elimination techniques since the system is full and non-symmetric. Both of these features have discouraged the use of iterative methods in the past. Since our work dealt with iterative techniques and vector and parallel algorithms we elected to explore the use of these

techniques for boundary element methods, previous perceptions of the problem notwithstanding. Accordingly, a boundary element program was developed and the ORTHOMIN strategy developed for the NSPCG iteration package in the Center for Numerical Analysis was incorporated as the system solver. Performance studies were made for boundary element discretizations of increasing size and the efficiency of the solution method compared with Gaussian elimination techniques. In particular, vectorized KJI and JKI Gaussian elimination techniques were utilized and the comparisons were made initially for uniprocessor vectorized calculations on the CRAY. In a later segment of the work this was expanded to include vector and parallel computations on the CRAY XMP 4-8. Numerical results on these performance studies were documented in a paper which was presented at the CRAY users conference in Minneapolis October, 1988. It transpires that the conditioning of the boundary element systems for the representative class of potential problems studied is relatively well behaved. As a consequence, the iterative ORTHOMIN method performs very effectively and is competitive with the special vectorized elimination techniques on grids that are as coarse as 32 boundary elements. For finer grids the performance of the iterative method is superior and the vector-parallel processing capabilities of the ORTHOMIN strategy can be exploited to significant advantage.

#### Navier Stokes Calculations

Returning to the more standard finite element techniques, we considered the use of accelerated gradient type iterative methods for Navier Stokes problems. Two formulations were in popular use -- the mixed finite element methods and the penalized formulations. Again the dominant solution techniques are based on Gaussian elimination and part of our objective was to assess the effectiveness again of the accelerated iterative methods in this context. Details of this study are given in the attached reprint of the paper by Carey, Wang and Joubert (1989). In this study we formulated both the mixed and penalty forms of the finite element method for viscous flow problems and developed associated finite element software.

This finite element program was then integrated with the iterative software developed by Young, Kincaid and associates in the Center for Numerical Analysis as part of this joint, interdisciplinary study. Consequently we were able to examine performance of a variety of accelerated iterative methods on this class of problems. Performance results were documented and comparison studies made. Some particular items of interest included the effect of the penalty parameter on the iterative performance and the influence of increasing asymmetry as the Reynolds number increases in the viscous flow problem.

Our results showed that the penalty method did in fact severely degrade the performance of iterative methods. This has led to a major open question in so far as the utility of these methods is concerned for this class of problems. The difficulty center about the use of a large penalty parameter to enforce the incompressibility constraint in the equations. The effect of this large parameter is to cause scaling and conditioning problems in the related discrete system of equations. Attempts to design an effective preconditioner for the penalized system were not successful. The standard Jacobi type preconditioning and various forms of incomplete factorization were applied but with very limited success. Despite this negative result, we were able to use Gaussian elimination to factor the linearized Stokes flow problem and then use this fully factored form for the nonlinear Navier Stokes problem. Using such a preconditioner removes the effect of the penalty parameter and allowed us to obtain efficient solutions to the nonlinear problem (which is of greater practical interest.) The work was extended to other types of generalized Newtonian flows including Bingham fluids and power law fluids such as those encountered in polymer processing.

#### Parallel Finite Element Methods

Our work on parallel processing continued concurrently with the above research. We focused primarily on the extension of our element-by-element techniques beyond the element-by-element conjugate gradient methods to nonsymmetric forms and in particular the biconjugate gradient (Lanczos method) and the conjugate gradient squared method. Both the BCG and CGS methods were implemented and were tested in our element-by-element solvers. The numerical experiments on the parallel element-by-element techniques were conducted on the Alliant FX-8 processor at Argonne Laboratory.

The parallel element-by-element solution scheme is described in the paper by Barragy and (1988). Of particular note here are the speed up curves in figures 2 through 5 which indicate that the element-by-element by conjugate gradient scheme for nonsymmetric problems produces almost linear speed up as the number of processors increases from 1 to 8 on the Alliant. Similar studies on the balance show inferior speed up for processors varying from 1 to 20. However, we made some other more recent calculations and obtained improved results, particularly for larger problems. The next step in this phase of the research was to utilize not only parallel scalar capabilities of the Alliant but also the parallel-vector combined schemes.

Several other theoretical and technical aspects were investigated in relation to the finite element and iterative work. For example, we developed some error estimates for nonlinear flows and a new class of least-squares finite element methods with

preconditioned conjugate gradient solution. The idea in the least-squares method is to cast the PDE as a first-order partial differential equation system and then use a least-squares residual formulation. One result of this approach is that the system of finite element equations is always symmetric, even if the original operator is not. This implies that conjugate gradient type iterative methods can be used successfully and one does not have to resort to the BCG and ORTHOMIN type of algorithm. However, effective preconditioning is important and in the paper we describe a very special class of preconditioners that proves effective in this formulation. Unfortunately, we are not able at this point to design similar preconditioners at the element level that can be utilized in the element-by-element parallel schemes.

As part of our work on applications to viscous flow and transport processes we considered analysis of a slow viscous flow with diffusion of a gas through a viscous fluid including reaction at a surface. The resulting equations are large, nonlinear, and amenable to both vector and parallel processing using the techniques developed here. We also conducted some work on moving grids for transport processes in reservoir engineering. Here the objective was to develop moving grid technology to better accommodate moving layers and fronts. This leads to a coupled system of ordinary differential equations for both the solution concentration variables at the nodes as well as the node point coordinates themselves. Part of the objective of this research study was to investigate techniques for decoupling the solution and coordinate variables so that integration of the semi-discrete system could be accomplished more efficiently. We are interested in the application of variable order-variable step methods to both the coupled and uncoupled form of the moving finite element system. One of the next steps in the research program was the extension of the element-by-element techniques to explicit and implicit time dependent integrators. This allows us to carry our vector and parallel capability across to semi discrete systems and classes of problems such as the moving grid example mentioned.

To summarize, in the first phase of the research, Dr. Carey's research focused on several fundamental issues. Of significance is the work on convection-dominated transport processes. These problems lead to highly non-symmetric algebraic systems which are not successfully treated with most standard iterative methods. To address this Drs. Carey and McLay and graduate students investigated BCG (Lanczos) and CGS (Conjugate Gradient Squares) schemes applied to our finite element formulations. Both standard Galerkin and also streamline upwind Petrov Galerkin schemes were investigated. This algorithm work is being developed for use in conjunction with our domain decomposition techniques on parallel shared-memory multiprocessors. We also investigated the use of gradient-type iterative methods for Navier-Stokes problems.



### Iterative Methods

Dr. Young, together with Dr. T. Z. Mai and Dr. C. Jea continued research on iterative algorithms for solving large sparse linear systems. The paper by Jea and Young (1988) concerning the effectiveness of adaptive parameters was accepted for publication. Two other papers concerning iterative algorithms for solving symmetric and nonsymmetric linear systems and the ITPACK 3A and 3B software packages appeared in technical journals. Dr. Mai and Dr. Young continued their research on composite adaptive procedures and on dual adaptive procedures. The work is described in Mai and Young (1988), respectively.

Dr. Young and Mr. Vona also worked on the development of various "high-level" methods for achieving parallelism for iterative methods and various approaches were described in a paper by Young. A number of promising procedures were described. These procedures were tested and refined.

Mr. Joubert, working with Dr. Young, continued to work on the development and testing of generalized conjugate gradient methods and related methods for solving nonsymmetric linear systems. Dr. Young and Mr. Joubert had intensive discussions with Dr. Tom Manteuffel about this problem area both at the University of Colorado at Denver and at the Los Alamos Scientific Laboratory.

A new computer package called NSPCG was completed by Tom Oppe and Wayne Joubert under the direction of Dr. David R. Kincaid. The package uses various acceleration techniques in conjunction with various preconditioners for solving large sparse linear systems by iterative methods. The package has accelerators for both symmetric and nonsymmetric systems. Moreover, a host of basic preconditioners are available including left-right-, and two-sided-preconditioners. Much of the code has been vectorized to work efficiently on supercomputers but has not been modified for use on shared or distributed memory parallel computers. This package is modular in nature so that almost any preconditioner may be used with any accelerator. Moreover, any preconditioner may be used with most all of the several allowable data storage formats. In addition, the package can be used in a matrix-free mode where the user supplies customized routines for performing all matrix operations. Testing of the package on application problems was done using several different problem test-beds such as sample reservoir simulation problems and systems derived from finite-element techniques.

Mr. Oppe, working with Dr. Kincaid, also did some preliminary studies on a parallel version of the conjugate gradient algorithm using various multitasking tools on the Cray X-MP/48 at Cray Research. (See the report by Oppe and Kincaid [1988a]). As an

extension of this report, similar tests were conducted on two parallel computers - the Sequent Balance (Computer Sciences Department, University of Texas at Austin) and the Alliant FX/8 (Parallel Computing Facility, Argonne National Laboratory). The parallel algorithm was used to solve a model partial differential equation on a simple region with various mesh sizes. In this report, speed-up factors are given, and the effects of bank conflicts on the Cray are noted.

As described in reports by Oppe and Kincaid [1987] and by Kincaid and Oppe [1988] an algorithm for computing in parallel the general LU-factorization of a matrix was presented. As special cases, one obtains the Doolittle, Crout, and Cholesky methods. This algorithm was implemented and tested on the Cray X-MP/48. This research led to the investigation by Oppe and Kincaid of several serial and parallel algorithms for computing the LU-factorization when L is unit lower triangular. Their report presented several numerical experiments and programming considerations to reduce bank conflicts on the Cray X-MP/48 parallel supercomputer. Speedup factors were given for the parallel algorithms. The two best algorithms tested in the paper performed at essentially the top speed of this supercomputer (817 million floating-point operations per second). It is felt that any further improvement would have to come from efforts to more delicately balance the four processors.

### RELATED ACTIVITIES

Alliant Acquisition. In July 1988 an Alliant Parallel/Vector processor was acquired by the Texas Institute for Computational Mechanics under an equipment grant from NSF to TICOM with additional support for the College of Engineering. Both Drs. Carey and Young are members of the Institute and we are now using the new facility which greatly facilitated our research. We were able to test algorithms and new ideas quickly.

Advanced Processing/Algorithm Symposium. A symposium dealing with algorithms and software for PDE's on advanced processors was organized by Dr. Carey at the Austin Capitol Marriott October 17,18.

Iterative Methods Conference. A conference on Iterative Methods was organized with support from DOE, AFOSR, and with the sponsorship of SIAM, CNA and the CFD Lab. Over 150 attendees from the US and overseas participated in the 3-day conference which was organized to honor Dr. Young's 65th birthday and longstanding contributions to this field.

### *Phase 2*

Several research issues were addressed in this phase of the research and are described in some detail in the attached papers. Part of the work was directed to the use of domain decomposition techniques on parallel processors. We considered both grid optimization and finite element solution strategies on subdomains. In the grid optimization research a Brackbill-Saltzman scheme is recast to a domain decomposition format using overlapping Schwarz subdomains. The local nonlinear elliptic problems defining the grid are solved in parallel using both shared memory and distributed architectures. Parallel efficiencies exceeding 90 percent are achieved in both configurations for representative test problems on realistic grids.

The approach was applied to a compressible flow problem with the mesh on the subdomains optimized to enhance grid orthogonality, smoothness and solution accuracy. Care must be taken in assigning the location of the interfaces to be in regions where the flow behavior is not changing dramatically since this can have some impact on the convergence of the Schwarz process. Since grid generation has become a major "bottle neck" and grid optimization may be computationally as intensive as flow solutions itself, there is a need for parallel algorithms in this area. Our work appears to be the first attempt to accomplish this.

We also presented some new results at the SIAM meeting on Parallel Algorithms in March 1991. In this work we used a spectral element domain decomposition with non-overlapping domains for nonlinear PDE solution. The nonlinear solution scheme utilizes a point relaxation SOR-Newton method previously studied by Carey and Krishnan (1981). This permits parallel asynchronous nonlinear iteration. Numerical experiments were carried out to examine the degradation in convergence associated with asynchronous updates in the nonlinear iteration on a shared-memory multiprocessor. The behavior of the scheme proved quite interesting and raised several theoretical questions related to the frequency of asynchronous updates when nonlinearities are present.

We pioneered the development of parallel element-by-element gradient solution schemes under the DOE support. This work attracted considerable attention since it is relatively straightforward to modify existing industrial software to exploit the main ideas. eg. We assisted colleagues at SANDIA and worked with EG&G and the USGS on using the approach in their analyses. The key idea was to use individual elements or groups of elements and parallelize the matrix-vector products and dot products over the elements. This implies that the global matrix need not be assembled and that parallelization is achieved very naturally within the framework of a standard finite element code.

Our work described in Barragy and Carey (1992) was directed to the use of this approach for high-degree ( $p$  or spectral) elements. Parallelization and good speedup is

achieved and demonstrated for typical problems. There are several important theoretical issues related to parallel preconditioning that we explored. The method was not only applied to standard model problems but, more importantly, to representative Navier Stokes problems.

Dr. Young and Mr. Vona worked on the development of special preconditioners, based on parallel multigrid methods developed by Frederickson and McBryan and other multilevel methods, for speeding up the convergence of iterative methods. One aspect of this work was the development of procedures for constructing polynomials satisfying certain weighted minimization properties. It was found that in many cases these polynomials can be accurately determined using three-term recurrence relations such as are satisfied by Chebyshev polynomials.

While iterative methods for solving linear systems with symmetric and positive definite coefficient matrices are fairly well understood, this is by no means the case for systems where the matrix of the systems is nonsymmetric and/or indefinite. Although such systems are becoming increasingly more important; nevertheless, it often appears that the choice of iterative method to be used in a given case is based more on "art" than "science". In his Ph.D. dissertation, Wayne Joubert obtained a number of important results in this difficult area concerning generalized conjugate gradient methods and Lanczos-type methods.

Dr. Kincaid and Dr. Young worked on stationary second-degree methods for large sparse linear systems. Two reports (Young and Kincaid, 1990) and (Kincaid and Young, 91) were completed.

Tom Oppe finished his Ph.D. work in 1990 and wrote a dissertation concerned with optimization of iterative methods for solving large sparse linear systems using vector supercomputers. An optimization technique proposed involves the use of a standardized set of computational kernels that are common to many iterative methods. These kernels are called "Iterative BLAS".

Oppe and Joubert working with Drs. Young and Kincaid wrote a new computer package employing new sparse matrix storage formats for solving sparse matrix problems on vector computers. This package uses many iterative BLAS constructs in the vectorization of iterative algorithms. Oppe's work has shown that the NSPCG package can be a useful tool for the evaluation of iterative methods on vector computers.

### *Phase 3*

Research continued with excellent progress and new results on methodology and algorithms. We also made supporting benchmark application studies on representative parallel computing architectures. Results from these research studies were reported at scientific meetings, as technical reports and as journal publications.

The work on parallel element-by-element techniques and domain decomposition schemes developed well. In particular, we focussed on the use of finite element spectral methods (or high  $p$  methods) on distributed massively parallel systems. The approach was 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 were studied since these are crucial to efficient iterative solution. We made performance comparison studies for several preconditioners. The main challenge was to develop an effective preconditioner which did not degrade the parallelism in the computation. We developed several new preconditioners that were quite useful. We also 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). We also carried out scalability studies for the parallel high  $p$  schemes and made performance studies on the NCUBE at Sandia (Barragy et al, 1993). This was part of a collaborative research activity with the Parallel Applications Group at Sandia. One of our PhD students (Alan Stagg) interned at Sandia and worked with Doug Cline on parallel parabolized Navier Stokes computations on the NCUBE. We obtained impressive results.

A new class of GMRES schemes was developed and their parallel implementation described (Joubert 1992). We also worked intensively on parallel iterative algorithms for nonsymmetric systems. Of particular interest were parallel non-symmetric libraries for the CM2. Performance studies were carried out for sparse systems arising from linear elliptic PDE's. We 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 were submitted to the Journal of Supercomputing. Several other presentations dealing with new contributions are listed in the attachments.

Work continued 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. Our work on nonsymmetric systems is described in various reports and papers.

Dr. Young and Mr. Vona continued their work on the development of rapidly convergent iterative methods that are suitable for vector and parallel computers. One class of methods studied is based on parallel multigrid procedures, which were introduced by Frederickson and McBryan. Another class of methods considered involved the use of rational iteration methods that are based on implicit methods for solving time dependent problems.

Drs. Kincaid and Young 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.

Dr. Kincaid continued to work on the vectorization and parallelization of ITPACKV 2D. 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.

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

#### *Phase 4*

The principal objectives of this research project concerned parallel distributed solution of partial differential equations using iterative techniques. The work embraced basic research on discretization strategies, finite element methods, gradient solution, non-symmetric problems, and complex large-scale applications. Some of the applications to three dimensional coupled fluid flow and transport problems can be regarded as "grand challenge applications."

This project concerned several issues that are directly related to the DOE mission and involves close interaction with several DOE Laboratories. The basic thrust of the research effort was directed to the national need to develop improved methods and algorithms on parallel computers. PDE applications to fluid flow and coupled transport processes were of the greatest concern to DOE in relation to fossil fuel and other energy

sources such as nuclear, solar, and geothermal energy. These applications also include contaminant transport problems in Waste Processing. They are relevant to many industrial technology and process problems in, for instance, casting and forming. Finally, the methodology and algorithms developed here are important to the success of more complex environmental models for studies of global warming, acid rain and industrial pollution.

Our research in the areas of finite elements and iterative techniques spans a considerable period. Under the support of DOE our activities were focused on large scale transport processes and on parallel methodology and algorithms. This interest led us to explore domain decomposition, element-by-element, multigrid and other schemes which lend themselves to the "divide and conquer" parallel philosophy. Consequently, we produced new theoretical results, and developed and implemented new algorithms to meet the goal of efficient parallel PDE solution. Our algorithms and software are being applied to Navier-Stokes problems and to other coupled fluid flow and transport applications at The University of Texas at Austin, Sandia and elsewhere in the U.S. Earlier iterative software from the ITPACK series is widely distributed in the U.S. and used by DOE Laboratories and contractors. This software has been extended to parallel architectures.

An important part of the work concerned "divide and conquer" parallel strategies. We made several advances with parallel element by element and domain decompositions techniques. This work will continue to be a major focal area. We also made benchmark studies for PDE applications on representative parallel architectures. Several calculations were made on the NCUBE and CM2 distributed processor systems. Work on the INTEL distributed system was begun and was accelerated by a hardware grant from INTEL. Other new and future systems such as the KS and TERA (currently a paper design only), and MOSAIC (only currently integer arithmetic) are of interest and may feature in future work. We developed and applied high-order ( $p$ ) (spectral) finite element methods for distributed parallel architectures. The approach was implemented in a prototype finite element program for solution of Navier-Stokes equations. Other block iterative strategies were studied for 3-D parabolized Navier-Stokes calculations. Software was developed for the NCUBE and DELTA machines. Performance studies and more extensive testing and refinement are planned. We also developed a new variant of the GMRES scheme for parallel systems and are carried out theoretical work on parallel preconditioners for the finite element iteration schemes. Work continued on parallel multilevel theory and algorithms.

Central to the research effort was the development of robust, fast parallel iterative methods for sparse systems obtained from finite difference or finite element discretizations. Of particular interests are gradient type iterative schemes for non-symmetric systems arising from transport equations. Applications described by such PDEs are pervasive through all

areas of engineering and applied science of interest to DOE such as viscous flow and heat transfer in heat exchangers, enhanced oil and gas recovery, nuclear power technology, and global warming.

Part of our work involved the development of improved parallel preconditioning schemes. We made comparison studies of several block preconditioners. Future work will consider optimal hierarchic preconditioners and is directed to parallel versions of the schemes. We will also continue our work on adaptive mesh refinement schemes and adaptive subdomain annealing schemes to maintain good load balance in parallel distributed systems. The work on parallel p schemes will be expanded to p-redistribution whereby the grid topology is invariance but clustering is permitted to accommodate singularities which might otherwise destroy the validity of the approximation.

An important part of our DOE research involves the development of new sparse iterative schemes for non-symmetric and indefinite systems. For such problems, numerical procedures often suffer from one or more of the following: large and irregular oscillations of the residuals; very slow convergence or stagnation; breakdown; and excessive computational or memory requirements.

Work continued on stationary second-degree methods for solving large sparse linear systems. These methods do not require the calculation of inner products for each iteration and therefore offer certain advantages over other iterative schemes on distributed parallel systems. Cyclic reduction schemes were also studied. We developed a new class of GMRES schemes and continued to explore their parallel implementation and limitations. Progress was made on the extension of parallel multi-grid procedures of the type introduced by Frederickson and McBryan. Another class of methods under development involves the use of rational iteration schemes that are based on implicit methods for solving time-dependent problems. We also developed and analyzed dual methods that can be used for parallel time-accurate solution of evolution PDEs or used as iterative methods for solution of the associated equilibrium PDE.

An example illustrating the importance of the work is Navier-Stokes flow with heat transfer. We set up a benchmark application using the above methods for flow through a cascade system with heat transfer. This study was relevant to heat exchanger design as well as other important application areas such as microelectronics cooling. For example, new experimental sub-micron devices were fabricated and the thermal management problem identified as a major design issue.

Applications to enhanced oil and gas recovery will also be impacted by the research. Currently, the petroleum industry and aerospace industries are the main users and industrial purchasers of supercomputing hardware. It is well known that a large fraction of US oil is



not recoverable by primary production techniques. (Moreover, approximately 800,000 wells have been drilled in the US and current oil output is of the same order as approximately 8000 wells in Saudi Arabia). Our technology has an important role to play in this industry. Hence, the methods, algorithms and software developed under this research project are of significant importance to DOE and US industry. Our interaction with DOE laboratories and with industry confirm this view.

Major recent accomplishments:

As indicated in the previous sections, we have made several important contributions. For example:

1. New parallel iterative schemes and algorithms have been developed
2. Some of the methods have been implemented on parallel distributed machines for the first time.
3. The complexity and scalability of the algorithms is being analyzed
4. New parallel preconditioning techniques have been developed and are being tested.
5. The methods and algorithms are being applied and tested in complex and large scale transport applications such as the coupled viscous flow and heat transfer problem.
6. Some prototype software on the NCUBE and CM has been developed. The NCUBE software is being moved towards a "semi-production" environment by Doug Cline at Sandia (for experienced users).
7. Work was carried out on the development of iterative methods for solving large sparse nonsymmetric linear systems.
8. A new method, called MGMRES, which can be viewed as a generalization of GMRES, was developed for solving linear systems of the form  $Au=b$  for cases where a symmetric matrix  $Y$  is available such that  $Y$  and  $YA$  are symmetric (but not necessarily symmetric and positive definite.)
9. Work on parallel multigrid methods was carried out. It was demonstrated that certain non-periodic problems can be transformed into periodic problems to which parallel multigrid methods can be applied and analyzed.
10. Some of our work has focused on the use of computational kernels (iterative BLAS) for solving sparse linear systems.

## Related Publications and Presentations

(\* Reprints enclosed)

G. F. Carey

### Publications

- Carey, G. F. and S. S. Chow, "Well Singularities in Reservoir Simulation," *Journal for the Society of Petroleum Engineers*, 713-719, November 1987.
- Carey, G. F. and Peter C. Patton, "Toward Expert Systems in Finite-Element Analysis," *Communications in Applied Numerical Methods*, 3, 527-533, 1987. \*
- Murray, Paul and G. F. Carey, "Finite Element Analysis of Mass Transport Through a Viscous Fluid with Reaction," *Journal of Chemical Engineering Science*, 42, No. 12, 2833-2846, 1987.
- Carey, Graham F., Alan Mueller, Kamy Sepehrnoori and Richard L. Thrasher, "Moving Elements for Transport Processes," *Journal for the Society of Petroleum Engineers*, 401-408, August, 1987. \*
- Barragy, E and G. F. Carey, "A Partitioning Scheme and Iterative Solution for Sparse Bordered Systems," *Computer Methods in Applied Mechanics and Engineering*, 70, 321-327, 1988. \*
- Barragy, E. and G. F. Carey, "A Parallel Element-by-Element Solution Scheme," *International Journal of Numerical Methods in Engineering*, 26, 2367-2382, 1988. \*
- Barragy, E. and G. F. Carey, "Parallel Element-by-Element Grid Generation," *Proceedings Numerical Grid Generation in Computational Fluid Mechanics Conference*, December 5-8, 1988, Miami Beach, Florida.
- Carey, G. F., D. Kincaid, K. Sepehrnoori and D. Young, "Vector and Parallel Iterative Solution of Large Sparse Systems for PDE's," *Proceedings Fourth Science and Engineering Symposium*, pp. 25-43, October 12-14, 1988, Mendota Heights, MN.
- Carey, G. F., E. Barragy, R. McLay and M. Sharma, "Element-by-Element Vector and Parallel Computations," *Communications in Applied Numerical Methods*, 4, No. 3, 299-307, 1988. \*
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## Related Publications and Presentations

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G. F. Carey

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- Carey, G. F. and S. S. Chow, "Well Singularities in Reservoir Simulation," *Journal for the Society of Petroleum Engineers*, 713-719, November 1987.
- Carey, G. F. and Peter C. Patton, "Toward Expert Systems in Finite-Element Analysis," *Communications in Applied Numerical Methods*, 3, 527-533, 1987. \*
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- Carey, Graham F., Alan Mueller, Kamy Sepehrnoori and Richard L. Thrasher, "Moving Elements for Transport Processes," *Journal for the Society of Petroleum Engineers*, 401-408, August, 1987. \*
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- 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.
- Joubert, Wayne. "On the Convergence Behavior of the Restarted GMRES Algorithm for Solving Nonsymmetric Linear Systems," (Submitted January 1992 to Journal of Numerical Linear Algebra with Applications, special issue on Iterative Methods and Preconditioners for Nonsymmetric Linear Systems.
- Wu, H. M. and G. F. Carey, Non-Linear Convective Effects on Moving Boundary AC Plasma Arcs, *IEEE Transactions on Plasma Science*, Vol 20, No. 6, 1992. \*
- MacKinnon, R. and G. F. Carey, Moving-Grid Finite Element Modelling of Thermal Ablation and Consolidation in Porous Media, *International Journal for Numerical Methods in Engineering*, 36, 717-744, 1993.
- Davis, M. and G. F. Carey, Iterative Solution of the Stream Function-Vorticity Equations Using a Multigrid Solver with Finite Elements, *Communications in Applied Numerical Methods*, 9, 587-594, 1993.
- Barragy, E., G. F. Carey and R. Walters, Application of Conjugate Gradient Methods to Tidal Simulation, *Advances in Water Resources*, 16, 163-171, 1993.
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- Runnels, S. and G. F. Carey, A Domain Decomposition Strategy for Finite Element Simulation of Phase Change, *Numerical Heat Transfer, Part B*, Vol 24, No. 2, 181-189, 1993. \*
- Barragy, E. and G. F. Carey, Stream Function Vorticity Solution Using High Degrees (p) Finite Elements and Element-by-Element Techniques, *CNME*, 9, 387-395, 1993. \*
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- Barragy, E., Parallel Finite Element Methods and Iterative Solution Techniques for Viscous Incompressible Flows, PhD Dissertation, The University of Texas at Austin, 1993.
- Carey, G. F., A. Pehlivanov and P. S. Vassilevski, Least-Squares Mixed Finite Element for Non-Selfadjoint Elliptic Problems: II. Performance of Block-ILU Factorization Methods, CNA Report 267, May 1994.
- Joubert, Wayne, and Graham F. Carey. "Embedded Gradient Iterative Solution of Nonlinear PDE's on the Connection Machine," *International Journal for High Speed Computing*, 6, 2, 277-286, 1994. \*

- Carey, G., F., J. Schmidt, V. Singh and D. Yelton, A Prototype Scalable, Object-Oriented Finite Element Solver for Partial Differential Equations on Multicomputers, *J. of Parallel and Distributed Computing*, 20, 357-379, 1994.
- Abbasian, Reza O. and Graham F. Carey, Hybrid Iterative-MPE Schemes for Nonsymmetric Problems, *Num. Linear Algebra with Applications*, Submitted 1994.
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- Lorber, A. A. and G. F. Carey, A Vector-Parallel Scheme for Navier-Stokes Computations at Multi-Gigaflop Performance Rate, *IJNMF*, Submitted 1994.
- Pehlivanov, A., G. F. Carey and P. S. Vassilevski, Least-Squares Mixed Finite Element for Non-Selfadjoint Elliptic Problems: I. Error Estimates, CNA Report 271, July 1994.
- Rahman, M. and G. F. Carey, Modeling Separated Forced Convection in Laminar Flow Past Cavities, *Numerical Heat Transfer, Part A*, Vol 25, 85-101, 1994. \*
- Rahman, M. and G. F. Carey, Nonlinear Dynamics of Heat Transfer Enhancement using Eddy Promoters, *J. of Numerical Heat Transfer, Part A*, Vol 25, 117-133, 1994.
- Stagg, A.K., D.D. Cline, J.N. Shadid, and G. F. Carey, A Parallel Scalable Parabolized Navier-Stokes Solver for Large-Scale Simulations, *AIAA Journal*, In press, 1994.
- Wu, H., G. F. Carey and M. E. Oakes, Numerical Simulation of AC Plasma Arc Thermodynamics, *Journal of Comp. Phy.*, 112, No. 1, 24-30, 1994. \*

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- Carey, G. F., A. I. Pehlivanov and P. S. Vassilevski, Least-Squares Mixed Finite Element for Non-Selfadjoint Elliptic Problems: II. Performance of Block-ILU Factorization Methods, CNA Report 267, May 1994.
- Pehlivanov, A. I., G. F. Carey and R. D. Lazarov, Least-Squares Mixed Finite Element for Second Order Elliptic Problems, CNA Report 268, May 1994.
- Pehlivanov, A. I., G. F. Carey and P. S. Vassilevski, Least-Squares Mixed Finite Element for Non-Selfadjoint Elliptic Problems: I. Error Estimates, CNA Report 271, July 1994.
- Joubert, W. D., Y. Shen and S. Swift, Getting Started with PCG, CNA Report 273, November 1994.

### Books

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

### Presentations

- In August, 1987, Dr. Carey delivered the keynote lecture opening the CTAC Computational Techniques and Applications conference in Sydney, Australia. The lecture will appear in the bound conference proceedings.

Dr. Carey gave an invited lecture at Griffiths University, Brisbane Australia, August 9, 1997, on "Supercomputers in Finite Element Computations".

Dr. Carey presented a paper at the SIAM 1987 annual meeting, Oct. 12 - 15, 1987 in Denver dealing with the research on parallel solution using element-by-element techniques.

"Some Aspects of Adaptive Grid Computations," Presented at Symposium on Advances and Trends in Computational Structural Mechanics and Fluid Dynamics, Arlington, VA, October 17-19, 1988, (with M. Sharma, K. C. Wang and A. Pardhanani).

An invited lecture was given by Dr. Carey on Superconvergence and Element-by-Element Techniques at Rice University in Houston, April, 1988.

An invited seminar on recent advances in supercomputing and computational fluid dynamics was given to the Fluids group at the University of Texas at Austin, April 1988.

Dr. Carey gave the distinguished Massman lecture on advances on finite element methods and supercomputing at the University of Notre Dame on May 4, 1988.

Element-by-Element Parallel-Vector Schemes, Specialty Workshop on Methods and Algorithms for PDE's on Advanced Processors, U.T. Austin, October 17-18, 1988. Seminar, Adaptive Grid Refinement and Supercomputing, The University of Washington, Seattle, WA, October 27, 1988.

In February 1988, Dr. Carey taught a short course on computational aspects of finite elements that included adaptive grid strategies, element-by-element techniques and advanced processors.

"Semiconductor Device Simulation Using Adaptive Refinement and Streamline Upwinding," NUPAD II Workshop, May 1988, San Diego, CA, (with M. Sharma).

Vector and Parallel Iterative Solution of Large Sparse Systems for PDE's Fourth CRAY Science and Engineering Symposium, October, 1988, Mendota Heights, MN (with D. Kincaid, K. Sepehrnoori and D. Young).

"Parallel Element-by-Element Grid Generation," Presented at Numerical Grid Generation in Computational Fluid Mechanics Conference, Dec. 5-8, 1988, Miami Beach, FL, (with E. Barragy).

"Parallel-Vector Computation with High Degree Element-by-Element Methods," Presented at the SIAM Domain Decomposition Meeting, March 20-22, 1989, Houston, TX (with E. Barragy).

"Adaptive Grids and Supercomputing," Presented at the International Conference on Computational Techniques and Applications, Griffith University, Brisbane, Australia, July 10-12, 1989, (with E. Barragy, S. Bova, R. McLay, A. Pardhanani, and K. C. Wang).

"Material Process Modelling Using Adaptive Finite Elements and Supercomputers," Presented at the CRAY Research Conference on Manufacturing, Minneapolis, MN, Sept. 11-13, 1989, (with R. McLay, P. Murray and K. C. Wang).

Keynote Lecture, Parallel Vector Supercomputing and Adaptive Grid Computations, Conference on Computational Techniques and Applications, Griffith University, Brisbane, Australia, July 10-12, 1989.

Adaptive Grid and Element-by-Element Techniques with Applications to Supercomputing, EG&G, Idaho Falls, Idaho, September 13-15, 1989.

Research on Adaptive Grids and Parallel Computing, TICOM Workshop for Reliability in Computational Mechanics, October 26-28, 1989, Lakeway, TX.

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.

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.

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

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).

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).

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

CRAY Lecture, Computational Techniques and Applications Conference (CTAC) '91, Adelaide, Australia.

Invited Talk, Special session on 'Recent Progress and Applications of Finite Element Methods in Computational Fluid Dynamics' at the 4th International Symposium on Computational Fluid Dynamics, Livermore, CA, September 9-12, 1991.

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).

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.

Carey, G. F., R. McLay, D. Hu and Y. Shen, Transport, Sedimentation and Mixing, Workshop on Finite Element Modeling of Environmental Problems, March 4-5, 1994, Thompson Conference Center, Austin, TX.

Carey, G. F. and R. Abbasian, MPE-Iterative Methods for Solving Reaction-Diffusion Problems, Fifth SIAM Conf. on Applied Linear Algebra, Snowbird, Utah, June 15-18, 1994.

Lorber, A. and G. F. Carey, Time-Iterative Recursion with Domain Decomposition for Viscous Flows, IMACS Conference, July 11-15, 1994, Atlanta.

Joubert, W. and G. F. Carey, PCG: A Software Package for the Iterative Solution of Linear Systems on Scalar, Vector and Parallel Computers, Supercomputing '94, Nov. 14-18, 1994, Washington, DC.



Carey, G. F., R. McLay and S. Swift, Maximizing Sparse Matrix Vector Product Performances in MIMD Computers, Conf. on Iterative Methods, April 1-9, 1994, Breckenridge.

Lorber, A. and G. F. Carey, Multi-Gigaflop Performance for Navier Stokes Problems on Cray Supercomputers, Cray-Day, Cray Research Grant Program Recipients, May 10, 1994, Austin, TX.

#### Shortcourses and Workshops

Finite Elements in Fluids and Heat Transfer, October 30-November 1, 1990, Thompson Conference Center, The University of Texas, Austin, TX.

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

Symposium/Workshop on CFD in Environmental and Manufacturing Problems, December 7-8, 1990, 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).

Carey, G. F., Finite Elements in Fluids and Heat Transfer, October 18-20, 1993, Thompson Conference Center, University of Texas, Austin, TX. (with D. Gartling, Sandia).

Carey, G. F., Workshop on Finite Element Modeling of Environmental Problems, March 4-5, 1994, Thompson Conference Center, University of Texas, Austin, TX.

Carey, G. F., Grid Generation, Adaptive Refinement and Redistribution, May 2-4, 1994, Thompson Conference Center, University of Texas, Austin, TX.

Carey, G. F., D. M. Young, D. Kincaid, and W. Joubert, Workshop on Iterative Methods and Software, Breckenridge Iterative Conf., April 1994.

Publications

Adams, Loyce M., LeVeque, Randall J. and Young, David M. [1988], "Analysis of the SOR Method for the 9-point Laplacian," SIAM Journal of Numerical Analysis, 25, 1156-1180.

Carey, G.F., Kincaid, D.R., Sepehrnoori, K. and Young, D.M. [1988], "Vector and Parallel Iterative Solution of Large Sparse Systems for PDEs". (To appear in the Proceedings of the Cray Supercomputer Conference to be held in Minneapolis, Minnesota in October 1988.)

Jea, Kang C. and Young, David M. [1988]. "On the Effectiveness of Adaptive Chebyshev Acceleration for Solving Systems of Linear Equations", Report CNA-218, Center for Numerical Analysis, The University of Texas, Austin, Texas. (This paper will appear in a special issue of the Journal of Computational and Applied Mathematics.)\*

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Oppe, Thomas C., and Kincaid, David R., [1987c], "Parallel LU-Factorization Algorithms for Dense Matrices", Report CNA-213, Center for Numerical Analysis, The University of Texas, Austin, Texas. (To appear in Proceedings International Conference on Supercomputers, Athens, Greece, June, 1987). \*

Oppe, T.C. and Kincaid, D.R. [1987b]. "Numerical Experiments with a Parallel Conjugate Gradient Method" Advances in Computer Methods for Partial Differential Equations VI, (eds. R. Vichnevetsky and R.S. Stepleman), IMACS, Department of Computer Sciences, Rutgers University, New Brunswick, NJ, 1987, 369-374.

Oppe, Thomas C., Joubert, Wayne A., and Kincaid, David R. [1988]. "NSPCG User's Guide Version 1.0, A Package for Solving Large Sparse Linear Systems by Various Iterative Methods", Report CNA-216, Center for Numerical Analysis, The University of Texas, Austin, Texas.

Young, David M. [1988], "The Search for 'High-Level' Parallelism for the Solution of Large Sparse Linear Systems", Report CNA-221, Center for Numerical Analysis, The University of Texas, Austin, Texas. (To appear in the Proceedings of the Second International Conference on Vector and Parallel Computing, Tromso, Norway, June 6-10, 1988.)

Young, David M. [1987]. "A Historical Review of Iterative Methods", to appear in The Proceedings of the Conference on the History of Scientific and Numeric Computing, sponsored by the Association for Computing Machinery, Princeton, May 13-15, 1987. Also appeared as Report CNA-206, the Center for Numerical Analysis, The University of Texas at Austin, Austin, Texas.

Young, David M. [1988a], "A Historical Overview of Iterative Methods", Report CNA-225, Center for Numerical Analysis, The University of Texas, Austin, Texas. (To appear in the Proceedings of the Workshop on Practical Iterative Methods for Large-Scale Computations, held at the Minnesota Supercomputer Institute, University of Minnesota, Minneapolis, Minnesota, October 23-25, 1988.) \*

Young, David M., Jea, Kang C. and Mai, Tsun-zee [1988]. "Preconditioned Conjugate Gradient Algorithms and Software for Solving Large Sparse Linear Systems", Linear Algebra in Signals, Systems, and Controls, edited by B. N. Datta, SIAM, Philadelphia, PA, 1988.

Young, David M. and Mai, Tsun-zee [1988]. "Iterative Algorithms and Software for the Solution of Large Sparse Linear Systems", Communications in Applied Numerical Methods, 4, 435-456. Also appeared as Report CNA-215, Center for Numerical Analysis, The University of Texas at Austin, 1987. \*

Young, David M. and Mai, Tsun-Zee [1988a], "The Search for Omega", Report CNA-223, Center for Numerical Analysis, The University of Texas, Austin, Texas. (To appear in the Proceedings of the Conference on Iterative Methods for Large Linear Systems, held at The University of Texas, Austin, Texas, October 19-21, 1988.)

## D. M Young and D. Kincaid

### Publications (Cont.)

Joubert, Wayne D. [1990]. "Generalized Conjugate Gradient and Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations", Report CNA-228, Center for Numerical Analysis, The University of Texas at Austin. (Also Ph.D. Dissertation). \*

Joubert, Wayne D. [1990]. "Iterative Methods for the Solution of Nonsymmetric Systems of Linear Equations," Report CNA-242, Center for Numerical Analysis, The University of Texas at Austin.

Kincaid, David and Ward Cheney [1991]. "Numerical Analysis: The Mathematics of Scientific Computing", Brooks-Cole Publishing Co., Pacific Grove, CA.

Kincaid, David R. and Oppe, Thomas C. [1989]. "Recent Vectorization and Parallelization of ITPACKV," Report CNA-233, Center for Numerical Analysis, The University of Texas at Austin. \*

Kincaid, D.R. and Oppe, T.C., [1991]. "Recent Vectorization and Parallelization of ITPACK", *Preconditioned Conjugate Gradient Methods*, pp. 58-78, (O. Axelsson and L.Y. Kolotilnia, eds.), *Lecture Notes in Mathematics* 1457, Springer-Verlag, New York, NY.

Oppe, Thomas C., [1990], "The Iterative Solution of Large Sparse Linear Systems Using Vector Computers," Report CNA-241, Center for Numerical Analysis, The University of Texas at Austin. (Also Ph.D. Dissertation).

Young, David M. [1989], "The Search for "High Level" Parallelism for Iterative Sparse Linear System Solvers", Chapter 7 of *Parallel Supercomputing: Methods, Algorithms and Applications*, edited by Graham F. Carey, John Wiley and Sons, Ltd. \*

Young, David M. [1990], "A Historical Review of Iterative Methods", appeared in *A History of Scientific Computing*, edited by Stephen G. Nash, History Series, ACM Press, New York, 180-194.

Young, David M. and Mai, Tsun-zee [1990], "The Search for Omega", Chapter 17 of *Iterative Methods for Large Linear Systems*, edited by David R. Kincaid and Linda J. Hayes, Academic Press, Inc.

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. \*

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*.

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.)

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. \*

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.

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.

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.

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. \*

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Young, David M., and B. Vona, "Parallel Multilevel Methods," *Studies in Computer Science*, John Rice and Richard Demillo, ed., Plenum Press, New York, 1994. \*

CNA-Related Activities: Seminars, conferences, lectures

Dr. Young spent the Fall semester in Knoxville, Tennessee while on Sabbatical from The University of Texas at Austin. He was a Visiting Professor of Mathematics at the University of Tennessee (UTK) and a Visiting Scientist in the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL). The visit was made in connection with the Special Year in Numerical Linear Algebra that was held under the Science Alliance Program which is jointly supported by UTK and ORNL. Two advanced graduate students Mr. B. Vona and Mr. S. Xiao also spent the Fall Semester in Knoxville. Dr. Young, Mr. Vona and Mr. Xiao attended a short course on parallel computers with emphasis on the Sequent Balance and on the Intel Hypercube, which are operated by ORNL. The machines were used to solve large sparse linear systems derived from partial differential equations using iterative methods. Various schemes were used to achieve parallelism. The work is continuing. Arrangements have been made so that ORNL machines can be accessed from The University of Texas.

While visiting ORNL and UTK Dr. Young, along with Dr. Alan George of UTK/ORNL and Dr. James Ortega gave a Short Course on the numerical solution of systems of linear algebraic equations.

Dr. Young and Dr. Kincaid attended the 35th SIAM meeting in Denver, Colorado in October 12-15, 1987. A number of interesting papers were presented on numerical linear algebra and on parallel processing. On the day before the meeting, Drs. Young and Kincaid attended a Short Course on Parallel and Vector Computing. The instructors in the course included Robert Schnabel of the University of Wisconsin, Dr. Oliver McBryan of the University of Colorado at Boulder and Dr. Harry Jordan of the University of Colorado at Boulder.

Dr. Young attended the Tenth "Gatlinburg" Conference on Numerical Linear Algebra that was held at Fairfield Glades, Tennessee on October 19-23. The Gatlinburg conferences have been held roughly every 3 years since 1960. They are extremely valuable as a means of keeping up with the latest developments in the field of numerical linear algebra. At this meeting there was considerable emphasis on software and on vector and parallel computation.

Dr. Young gave a talk "Vector and Parallel Methods for Solving Partial Differentiated Equations at a Seminar at The University of Tennessee on November 23, 1987.

Dr. Young and Dr. Kincaid attended the "Third SIAM Conference on Parallel Processors for Scientific Computing" that was held in Los Angeles on December 1-4, 1987. A number of very interesting papers on the use of vector and parallel computing were presented.

Laboratory have begun a program of joint work on iterative algorithms for parallel computers such as the NCUBE and Intel Hypercube. Dr. Robert Benner of Sandia visited the CNA on three separate occasions (January 22-23, April 23, and October 21, 1987) to discuss this work. Tom Oppe visited Sandia February 22-23, 1988, and gave a talk on "Iterative Solution Methods on Vector and Parallel Computers."

Dr. Young and Dr. Kincaid attended the Short Course on "Matrix Eigenvalues and Singular Values," which was held in Knoxville in January 11-15, 1988. This course was given as part of the "Special Year on Numerical Linear Algebra" sponsored by the Oak Ridge National Laboratory and the University of Tennessee. The lecturers included Dr. Beresford Parlett, Dr. James Demmel, and Dr. Danny Sorensen.

Dr. David R. Kincaid attended a workshop on "Supercomputer Applications of Sparse Matrix Algorithms," which was held at Santa Cruz, California, March 27-30, 1988. He was one of the recording secretaries in a session on "Applications of Iterative Methods." Dr. Kincaid also made a short presentation during this session on current research (with Thomas C. Oppe) on developing parallel algorithms on the Cray X-MP4 Supercomputer" that will appear in the proceedings of this workshop.

Dr. Young and Mr. Joubert visited Dr. Tom Manteuffel at the University of Colorado in Denver to continue their collaboration on generalized conjugate gradient methods for solving large, sparse nonsymmetric systems. Mr. Joubert gave a talk, "Improving Orthomin-Like Iterative Methods for Solving Nonsymmetric Systems of Linear Equations."

Dr. Kincaid visited the People's Republic of China on May 16-29 and gave some lectures on iterative algorithms and software at Zhongshan University, Guangzhou; Guangxi Normal University, Guilin; Fudan University, Shanghai; Computing Center, Academia Sinica, Beijing; Nanjing Normal University and Nanjing University, Nanjing.

Dr. Young and Mr. Oppe attended the "Third SIAM Conference on Applied Linear Algebra," which was held in Madison, Wisconsin in May 1988. Mr. Oppe presented a paper with Dr. Kincaid and Mr. Joubert, "NSPCG-Nonsymmetric Preconditioned Conjugate Gradient Package".

Drs. Young and Kincaid attended the "Second International Conference on Vector and Parallel Computing," which was held in Tromsø, Norway in June 6 - 10, 1988. Dr. Young gave a talk, "The Search for 'High Level' Parallelism for the Iterative Solution of Large Sparse Linear Systems". Dr. Kincaid gave a talk "Numerical Experiments Using the NSPCG Computer Package." Following the conference, Drs. Young and Kincaid visited several institutions in the London area including Brunel University, The University of Reading, The University of Bristol, Oxford University and the Central Electric Co. Research Laboratory near London.



Dr. Kincaid organized a conference "Iterative Methods for Large Linear Systems" which was held in Austin in October 19-21, 1988. Dr. Young was an invited speaker and presented the paper by Young and Mai [1988a]. He was co-author of two other papers including Mai and Young [1988] and Jea and Young [1988]. Dr. Kincaid gave a talk on the status of the ITPACK Project.

Dr. Young was an invited speaker at the Workshop on "Practical Iterative Methods for Large Scale Computers" which was held in Minneapolis on October 23-25, 1988. He presented the paper Young [1988]. Dr. Kincaid gave a presentation on the NSPCG software package.

### CNA Related Activities (Cont.)

Dr. Young and Dr. Kincaid attended a conference that was held at Texas A & M University in March 1990 in honor of Professor George Lorentz. Dr. Young gave an invited talk "Applications of Approximation Theory to the Iterative Solution of Linear Systems." Dr. Kincaid gave a talk on "Recent Vectorization and Parallelization of ITPACK."

Dr. Young visited the Computer Science Department of Virginia Polytechnic Institute in March 1990 and gave two talks: "Iterative Algorithms and Software for Large Sparse Linear Systems" and "Parallel Multilevel Methods."

Dr. Young Dr. Kincaid attended the Parallel Circus that was held at Stanford University in March 1990. Dr. Kincaid gave a talk on "Recent Parallelization and Vectorization Research on Iterative Software and Algorithms."

Dr. Young and Dr. Kincaid served on the Organizing Committee for a Conference on Iterative Methods that was held at Copper Mountain, Colorado in April 1990. Dr. Young was scheduled to be an invited speaker but could not attend due to illness. His collaborator, Mr. Vona gave the talk, "Parallel Multilevel Methods." Dr. Kincaid gave a talk "Are There Sparse BLAS?" This talk was based on the joint work with Mr. Oppe, who also attended the conference and gave a talk on his dissertation research on sparse kernels. Mr. Joubert gave a talk "Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations." Dr. Kincaid helped organize a special evening session on "Standards for Sparse Matrix Software" and also gave a talk on sparse kernels.

In June 1990, Dr. Young visited Taiwan, ROC, and gave a series of three lectures at three universities. He gave a talk on "The Iterative Solution of Nonsymmetric Systems: An Art or a Science?" at the National Tsing Hua University in Hsinchu. He gave a talk "Iterative Algorithms and Software for Solving Large Linear Systems" at the National Cheng Chi University in Taipei. He gave a talk "Parallel Multilevel Methods" at the Fu Jen University in Taipei.

Dr. Young attended the Householder XI Conference on Numerical Linear Algebra that was held in Halmstad, Sweden, in June 1990. He organized a special evening session on "Multilevel Methods and Related Iterative Method" and gave a talk on "Parallel Multilevel Methods."

Dr. Young participated in a Workshop on Numerical Linear Algebra that was held at the Numerical Analysis Department at the Soviet Academy of Sciences in Moscow, USSR. He gave a talk on "Parallel Multilevel Methods."

Dr. Elizabeth Ong of the University of California at Los Angeles visited the Center for Numerical Analysis in July 1990, and gave a talk on "The 3D Linear Hierarchical Basis Preconditioner for Second Order Elliptic Problems."

Professor Cecilia Jea of the Fu Jen University in Taipei, Taiwan is visiting the Center for Numerical Analysis during the academic year 1990--91. She is working with Dr. Young on adaptive methods for choosing iteration parameters and on iterative methods for solving nonsymmetric linear systems.

Dr. Kincaid and Dr. Young visited the Center for Parallel Computation (RIACS) in

November 1990 and participated in discussions with Dr. Paul Frederickson and others concerning parallel computers and solving partial differential equations. Dr. Young gave a talk "Parallel Multilevel Methods."

Dr. Kincaid and Dr. Young attended the SIAM Conference on Systems, Signals, and Controls in San Francisco in November 1990. Dr. Kincaid organized a Minisymposium on "Iterative Methods and Algorithms." Dr. Kincaid presented a paper "Linear Stationary Second-Degree Methods for the Solution of Large Linear Systems."

Dr. Kincaid and Dr. Young attended the Supercomputing '90 Conference in New York in November 1990. They, along with Professor James Ortega of the University of Virginia, presented a tutorial "Iterative Methods: Basic Concepts and Recent Research Developments."

Dr. Kincaid gave a talk on "Numerical Mathematics and Computing: Software" at the AFIPS Workshop on Computational Science, University of North Carolina at Asheville, August 1990.

Dr. Kincaid presented a poster session on "Paralleling ITPACKV 2D for the Cray Y-MP" (joint work with M. Ramdas) at the SIAM Conference on Parallel Processing, Houston, TX, March 25-27, 1991. He also chaired a session on "Iterative Linear Algebra".

Dr. Kincaid gave an invited talk on "Stationary Second-Degree Iterative Methods and Recurrences" (joint work with Dr. Young) at the IMACS International Symposium on Iterative Methods in Linear Algebra, Brussels, Belgium, April 2-4, 1991. Dr. Kincaid and Dr. Wu co-organized and chaired a session with over a dozen papers on "Parallel and Vector Methods" for this conference. Dr. Kincaid presented a paper in this session on "Parallelizing ITPACKV 2D for the Cray Y-MP" (joint work with M. Ramdas).

Dr. Kincaid has organized a session on "Parallel Vector Iterative Methods" for the "13th IMACS World Congress on Computation and Applied Mathematics" to be held in Dublin, Ireland, July 22-26, 1991. He will speak on his current research during this session.

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".

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.

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