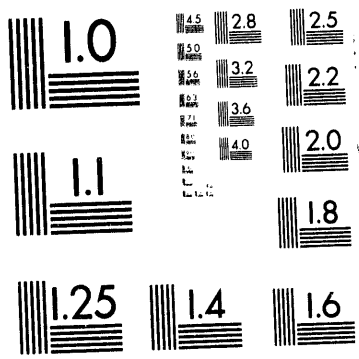
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PARALLEL SUPERCOMPUTING: ADVANCED METHODS, ALGORITHMS, AND SOFTWARE FOR LARGE-SCALE LINEAR AND NONLINEAR PROBLEMS

G.F. Carey, Director
Computational Fluid Dynamics Laboratory

D.M. Young, Director
Center for Numerical Analysis

DISCLAIMER

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1. SUMMARY

The program outlined here is directed to research on methods, algorithms, and software for distributed parallel supercomputers. Of particular interest are finite element methods and finite difference methods together with sparse iterative solution schemes for scientific and engineering computations of very large-scale systems. Both linear and nonlinear problems will be investigated. In the nonlinear case, applications with bifurcation to multiple solutions will be considered using continuation strategies. The parallelizable numerical methods of particular interest are a family of partitioning schemes embracing domain decomposition, element-by-element strategies, and multi-level techniques. The methods will be further developed incorporating parallel iterative solution algorithms with associated preconditioners in parallel computer software. The schemes will be implemented on distributed memory parallel architectures such as the CRAY MPP, Intel Paragon, the NCUBE3, and the Connection Machine. We will also consider other new architectures such as the Kendall-Square (KSQ) and proposed machines such as the TERA. The applications will focus on large-scale three-dimensional nonlinear flow and reservoir problems with strong convective transport contributions. These are legitimate grand challenge class computational fluid dynamics (CFD) problems of significant practical interest to DOE. The methods developed and algorithms will, however, be of wider interest.

The research will be led by Dr. G.F. Carey (Director, Computational Fluid Dynamics Laboratory) and Dr. D.M. Young (Director, Center for Numerical Analysis). Dr. Carey and Dr. Young are internationally known for their work on finite elements and iterative methods, respectively, and these topics are central to the proposed research. Dr. D. Kincaid (Computer Sciences), Dr. K. Sepehnoori (Petroleum Engineering) and Dr. R. McLay (Computational Mechanics) will participate as co-investigators in the research program. This program will also support graduate students and post-doctoral training in this rapidly evolving area. The research builds on our current efforts in developing methods, algorithms and software for advanced architectures. Large scale applications include, in particular, three dimensional Navier-Stokes calculations and reservoir simulation. We have received awards for our work on high performance computing and large-scale applications related to the proposed research. A list of related reports and publications are given later.

The research will be facilitated by a recent (1992) grant of an Intel distributed processor to Dr. Carey and other researchers at UT. We also anticipate that the UT Center for High Performance Computing which now has a CRAY-YMP will also acquire a distributed memory supercomputer during the proposed period of funding. The proposed research also receives support in the form of supercomputer access at several national facilities. In particular, we have been working closely with the Parallel Research Groups at Sandia and Los Alamos and have ongoing studies using the NCUBE and CM Machines at these sites.

2. OVERVIEW OF THE RESEARCH

2.1 Background and Motivation

Conventional serial computers are limited by certain factors such as the need to dissipate heat and the difficulty of fabricating sub-micron devices at significantly smaller scales. Short of major breakthroughs using radical new technologies (e.g., superconductors or optics), the traditional approach of miniaturization is reaching a point of diminishing returns. This, together with the economics of chip production, has led to the evolution of several parallel and parallel-vector architectures. These range from shared-memory supercomputers of coarse granularity (such as the CRAY Y-MP) to massively parallel distributed memory architectures (such as the Connection Machine, Intel Paragon, NCUBE and CRAY-MPP).

A major use of these advanced scientific computers is for the approximate solution of linear and nonlinear partial differential equations (PDE's) describing natural processes and

characterizing engineering design systems. Typically, the discretization process leads to large-scale computationally-intensive sparse linear and nonlinear algebraic systems. For realistic 3D applications of engineering and scientific interest, many of these problems are beyond the scope of conventional computer systems.

Hardware advances have attained the point where powerful parallel and vector-parallel computers are now emerging that can provide multi-Gigaflop speeds (billions of floating-point operations per second). However, the effective exploitation of these machines for science and engineering applications necessitates a radical change in the way we think about numerical methods and algorithms (e.g., see Young [1989]). So far, the rapid progress in hardware developments has understandably overshadowed research on parallel numerical methods, algorithms, and software. Promotion of basic research in these areas is essential; otherwise the realization of the full potential of these new hardware designs will be unnecessarily delayed. Moreover, scientific software for parallel architectures must be developed as soon as possible to accelerate transition of basic research discoveries to the user community. The present research is directed to these issues.

2.2 Research Objectives

The focus of the proposed research concerns parallel methods, algorithms, and software for complex applications such as those in coupled fluid flow and heat transfer. It is 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. Details are given in Section 3.

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 is to be incorporated with "intelligent" finite difference and finite element schemes with adaptive refinement capabilities that permit the grid and solution to evolve concurrently.

Our recent research in computational fluid dynamics (CFD) has 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 have focused on Navier-Stokes problems (Dr. Carey) and on chemical-recovery-reservoir simulation (Dr. Sepehrnoori). Three-dimensional applications will be central to the new work. 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.

Part of the work will focus on large scale three-dimensional applications and on massively parallel systems. With current systems capable of multi-Gigaflop performance, massively parallel systems may potentially deliver an order of magnitude improvement soon, and we are witnessing progress towards a Teraflop (a trillion floating-point operations per second) which will permit direct 3D Navier Stokes simulation, complex 3D simulation of natural processes such

as global warming, full integrated design of engineering systems (reactors, solar exchangers, etc.), and 3D multicomponent-multiphase reservoir and containment transport simulation.

2.3 Personnel and Personnel Organization

The research involves collaboration of principal investigators in Computer Sciences, Mathematics, and Computational Fluid Dynamics. The program will be coordinated by Dr. G.F. Carey, (Director, Computational Fluid Dynamics Laboratory), and Dr. D.M. Young, (Director, Center for Numerical Analysis), as principal investigators. Dr. K. Sepehrnoori (Petroleum Engineering) and Dr. D. Kincaid (Computer Sciences) will participate as co-investigators. Dr. Sepehrnoori is developing methods for 3-D reservoir simulation in enhanced oil recovery and Dr. Kincaid is developing iterative Basic Linear Algebra Subroutine (BLAS) kernels for transportable vector-parallel iterative software. Dr. R. McLay (TICOM) will be involved in 3D parallel finite element computations for viscous flow and heat transfer. This work will be carried out jointly with Dr. Carey for applications to manufacturing processes. A postdoctoral research fellow, as well as graduate research assistants, will also be supported. This support will allow us to continue our activities both on the algorithms and the software at a critical time in the development of this research area, since new and expanded hardware capabilities are becoming more widely available.

2.4 Interaction and Dissemination

During the past three years, we have conducted a joint seminar on "finite elements, iterative methods, and advanced computers" associated with our research program. This, together with regular discussion meetings between the investigators and graduate students, permits close coordination of our joint research. The investigators also jointly serve on related PhD committees and work closely with the graduate students on this research. A workshop on supercomputing was sponsored by us and held in Austin in conjunction with a conference on Iterative Methods honoring Dr. Young. These efforts have led to archival volumes and special journal issues related to the research. Dr. Young and Dr. Carey organized a workshop on Iterative Methods for Nonsymmetric Systems (Jan. 1992) in conjunction with the conference in Austin on Approximation Theory. A special journal issue on Multigrid methods co-edited by Drs. Carey and Mandel recently appeared (Dec. 1992). There is a close interaction with the parallel applications groups at Sandia and Los Alamos. Research contact with industrial associates also aids in dissemination of new material. Part of the proposed research dealing with manufacturing applications will be coordinated with Dr. David Gartling at Sandia.

3. DESCRIPTION OF THE RESEARCH

The focal points of the proposed research during the next three-year period involve parallel gradient-based solution strategies, parallel domain decomposition, parallel multilevel schemes, parallel local timestepping and asynchronous parallel strategies. Supporting software will be developed for both structured grids with finite differencing and unstructured grids for finite elements with parallel and parallel-vector iterative solution methods. Related issues involve some aspects of element-by-element and matrix-free methods, transient techniques and rational iteration, additive correction and nonsymmetric systems. Linear and nonlinear problems will be investigated. The research will primarily deal with distributed parallel-vector systems such as the Intel Paragon, NCUBE3, Connection Machine and CRAY MPP. However, other new parallel supercomputers such as the Kendall-Square (KSQ) Supercomputer and machines with data that "streams through memory" such as the proposed TERA will also be considered. Of particular interest are iterative methods, artificial transient techniques, nonsymmetric systems, and high p-spectral elements for linear and nonlinear three-dimensional applications. Consequently, we will be developing and applying new methods to 3D engineering applications of significant practical interest. These include 3D Navier Stokes, 3D reservoir simulation, 3D

contaminant transport for hazardous waste, and 3D flow and transport for industrial processes. Another component of the research is the development of parallel basic iterative "kernels" to facilitate a modular software design. Further details of the research program are given in the following subsections.

3.1 Domain decomposition techniques

Domain decomposition techniques are closely tied to the partitioning of the domain on which the PDE is defined. Subdomains may themselves consist of a large number of elements in the finite-element, finite volume, or finite-difference discretization. In a finite element analysis, the mathematical formulation is based on a weak integral statement of the PDE problem. If this is restructured over the subdomains, then "natural" interface jump conditions apply across the interior boundaries between subdomains. This restructuring of the mathematical problem supports several opportunities for developing accelerated parallel iterative algorithms over the subdomains. For example, large contiguous subdomains can be distributed to parallel processors in a "divide-and-conquer" strategy with block-iterative solution techniques introduced on the subdomains. The interface relation provides the connection between subdomain block iteration, block preconditioning strategies, and effective supercomputer techniques. Families of methods are being developed for both overlapping and non-overlapping parallel domain decomposition. In particular, some of our recent work on superconvergent flux post-processing (Carey et al 1992) is being reformulated to apply to the interfaces of the subdomain problems in the non-overlapping algorithm. This promises to yield faster convergence for both the serial and parallel schemes. Hierarchic imbeddings of grids can be exploited for both the domain decomposition schemes and the parallel multigrid methods, as described later.

We are developing parallel grid generation and optimization schemes based on domain decomposition. Grid generation for complex 2- and 3-dimensional domains has become a major "bottleneck" in large scale computations. At a meeting on grid generation, Paul Kutler of NASA Ames observed that "preparation of a good grid for large-scale shuttle-aerodynamic calculations requires a man-month or more" and that grid optimization calculations can rival the actual flow solution of the associated PDE's. We have developed an approach for local grid generation and optimization in a parallel system. By block iteration, an "optimal" local grid can be generated over the distributed processors and, moreover, the flow solution can be constructed concurrently with the grid. There are several open questions related to subdomain partitioning algorithms and load balance.

The present research will explore this domain decomposition work for distributed systems. We have access to the Connection machine at the Schlumberger Computer Research Group in Austin and at Los Alamos. Our collaborative work with the parallel applications group at Sandia is being coordinated with Dr. D. Cline (Sandia) who has been working with Dr. Carey and a graduate student (Alan Stagg) on parallel parabolized Navier Stokes computations for grand challenge applications on the NCUBE using domain decomposition. We plan to expand this activity to the Intel Paragon next year.

3.2 Spectral and hierarchic *p* schemes

Some of the proposed finite element research involves adaptive mesh and spectral elements - so called *"h"* and *"p"* methods. The standard finite-element error-estimates for regular problems have the form (Oden and Carey, 1985)

$$\|e\|_m \leq Ch^p \qquad (1)$$

where $C=C(p)$ and the rate p depends on the polynomial degree of the basis; e.g., $p=k-m$, where k is the polynomial degree. Here $\|.\|_m$ denotes the H^m norm and $e=u-u_h$ is the approximation error for a discretization with characteristic mesh size h. The error can be reduced by decreasing

h or increasing k (or both). Clearly, for regular problems, the error reduction is greater if the polynomial degree is increased ($C(p)$ also decreases as p increases). This idea is the basis for high-degree spectral elements. A second consequence is that the element matrices are larger and more dense. Hence fewer elements are needed per subdomain to achieve the same accuracy; e.g. in 3-D, a tensor-product basis of degree 7 generates 2^9 nodes per element for a scalar problem so the dense element matrices are of size $2^9 \times 2^9$ for the scalar field problem. For less regular problems, the power p in (1) is limited by the solution smoothness and increasing p will not improve the global asymptotic rate. Here both mesh grading and polynomial enrichment are used. This will complicate the data structure.

We can develop a hierarchic multilevel p scheme by introducing a hierarchic basis. In an hierarchic family, all lower-degree bases are nested as p increases. This implies that new element matrices can be constructed by simply adding a row and column border to the current (p-1) matrix. There are some interesting opportunities for economizing the element calculations that we also plan to pursue here. Moreover, the structure of the bordered submatrix systems can be exploited in associated gradient iterative schemes. Also note that the projection from the high level operator to lower levels simply involves removing rows and columns from the element matrices. We discuss this further in the treatment of element-by-element parallel schemes below.

3.3 Element-by-Element Parallel Strategies

In a previous phase of our work on subdomain techniques, we made an important breakthrough in the area of abstract domain decomposition techniques and iterative methods. This is in the form of an element-by-element scheme together with conjugate-gradient-like iterative solution of the finite element system for PDE problems. Indeed, these ideas are now becoming widely adopted for both serial and parallel computation. The essential idea in the element-by-element approach is to utilize the independent element calculations in the finite element approximation to parallelize the method. Moreover, appropriate iterative methods such as block-preconditioned conjugate gradient schemes can be recast at the element level to define a powerful new method in which much of the solution step can be parallelized. This method relies on the observation that conjugate-gradient-iterative methods involve repeated matrix-vector products and inner products. Rather than assembling the element contributions in the traditional fashion and then solving the merged sparse system, we write

$$\sum_{e=1}^{E} \hat{A}_e = \sum_{e=1}^{E} C_e^T A_e C_e \tag{2}$$

where C_e is the Boolean transformation defining a map between local element numbering and the global node system. Here e is the element index, A_e is the dense local element matrix and $\hat{A}_e$ is the element matrix expanded to global matrix system size. In the subsequent matrix-vector products of the gradient iterative method, we can write

$$v = Aw = \left(\sum_{e=1}^{E} \hat{A}_e \right) w = \left(\sum_{e=1}^{E} (C_e^T A_e C_e w) \right) = \sum_{e=1}^{E} C_e^T A_e w_e = \sum_{e=1}^{E} C_e^T v_e \tag{3}$$

It follows that the global matrix product can be carried out at the element level as $A_e w_e = v_e$, thus circumventing the usual matrix assembly step. More importantly, since the element contributions can be evaluated independently and in parallel, this implies that parallel and parallel-vector schemes can be developed from this framework in a natural and elegant manner. Further details are given in Carey [1993]. There are some important issues that arise in

connection with communication on distributed systems and memory conflicts on shared parallel systems that warrant further study. For example, the extraction operation $w_e = C_e w$ must distribute parts of the global vector to respective processors. Similarly, the residual accumulation of element vectors to a global vector requires special attention.

One of the key features of the element-by-element approach is the fact that it is posed on an element-based data structure rather than a node-based structure. This implies that irregular unstructured grids can be utilized that may employ elements of different types, e.g., singular elements can be used near a fracture tip, polynomial (spectral) elements in the main field and "infinite" elements in the far-field. The method, therefore, lends itself to general parallel utilization and can be applied in conjunction with adaptive refinement to highly unstructured grids. This is particularly important since the preceeding approach may be combined with adaptive grid refinement to provide more efficient solution schemes for large-scale 3D applications. In the adaptive refinement procedure, the solution is computed on a coarse grid, an *a posteriori* analysis permits construction of error indicators that locate regions where grid refinement is warranted, and then the grid cells in these regions are locally refined. The solution-refinement process is repeated until a desired accuracy is met.

The key ingredient here is the data structure that supports the refinement process. We have developed a scheme whereby quadrilateral or triangular elements are subdivided to quartets of sub-elements to generate a quadtree (Carey et al, 1988). The procedure can be extended to 3-D in the form of an octree data structure that is more complex and will be investigated as part of the proposed research. Since we are able to parallelize over elements in a block iterative solver, this implies that the scheme should be applicable to unstructured adaptive grids with little degradation in parallel performance. We also propose to extend this approach to nested (hierarchic) bases in which the polynomial degree is increased automatically to meet a desired solution accuracy. One of the main difficulties associated with p methods is the significant degradation in conditioning as the element degree is increased. This has led to renewed interest in the selection of basis functions and the development of element block preconditioners that utilize special bases. We are currently investigating basis transformation techniques as a mechanism for generating good preconditioners within the framework of the element-by-element spectral methods (Barragy and Carey, 1991).

3.4 Multilevel/Multigrid Decomposition

The need to treat 3D problems has also motivated some of our work on hierarchic elements and multilevel schemes. We propose to implement the multilevel strategy in conjunction with both the spectral element procedure (multi-p) and also develop a parallel hierarchic h scheme. In the hierarchic method, a macro element is repeatedly refined to produce a nested hierarchy of local refinements but, as in the p scheme, the h-basis is constructed in a hierarchy rather than in the usual Lagrange manner. This leads to a nesting of matrix families in which rows and columns are simply added as the mesh is refined or "turned off" as the mesh is coarsened. The hierarchic h-method can be utilized in a multigrid-multilevel algorithm and the effect of the multigrid projections is to achieve a preconditioning so that the number of iterations of the parallel solver is independent of the mesh size h. (Of course, the work per solve still scales with the matrix size so scalability is still an issue.) Most of our work to date has involved 2D model problems. In the proposed work, the emphasis will be on the 3D case. The extension from 2D to 3D is far from routine; e.g., in 2D a quadrilateral element has four edge neighbors and four vertex neighbors whereas a "quadrilateral brick" in 3D has 6 face neighbor elements, 12 edge neighbors and 8 vertex neighbors. The situation for unstructured 3D tetrahedral grids is more complex. This implies parallel communication will be a more significant issue in 3D.

Another difficulty with the 3D problem is that, even for single element subdomains, the memory requirements may be too demanding for some distributed systems. To circumvent this, we propose to develop and study element matrix-free schemes. That is, by using the tensor product structure of the finite element basis and the associated Gaussian quadrature, we are able to restructure the element calculations and the steps in the gradient iterative scheme to be less

demanding with respect to local memory requirements for the distributed system. These ideas can also be applied in the context of time-dependent techniques.

Parallel preconditioning accelerators will be developed and tested as part of the study. In the proposed research, we plan to continue this work in the context of spectral finite-elements and hierarchic h schemes with element-by-element domain decomposition as indicated previously. Additional work on transient methods has been initiated and is directed to both stable time-accurate methods and also stable steady solution (not time accurate). More details are given later.

3.5 Iterative Methods for Large Sparse Systems of Linear Algebraic Equations

At the core of many problems involving the solution of partial differential equations is the problem of solving multiple systems of linear algebraic equations. Typically, the coefficient matrices for such systems are very large and very sparse. Our research is concerned with the development of rapidly converging iterative methods which make maximum use of highly parallel computer architectures such as the Connection Machine, the Intel Paragon and the Cray MPP.

There are two levels of parallelism to be considered in designing algorithms and programs for highly parallel computer systems. At one level we have "low level" or fine grain parallelism which is needed to ensure that each individual iteration is carried out efficiently. To do this one must consider questions of sparse data structures and the efficient manipulation of vectors and sparse matrices. In addition to this there is a need to consider "high level" parallelism which involves designing the overall iterative algorithm to obtain rapid convergence and, at the same time, retaining the fine grain parallelism.

Many of the standard iterative methods parallelize well but their convergence rates often leave something to be desired. For example, the use of a basic iterative method, such as the Jacobi method, combined with Chebyshev acceleration or conjugate gradient acceleration typically requires on the order of $K(A)^{1/2}$ iterations, where $K(A)$ is the condition of the matrix of the linear system. (For a typical elliptic equation defined over a grid of size h, $(K(A))^{1/2}$ is in the order of h^{-1}.) On the other hand, the accelerated Jacobi method is highly parallelizable. With some basic iterative methods, such as the accelerated SSOR method, it is sometimes possible to get $O(h^{-1/2})$, convergence if one uses the "natural" ordering of the grid points. However, the use of that ordering degrades parallelism. If one uses the "red-black" ordering of the grid points instead of the natural ordering, the accelerated SSOR method is highly parallel but the number of iterations increases from $O(h^{-1/2})$ to $O(h^{-1})$.

For certain types of problems, including "separable" elliptic problems in two- and three-dimensions, one can often achieve convergence in $O(\log K(A))$, or $O(\log h^{-1})$ iterations by the use of alternating direction implicit methods (ADI methods). While the commutativity of certain matrices is required to rigorously guarantee the rapid convergence, the method actually works well in many cases where the commutativity does not hold. To carry out the method requires the solution of a large number of tridiagonal linear systems. However, the solution of these systems can be carried out in parallel. Unfortunately, the ADI method is less robust than many other methods and often does not work well for problems involving coefficients which are discontinuous or highly variable.

3.6 Adaptive Parameter Determination and Error Purification

Conjugate gradient acceleration leads to more rapid convergence than Chebyshev acceleration. However, with conjugate gradient acceleration several inner products must be evaluated for each iteration. This is a disadvantage with distributed memory computers since inner products involve communication between processors. On the other hand, Chebyshev acceleration, though not requiring inner products, does require the use of one or more iteration parameters which are related to the largest and smallest eigenvalues of the iteration matrix.

Procedures for finding those parameters use relatively elementary methods to estimate the extreme eigenvalues of the iteration matrix.

We propose to investigate the use of more sophisticated procedures for approximately determining extreme eigenvalues and other eigenvalues of the iteration matrix as well as some of the associated eigenvectors. The eigenvalues thus obtained can be used to change the iteration parameters to make the Chebyshev acceleration process converge more rapidly. In addition, the eigenvectors can be used to "purify" the approximate solution. Thus, if an eigenvector of the iteration matrix is known, the approximate solution of the linear system can be modified so that the component of the error with respect to that eigenvector is reduced or eliminated. The elimination of several such eigenvector components can result in a substantial speeding up of the iterative process. The procedure is expected to be particularly effective in the case of singular and nearly singular systems. It should be noted that the parameter estimation and purification procedures do not have to be synchronized with the main iteration procedure since the timing of the parameters changes and of the purification procedures is not critical. Moreover, Ritz values and vectors can be determined based on the set of Krylov vectors generated by the main iterative process and these can be used to carry out simultaneous purifications of the errors. It should also be noted, that eigenvalues and eigenvectors generated in the process of solving a given system can be saved and reused later to speed up the solution of related systems. This should be particularly useful in the solution of time dependent equations by implicit methods and for nonlinear problems solved using nonlinear successive approximation.

3.7 Parallel Multigrid Methods

Multigrid methods, when applied appropriately to linear systems arising from elliptic partial differential equations, often converge very rapidly. Frequently the number of cycles required is independent of the grid size h. Standard multigrid methods are not completely parallelizable since as one progressively considers coarser and coarser grids fewer points are involved and a point of diminishing parallel return is ultimately reached. Frederickson and McBryan [1991] considered the use of parallel multigrid methods where, at each coarse grid level, several coarse grids are used in parallel so that the total number of grid points used is the same for all levels. The advantages of this class of parallel multigrid methods include the fact that all processors are kept busy at all levels and that the problem of "aliasing", which frequently occurs with standard multigrid methods, is eliminated. Also, the analysis of parallel multigrid methods, at least for some model problems, is much simpler than for standard multigrid methods.

Dr. Vona and Mr. Xiao, together with Dr. Young have worked extensively with Dr. Frederickson on the analysis of the convergence properties of parallel multigrid methods and other multilevel methods in terms of the standard theory of iterative methods. (See Young and Vona [1990] and Vona [1992]). The focus of the work has been on the application of parallel multigrid methods to several types of elliptic problems including anisotropic problems. We are planning to test these algorithms and implement them on distributed memory computers. We also plan to work on the application of the algorithms to more general problems.

3.8 Time Dependent Problems and Rational Iteration

We plan to work on the development of iterative methods based on rational iteration for solving the system

$$Au=b. \tag{4}$$

The motivation for considering rational iterative methods is the fact, that for the time dependent problem

$$\begin{cases} \dfrac{du(t)}{dt} = -Au(t) + b \\ u(0) = u^{(0)} \end{cases} \tag{5}$$

where A is a symmetric and positive matrix, the solution is

$$u(t) = \bar{u} + e^{-At}(u^{(0)} - \bar{u}) \tag{6}$$

where $\bar{u} = A^{-1}b$ is the solution of (4). Moreover $u(t) \to \bar{u}$ as $t \to \infty$. Many of the standard methods for solving the time dependent problem (5) correspond to iterative methods for solving the linear system (4). For example, the extrapolated Richardson method given by $u^{(n+1)} = u^{(n)} + \gamma(b - Au^{(n)})$ corresponds to the forward difference method for integrating (5).

It is well known that, if explicit methods are used to solve (5), then a very severe limitation on the time step Δt must be imposed in order to avoid instability. In order to be able to use a larger step size without loss of stability, implicit methods such as the backward difference method or the Crank-Nicolson method are often used. These implicit methods correspond to the following rational iterative method:

$$(A + \rho I)u^{(n+1)} = [(1 - \gamma)A + \rho I]u^{(n)} + \gamma b \tag{7}$$

Here ρ is a parameter and γ is an extrapolation factor. (The choice γ=1 corresponds to the backward difference method with $\Delta t = \rho^{-1}$, while the choice γ=2 corresponds to the Crank-Nicolson method with $\Delta t = 2\rho^{-1}$).

Rational iteration has several potential advantages including the following

(a) by the use of partial fraction decompositions several iterations with different values of ρ can be carried out in parallel. (This was done by Gallopoulos and Saad [1992] for carrying out several time steps in parallel for the time-dependent problem (5)).

(b) by choosing an appropriate set of values $\rho_1, \rho_2, \ldots \rho_n$, (see Young and Vona [1992])the number of rational iterations required for convergence is $O(\log K(A))$.

A major obstacle to the use of rational iteration is the need to solve many linear systems of the form $(A + \rho I)x = y$ for some $\rho > 0$. This, of course, becomes increasingly difficult as ρ decreases. We plan to investigate several methods for carrying out rational iteration. One procedure is to consider a family of related systems

$$(A + \rho_i I)x^{(i)} = y^{(i)} \tag{8}$$

for a set of values $\rho_1 > \rho_2 > \ldots > \rho_m$. If ρ_1 is large, then the system can be easily solved by a standard iterative method. The subsequent systems will then be solved by a continuation process which is related to the problem of solving the time-dependent equation. Since the systems to be solved are related, any information, such as eigenvalue/eigenvector estimates obtained for

solving one system can be saved and used on the next system. We also plan to consider other methods for solving sets of related systems including those described by Van de Vorst [1987] and Saad [1985].

3.9 Nonsymmetric Systems

If the matrix A of a given linear system $Au=b$ is symmetric and positive definite (SPD) then many of the standard basic iterative methods such as Richardson's method, the Jacobi method, and the SSOR method are "symmetrizable". This implies, among other things, that the eigenvalues of the iteration matrix G are real and less than one. Because of this, the rate of convergence can be greatly accelerated by the use of Chebyshev acceleration or by conjugate gradient acceleration; see for instance Hageman and Young [1981].

For many practical problems involving convective transport such as the fluid flow and reservoir problems mentioned previously, the linear system $Au=b$ corresponding to the central-difference finite difference method or Galerkin finite elements is not SPD. For such problems, the standard basic iterative methods are not symmetrizable. However, in many cases the basic iterative method can still be accelerated by the use of generalized conjugate gradient methods (which are often referred to as "Krylov space methods".) Young and Jea [1980] considered three Krylov space methods, namely ORTHODIR, ORTHORES, and ORTHOMIN. The ORTHOMIN form is closely related to the classical form of the conjugate gradient method given by Hestenes and Stiefel [1952] while ORTHORES is a three-term method which was considered by Concus, Golub and O'Leary [1976]. The ORTHODIR form is in theory the most robust since if either of the other two methods converges then ORTHODIR converges. On the other hand ORTHODIR requires somewhat more work per iteration and is subject to rounding errors; see e.g. Abbassian [1983].

A significant disadvantage of Krylov subspace methods is that the amount of work required to carry out a given iteration increases linearly as the number of iteration increases. This can be avoided by using "truncation" or "restarting". However, this may result in slower convergence or failure to converge. Lanczos methods are similar to Krylov space methods but the work required per iteration does not increase with the number of iterations. Jea and Young [1983] considered three Lanczos methods, namely LANDIR, LANMIN, and LANRES. (In Jea and Young [1983] these methods were referred to as "Lanczos/ORTHODIR", "Lanczos/ORTHOMIN", and "Lanczos/ORTHORES," respectively). LANDIR, LANMIN, and LANRES correspond to applying ORTHODIR, ORTHOMIN and ORTHORES, respectively, to a "double system" derived from the given system. LANMIN is equivalent to the "biconjugate gradient method" (BCG method) presented by Fletcher [1976]. It can be proved that LANDIR converges whenever either LANMIN or LANRES converge. However, numerical studies indicate that LANDIR suffers from degradation due to roundoff effects.

The BCG method is a widely used method which has been the subject of a considerable amount of research over the past few years. The method is subject to the possibility of breakdown and, even when breakdown does not occur, the convergence behavior is often very irregular. Also, the method requires the use of A^T as well as A and this may be a serious disadvantage especially with highly parallel computers. Some of the recent results obtained for BCG are described in the work of Joubert [1990] (for coping with breakdown), Van der Vorst [1992] (for modifying BCG to obtain BCGSTAB which exhibits more regular convergence behavior) and Freund and Nachtigal [1991] (for modifying BCG to obtain QMR which does not require the use of A^T) and still has more regular behavior.

We plan to study the behavior of LANDIR to determine why there are serious roundoff problems and how they can be avoided. We will also study a new procedure which we call "LANGMRES" and which is based on the application of GMRES to the double systems referred to earlier. (GMRES was introduced by Saad and Schultz [1986], and is mathematically equivalent to ORTHODIR but requires less work per iteration and is less subject to rounding errors).

We also plan to study the use of LANDIR or LANGMRES as auxiliary procedures to be used in case of breakdown for algorithms where BCG or LANRES is used as the primary procedure.

3.10 Software Research

The Center for Numerical Analysis has a continuing program of research on iterative algorithms for solving sparse linear systems of algebraic equations with special emphasis on systems arising in the numerical solution of partial differential equations. An important aspect of the work has been the development of several research-oriented software packages developed as part of the ITPACK Project. These packages allow for the use of a wide variety of iterative algorithms suitable for use on vector and parallel supercomputers for both symmetric and nonsymmetric systems.

In the proposed research, we will focus on iterative algorithms from these packages and new extensions of these algorithms that are the best candidates for parallelization. Prototype codes will be implemented on various parallel computers and benchmark performance studies made. The algorithms will also be utilized in large-scale applications.

ITPACKV 2D is a package of seven iterative algorithms for solving sparse linear systems with symmetric and positive definite or mildly nonsymmetric coefficients matrices. The iterative algorithms in this package have been implemented for efficient use on vector supercomputers. A parallel version of the package has been developed for use on the 8-processor Cray Y-MP.

NSPCG (Non-Symmetric Preconditioned Conjugate Gradient methods) contains acceleration techniques in conjunction with various preconditioners for solving large sparse nonsymmetric linear systems by iterative algorithms. This package is modular in nature so that almost any preconditioner may be used with any accelerator.

Part of the research involves the problem of extending this software capability to parallel machines. We also plan to consider parallel variants of recent stabilized schemes such as the Quasi-minimum Residual (QMR) method and Stabilized Biconjugate Gradient (BCGSTAB). The software will be applied to convective transport applications in 3D.

Recent work here and elsewhere has focused on the establishment of a set of computational kernels related to iterative methods for solving sparse linear systems. It can be shown that many iterative algorithms can be decomposed into a relatively small set of basic computational operations. These computational kernels provide a flexible platform and would be particularly advantageous for software developed for use on different advanced parallel architectures. Since these would be the most computationally intensive parts of an iterative algorithm, it should be possible to develop efficient iterative algorithms for different parallel computers by writing code in terms of these basic building blocks. Like the original Basic Linear Algebra Subprograms (BLAS), these computational kernels would be defined in terms of fundamental operations independent of the computer architecture and without giving the exact implementation details for the particular underlying parallel computer architecture. Obviously, different hardware characteristics (shared versus distributed memory) would require different programming strategies to achieve optimal performance. Also, an iterative code could use the computational kernels tailored for a particular parallel computer and thereby be optimized in some sense. Moreover, the same code would be portable to other parallel computers having a similar set of optimized computational kernels.

During the development of the NSPCG software package, computational kernels were used related to vectorization. These were the key routines in the iterative algorithms that were optimized for efficient execution on vector computers. Several different sparse matrix data storage schemes were available in NSPCG for representing matrices ranging from unstructured to diagonally structured. By writing the iterative algorithms in terms of computational kernels, basic operations were vectorized using these storage schemes. While these computational kernels proved to be quite useful on vector computers, it is unclear if the same set of kernels or a different one will be need on parallel computers.

The development of these parallelizable computational kernels are complicated by the various sparse matrix storage formats to be treated and the different parallel computer

architectures involved. The communication overhead is also an issue to be investigated. Part of the research involves developing a taxonomy of iterative kernels and analyzing their computational complexity. Then representative parallel kernels will need to be developed and tested in PDE applications.

As an example of what we have in mind, some of the "Iterative BLAS" from Oppe and Kincaid [1990] are presented next. The Iterative BLAS are organized into three groups: general vector update operations, linear recursions, and stencil-specific vector update operations. We give the first two here.

We define the following *General Vector Update Operations* routines. Let x, y, and a be real vectors, α be a real scalar, and m and n be integer vectors.

YAX (y plus a times x) $y_i \leftarrow y_i + \alpha a_i x_i$.

YASX (y plus a times sparse x) $y_i \leftarrow y_i + \alpha a_i x_{m_i}$.

SYAX (sparse y plus a times x) $y_{n_i} \leftarrow y_{n_i} + \alpha a_i x_i$.

SYASX (sparse y plus a times sparse x) $y_{n_i} \leftarrow y_{n_i} + \alpha a_i x_{m_i}$.

YAX2 (y plus a times x, Level 2) $y_i \leftarrow y_i + \alpha \sum_{j=1}^{k} a_{i,j} x_{i+m_j}$.

YASX2 (y plus a times sparse x, Level 2) $y_i \leftarrow y_i + \alpha \sum_{j=1}^{k} a_{i,j} x_{m_{i,j}}$.

We define the following *Linear Recursion* routines. Let α be a real scalar and x, a, b, and d be real vectors.

FOLR (first order linear recursion) $x_i \leftarrow x_i + \alpha a_i x_{i-1}$.

SOLR (second order linear recursion) $x_i \leftarrow x_i + \alpha(a_i x_{i-1} + b_i x_{i-2})$.

MFOLR (multiple first order linear recursion) $x_{i,j} \leftarrow x_{i,j} + \alpha a_{i,j} x_{i-1,j}$.

MSOLR (multiple second order linear recursion) $x_{i,j} \leftarrow x_{i,j} + \alpha(a_{i,j} x_{i-1,j} + b_{i,j} x_{i-2,j})$.

One of our goals is to develop and test software for computational kernels that are common to a large class of iterative methods. These kernels can then be used in the development and testing of software for large systems arising from applications. Several different researchers have begun to write software for computational kernels to be used in developing efficient and portable implementations of iterative algorithms for sparse matrix problems on high performance computers. Some of the problems that have to be overcome concern keeping the interface for the suite of codes simple yet functional and flexible for many different data structures and for various iterative algorithms. This is particularly difficult to achieve on different parallel architectures.

Some related work for iterative software is summarized below:

Ashby and Seager [1990] propose a standard user interface for iterative linear system solvers. They discuss how the matrix-vector multiplication, preconditioning, and stopping criterion routines might be standardized as well as the overall design of iterative packages. Their goal is to make it easier for users to integrate, experiment,and combine iterative software into scientific simulation codes.

Saad [1991] describes the main features of a *toolkit* for manipulating and working with sparse matrices. He states that one of the goals of the package is to provide basic tools to facilitate the exchange of software and data between researchers in sparse matrix computations.

The package provides programs for converting data structures, printing simple statistics for a matrix, plotting a matrix profile, performing basic linear algebra operations with sparse matrices, etc. Recently, a version has been developed for use on a workstation with color graphics.

Oppe [1992] is developing a software package call STENCIL to solve linear systems by various iterative methods. The package contains several acceleration methods in conjunction with a number of preconditioners. The coefficient matrix is assumed to arise from the use of certain stencils in either a 2-D rectangular or 3-D box domain.

Joubert and Carey [PCG] are developing a package called PCG designed to solve linear systems by iterative methods on a variety of parallel architectures. Uniformity of calling sequences and near-uniformity of matrix storage formats are maintained across shared memory, data parallel, and message passing computers.

Heroux [1992] presents a proposal for a toolkit of kernel routines for some of the basic operations in iterative methods for sparse linear systems. He describes an interface for routines that perform the product of a sparse matrix times a dense matrix, the solution of a sparse triangular system with multiple right-hand-sides, the right permutation of a sparse matrix, and a check for the integrity of a sparse matrix representation. The interfaces for these four operations are defined for a variety of common data structures and a set of guidelines is given for defining the interfaces for new data structures. Heroux indicates that the primary purpose of his toolkit is to provide a set of basic routines upon which Duff, Marrone, and Radicati [1992] can build their user level sparse BLAS.

Duff, Marrone, and Radicati [1992] describe a set of level 3 basic algebra subprograms for sparse matrices. They discuss the design, implementation, and use of routines for the multiplication of a full matrix by a sparse matrix, for the solution of triangular systems with one or more (full) right-hand sides, for transforming sparse data structures, and for permuting sparse and full matrices. The objective is to develop standard software for use in the development of efficient and portable codes using iterative algorithms with sparse matrices on high performance computers. Their work is intended to be complementary to the toolkit of Heroux [1992].

Barrett, Berry, Demmel, Dongarra, Eijkhout, and Pozo [1992] describe a software system based on *templates* and *tool boxes* designed to facilitate the preparation of programs for implementing iterative algorithms for solving large sparse linear systems. The main component of the environment is a sparse matrix package for handling operations involving sparse matrices and vectors. The use of the system is illustrated for a number of iterative algorithms. The algorithms are described in three ways: first using an Algol-like language; second using a Matlab implementation; and third using Fortran. Extensive use is made of subroutines for carrying out various operations involving matrices and vectors. One of the goals is to be able to write a new program and to modify an existing program for describing an iterative algorithm using a relatively small number of statements.

Each of theses approaches has considerable merit but there is no clear consensus in this active research area. Our proposed work on iterative kernels will complement these activities. Hence we anticipate continuing collaboration with several of the above researchers on this subject.

3.11 Applications

Navier Stokes problems and reservoir simulation are two of the main applications areas to be considered in the reserach. For brevity we will give here only a brief description of the reservoir problem. Further details are given in the references cited and in the Appendix.

Numerical reservoir simulation involves the development and usage of a mathematical model and simulator which describes the flow of fluids in a permeable medium. The most complex simulators are those used for enhanced oil recovery processes. These processes involve the injection of chemicals, solvents, or heat into underground reservoirs in order to increase the recovery of trapped oil from the reservoir rock. Processes using chemicals such as detergents, caustics, and polymers are called chemical flooding and typically involve the multiphase flow of a large number of components that interact with the permeable medium. This can be represented

by a mathematical formulation that involves a set of coupled, highly nonlinear, time-dependent partial differential equations that must be solved by using numerical methods such as finite-difference or finite-element methods. This leads to a system of algebraic equations that must be solved at each time level using a numerical technique.

Due to the complexity of the governing nonlinear chemical flooding equations, both a fine mesh and very small time steps are needed to obtain an accurate solution (Datta Gupta *et al.*, 1986; Pope *et al.*, 1990; and Saad, 1989). Thus, for field simulations, a very large amount of computer time, as well as a large amount of storage, is required. As a consequence, supercomputers are needed to solve such enhanced oil recovery simulation problems. Even then, a highly optimized vector-parallel code is essential for practical and affordable simulation.

Over the past several years, we have developed two major compositional reservoir simulators (Chang *et al.*, 1990; Datta Gupta *et al.*, 1986; Saad *et al.*, 1989; and Saad *et al.*, 1990). One is for simulating enhanced oil recovery by chemical methods and is called UTCHEM. The second is for simulating enhanced oil recovery by miscible agents such as solvents, enriched gases, and carbon dioxide and is called UTCOMP. Both are compositional simulators, by which we mean that compositional phenomena such as phase behavior are modeled. These simulators employ finite-difference algorithms that discretize the nonlinear partial differential conservation equations describing the pertinent chemical and physical phenomena in three dimensions.

We, and others in industry use these simulators for research into process mechanisms, reservoir studies, interpretation of coreflood experiments, evaluation of numerical methods and solution algorithms, and optimization of oil recovery methods, among other uses. Versions of our codes have been developed for Cray computers and VAX computers. The Cray version of UTCHEM is highly vectorized and executes on a CRAY Y-MP 8 using Multitasking™. UTCOMP has only been partially vectorized, so it does not execute nearly as efficiently as UTCHEM. In both cases, there are many problems that require very large computational times and storage. Single-well patterns can be simulated in most cases without excessive cost, but as an application expands to include many patterns or an entire field of even moderate size, the cost often becomes prohibitive. Even laboratory-scale simulations can be very expensive when high-resolution simulation of unstable displacements and/or displacements with large crossflow are needed for fundamental investigations. It follows that high performance parallel schemes are needed. A brief description of the UTCHEM simulator and governing equations is provided in Appendix I.

As indicated above, the discretization of the governing partial differential equations describing fluid flow through a permeable medium leads to systems of linear equations. The numerical solution of the resulting systems of equations is very time consuming, especially as the number of equations becomes large. Furthermore, an actual field simulation may require solving these systems thousands of times. It is clear that a significant portion of the computational cost of a reservoir simulation study is incurred by the solution of the linear systems of equations. Hence, the development of efficient solvers is an important aspect of reservoir simulation.

As a part of our ongoing effort on improving our computational techniques for reservoir simulation, we are working on the development of a fully implicit polymer flooding simulator. In this simulator, the governing component conservation and overall material balance (pressure) equations are solved implicitly using a higher-order finite-difference method. The new simulator has improved stability properties over those of the UTCHEM simulator using an IMPES-like formulation. However, the solution of the resulting systems of linear equations is much more complicated and time consuming than the linear systems obtained in UTCHEM. Figure 1 shows the representative matrix structure for a two-dimensional problem with a very coarse grid having $N_x = 6$ and $N_y = 6$. The matrix has a large and dense bandwidth and although the structure is symmetric the entries are not. The bandwidth becomes larger as additional components and gridblocks are used (bandwidth = $12\ N_x + N_c$, where N_c is the number of components used in the problem). Fast and robust system solvers are crucial for practical usage of this simulator since over 90% of the computation time is spent in this portion of the simulator. Our preliminary results with NSPCG show that some nonsymmetric iterative solvers can outperform band solvers.

Part of the proposed research concerns the development and application of higher order non-oscillating schemes for this class of transport problem. Another important goal is the efficient solution of the resulting sparse systems using iterative methods. Finally, the problem of developing an effective, scalable parallel implementations will be a focal point of the research.

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4. Institutional Commitment and Other Support

The Center for Numerical Analysis is an organized research activity within the College of Natural Sciences. The emphasis of the research is on computer solution of partial differential equations and on the iterative solution of large sparse linear systems. A number of research-oriented software packages have been developed in the Center as part of the ITPACK project to aid in the research.

The CFD Laboratory of the College of Engineering is an endowed Laboratory equipped with several Sun microsystem scientific workstations, x-window terminals and Macintosh PC's networked to a Laserwriter. Both the CNA and CFD Labs are linked externally to the U.T. System CRAY YMP via a high-speed line and to national supercomputer centers. An Intel i860 distributed parallel system was obtained through a grant from Intel last year and will be utilized in the research.

We have initiated cooperative efforts with government and industrial researchers in this area. Of particular relevance is the collaboration with the Parallel Processing Institutes and researchers at Sandia and Los Alamos. This association also gives us access to a variety of advanced experimental parallel processors such as the NCUBE and the Connection Machine. Other related cooperative work is underway and industrial support is being requested through fellowships to students working on the project and as summer industrial interns.

5. Impact on Infrastructure of Science/Engineering

An important outcome will be not only the algorithm research, but also the software for generic parallel architectures. As in the past, this software will be made available to graduate students and to other researchers. The support will also enhance the academic preparation of graduate students in parallel computing, an area of current need. We hope to move our research forward to lead to major new research contributions in computational modeling on supercomputers. The ITPACK software library is widely distributed and our finite element and grid programs are used in industry and by government research laboratories. (Industrial shortcourses are offered each Fall and Spring on "Computational Aspects of Finite Elements" and include some aspects of high performance computing.)

11. BIOGRAPHICAL DATA

Dr. Graham F. Carey

Dr. Graham F. Carey is currently a Professor in the Department of Aerospace Engineering and Engineering Mechanics at the University of Texas at Austin. He has a B.S. (Hons.) degree from Australia, and M.S. and Ph.D. degrees from the University of Washington at Seattle. His research and teaching activities primarily deal with techniques in computational mechanics, particularly finite element methods. Related research experience includes periods as a research faculty member in Civil Engineering Australia (1966-68), and as a research engineer at the Boeing Company, Seattle (1968-70), during which time he worked in finite element formulation and computation of nonlinear problems. Prior to joining the University of Texas faculty, he held the positions of Research Assistant to Research Associate Professor at the University of Washington (1974-76), working on computational problems in mechanics. He is now Director of the CFD Laboratory and a member of the Texas Institute for Computational Mechanics, Fluids Group, Center for Numerical Analysis and the Center for Enhanced Oil and Gas Recovery Research, where these research activities are being continued.

Publications include a textbook co-authored with H.C. Martin, entitled Introduction to Finite Element Analysis (McGraw-Hill, 1973), co-authorship of a series of six graduate level monographs entitled Finite Elements (Prentice Hall), and co-editorship of the book Finite Elements in Fluids (1985). Dr. Carey has edited a monograph entitled Parallel Supercomputing Methods and Algorithms (Wiley, U.K., 1989) and a monograph on Grid Generation, Redistribution and Refinement is in preparation. He has also authored over 130 publications in the general area of computational mechanics, finite element technology and parallel computing and is editor of the Wiley International Journal, Communications in Applied Numerical Methods.

Additional activities in computational mechanics include membership in the American Academy of Mechanics, SIAM, the Society for Engineering Sciences, Committee on Computational Methods in Engineering Mechanics, with listings in the International Directory of Engineering Analysts, Who's Who in the South and Southwest, Who's Who in Frontiers of Science and Technology, and Who's Who in the World. Dr. Carey is an adjunct fellow of the Minnesota Supercomputer Institute. Dr. Carey has held the W. J. Murray Centennial Teaching Fellowship and has recently received an Engineering Foundation Excellence Award. He is a recipient of an Endowed Engineering Foundation Professorship and received a high performance computing "Gigaflop" award.

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Dr. David M. Young

Dr. Young received his PhD from Harvard University in 1950. He has had experience as a Research Mathematician at the Computing Laboratory at the Aberdeen Proving Ground (1951-52), Associate Professor of Mathematics, University of Maryland (1952-55) and Manager, Mathematical Analysis Dept. of the Ramo-Wooldridge Corporation (1955-58). He joined the faculty of the University of Texas at Austin in 1958 as Professor of Mathematics. In 1967 he helped establish the Department of Computer Sciences. Dr. Young was Director of the Computation Center from 1958 until 1970. Since 1970 he has been Director of the Center for Numerical Analysis.

Dr. Young has worked extensively on the numerical solution of partial differential equations. He has been particularly concerned with effective iterative methods for solving large sparse linear systems which typically arise when discretization methods such as finite difference methods and finite element methods are used. He has been involved with the development and evaluation of various iterative algorithms using both theoretical analysis and also numerical experimentation. He has also been concerned with the actual implementation of iterative algorithms which are suitable for use on vector and parallel computers.

Dr. Young is the author of a number of research papers and reports. Selected papers and reports appearing since 1984 are listed below. He is the author of three books which are listed below.

For several years Dr. Young, along with Dr. Kincaid and others, has worked on the ITPACK project for developing research-oriented mathematical software for solving large sparse linear systems using iterative methods. Dr. Young was also a participant on the ELLPACK project for the development of software for solving partial differential equations.

Selected Publications Since 1984

Kinciad, D.R. and Young, D. M. [1984]. "The ITPACK Project: Past, Present, and Future," *Elliptic Problem Solvers II*, (Garrett Birkhoff and Arthur Schoenstadt, eds), Academic Press, New York, 53-63.

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Dr. David R. Kincaid
Co-Investigator

Dr. Kincaid received the B.S. (*cum laude*) degree from Lamar University and the M.A. and Ph.D. degrees from The University of Texas at Austin. He taught in the Computer Science Department at Purdue University before returning to The University of Texas at Austin. Currently, Dr. Kincaid is a Research Scientist in the Computation Center, a Senior Lecture in the Computer Sciences Department, and the Associate Director of the Center for Numerical Analysis. He is also a member of the Texas Institue of Computational Mechanics.

Dr. Kincaid is actively involved in numerical analysis research, especially numerical linear algebra and iterative methods, with emphasis on the use of high performance computers. His participation in the project includes supervising the development of software packages based on iterative algorithms, learning and utilizing parallelization techniques and testing the resulting software on parallel architectures.

Dr. Kincaid has had extensive experience in programming and in the supervision of programming activities. For example, he was involved in the development of three well-known software packages: `BLAS`, Basic Linear Algebra Subprograms; `ITPACK`, an iterative package for solving symmetric positive definite linear systems; and `NSPCG`, an nonsymmetric preconditioned conjugate gradient package. Recently, he has gained considerable experience on supercomputers with the adaptation of software for use on vector and parallel computers. Dr. Kincaid was a contributor to the ELLPACK package (Purdue University) for the development of software for solving partial differential equations.

Drs. David Kincaid and Ward Cheney have written two textbooks: an advanced textbook *Numerical Analysis: Mathematics of Scientific Computing* and an introductory textbook *Numerical Mathematics and Computing, 2nd Edition.*

Dr. Kincaid is the author of a number of research papers and technical report. Those published since 1984 are listed below.

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KAMY SEPEHRNOORI
Professor of Petroleum Engineering

EDUCATION

B.S. (Mechanical Engineering) The University of Texas, 1973; M.S. (Engineering) The University of Texas, 1974; Ph.D. (Petroleum Engineering) The University of Texas, 1977.

EDUCATIONAL EXPERIENCE

1989-present Frank W. Jessen Professor in Petroleum Engineering; 1985-1989 Associate Professor of Petroleum Engineering, The University of Texas at Austin; 1981-1985 Assistant Professor of Petroleum Engineering, The University of Texas at Austin; 1982-Summer Visiting Professor, Department of Petroleum Engineering, The University of Southwestern Louisiana; 1975-Fall Teaching Assistant, Department of Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin.

OTHER EXPERIENCE

1983 - Summer Summer job training at Dresser Atlas and Shell Oil Company - Houston; 1978 - 1981 Research Engineer - Scientist Associate, Center for Energy Studies and Petroleum Engineering Department, The University of Texas at Austin; 1979 - Summer Research Associate, Department of Petroleum and Geological Engineering University of Oklahoma; 1973 - 1977 Research Engineer - Scientist Assistant, Bureau of Engineering Research, The University of Texas at Austin.

HONORS AND AWARDS

Honor Roll, College of Engineering, The University of Texas. Sigma Gamma Tau, Phi Theta Kappa, Phi Kappa Phi, Recipient of Digital Equipment Corporation Grant for the Development of Computer Graphics in the Petroleum Engineering Department, 1982. Award of Excellence, Halliburton Education Foundation, September, 1984. Recipient of Sun Exploration and Production Company Centennial Fellowship, 1983-1989. GIGAFLOP Performance Award from Cray Research, Inc., 1989. Frank W. Jessen Professor in Petroleum Engineering, 1989-present.

MEMBERSHIPS

Society for Industrial and Applied Mathematics (SIAM) - Society of Petroleum Engineers (SPE)

UNIVERSITY ASSIGNMENTS

Computer Committee, Dept. of Pet. Eng. - Admission Committee, Dept. of Pet. Eng., Graduate Studies Committee, Dept. of Pet. Eng., Chairman, Library Committee, Dept. of Pet. Eng., Engineering Computer Committee.

NON-UNIVERSITY ASSIGNMENTS

General Editor, *In Situ*

CONSULTING

Digital Equipment Corporation

PUBLICATIONS

Dr. Sepehrnoori has published over 100 technical articles and reports in his research related areas.

AREAS OF INTEREST

Reservoir Simulation
Computational Methods
Applied Mathematics
Enhanced Oil Recovery
Database Application in Petroleum Engineering
Vector/Parallel Computations

MOST RECENT PUBLICATIONS

"An Expert System for Miscible Gas Flooding," with S.A. Khan and G.A. Pope, to appear in *SPE Computer Applications*, February 1993.

"An Expert System to Select Acid Gas Treating Processes for Natural Gas Processing Plants," with H. Kurimura and G.T. Rochelle, accepted for publication by *J. Gas Separation and Purification*, 1992.

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"Analysis of Tertiary Injectivity of Carbon Dioxide," with M.K. Roper, Jr. and G.A. Pope, SPE 23974 presented at the SPE/DOE 8th Symposium on Enhanced Oil Recovery, Tulsa, OK, April 22-24, 1992, and the SPE Permian Basin Oil and Gas Recovery Conference, Midland, TX, March 18-20, 1992.

"Interpretation of a CO_2 WAG Injectivity Test in the San Andres Formation Using a Compositional Simulator," with M.K. Roper, Jr., C.T. Cheng, J. Varnon, and G.A. Pope, SPE 24163 presented at the SPE/DOE Eighth Symposium on Enhanced Oil Recovery, Tulsa, OK, April 22-24, 1992.

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"Comparisons of Counter-Current Imbibition Transfer Functions in Dual Porosity Models of Naturally Fractured Reservoirs," with J. Chen and M.A. Miller, *In Situ*, 15(2), 1991.

"Simulation of Heterogeneous Sandstone Experiments Characterized Using C.T. Scanning," with S. Ganapathy, D. Wreath, M.T. Lim, B. Rouse, and G.A. Pope, SPE 21757 presented at the SPE Western Regional Meeting, Long Beach, CA, March 20-22, 1991.

"Development of a Thermodynamically Consistent, Fully Implicit, Equation-of-State, Compositional Steamflood Simulator," with K. Brantferger and G.A. Pope, SPE 21253 presented at the SPE Symposium on Reservoir Simulation, Anaheim, CA, February 17-20, 1991.

"Analysis of Field Tracers for Reservoir Description," with S.B. Allison and G.A. Pope, *J. of Petroleum Science and Engineering*, 5(2), January, 1991.

"Benchmark of UTCHEM Reservoir Simulator on Various Cray Computers," with G. Shiles and G.A. Pope, *Communications in Applied Numerical Methods*, 7 (1), January, 1991.

"The Effects of Gravity on Micellar-Polymer Flooding Under North Sea Conditions: A Simulation Study," with M. Shook and G.A. Pope, *In Situ*, 15(1), January, 1991.

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"Numerical Simulation of Interwell Tracers," with G.A. Pope and G. Shiles, accepted by *In Situ*, October 1990.

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APPENDIX I

UTCHEM SIMULATOR AND GOVERNING EQUATIONS

In UTCHEM, the material balance equations are solved for up to nineteen components: water, oil, surfactant, polymer, anions, divalent cations, cosurfactant-1, cosurfactant-2, three tracers, sodium dichromate, thiourea, trivalent chromium, gel, hydrogen, carbon, silicon, and organic acid species. These components may form up to three phases–aqueous, oleic, and microemulsion–depending on the relative amounts and effective salinity of the phase environment.

The major physical phenomena modeled in the simulator are phase density, phase viscosity, phase behavior, dispersion, adsorption, interfacial tension, relative permeability, capillary pressure, capillary trapping, cation exchange, and polymer properties. The latter includes permeability reduction, inaccessible pore volume, and shear-thinning. Depending on the process and components injected, various chemical reactions to form gel or precipitation-dissolution reactions are modeled.

Next, we present the material balance equations and the pressure equation used in the simulator as well as a brief description of the numerical schemes.

Material balance equations

The material balance equations solved in UTCHEM are given below. A detailed description of these equations can be found in Datta Gupta *et al.* (1986), Pope *et al.* (1990), and Bhuyan *et al.* (1990).

$$\frac{\partial}{\partial t}\left[\phi \tilde{c}_i\left(1+c_i^{\circ}\Delta P\right)\right] +$$

$$+\frac{\partial}{\partial x}\left\{\sum_{j=1}^{n_p}\left(1+c_i^{\circ}\Delta P\right)\left[c_{ij}u_{xj}-\phi S_j\left(K_{xxij}\frac{\partial c_{ij}}{\partial x}+K_{xyij}\frac{\partial c_{ij}}{\partial y}+K_{xzij}\frac{\partial c_{ij}}{\partial z}\right)\right]\right\} +$$

$$+\frac{\partial}{\partial y}\left\{\sum_{j=1}^{n_p}\left(1+c_i^{\circ}\Delta P\right)\left[c_{ij}u_{yj}-\phi S_j\left(K_{yxij}\frac{\partial c_{ij}}{\partial x}+K_{yyij}\frac{\partial c_{ij}}{\partial y}+K_{yzij}\frac{\partial c_{ij}}{\partial z}\right)\right]\right\} +$$

$$+\frac{\partial}{\partial z}\left\{\sum_{j=1}^{n_p}\left(1+c_i^{\circ}\Delta P\right)\left[c_{ij}u_{zj}-\phi S_j\left(K_{zxij}\frac{\partial c_{ij}}{\partial x}+K_{zyij}\frac{\partial c_{ij}}{\partial y}+K_{zzij}\frac{\partial c_{ij}}{\partial z}\right)\right]\right\} =$$

$$Q_i \qquad i = 1,\ldots,n_c, \tag{1}$$

where $\Delta P = P_j - P_R$ and $\bar{c}_i = \left(1 - \sum_{i=1}^{n_c} \bar{c}_i\right) \sum_{j=1}^{n_p} (c_{ij} S_j) + \bar{c}_i$.

The overall material balance equation is obtained by summing the material balance equation (Eq. 1) over all components:

$$\phi c_t \frac{\partial P}{\partial t} + \frac{\partial}{\partial x} \sum_{j=1}^{n_p} \left[u_{xj} \sum_{i=1}^{n_c} \left(1 + c_i^\circ \Delta P\right) c_{ij} \right] +$$

$$+ \frac{\partial}{\partial y} \sum_{j=1}^{n_p} \left[u_{yj} \sum_{i=1}^{n_c} \left(1 + c_i^\circ \Delta P\right) c_{ij} \right] +$$

$$+ \frac{\partial}{\partial z} \sum_{j=1}^{n_p} \left[u_{zj} \sum_{i=1}^{n_c} \left(1 + c_i^\circ \Delta P\right) c_{ij} \right] = \sum_{i=1}^{n_c} Q_i , \qquad (2)$$

where $c_t = c_f + \sum_{i=1}^{n_c} c_i^\circ \bar{c}_i$.

Pressure equation

The pressure equation is obtained by substituting the multiphase flow version of Darcy's law given below for the flux terms u_{xj}, u_{yj}, and u_{zj}, in (2):

$$\vec{u}_j = - \vec{\vec{k}} \lambda_{rj} \left(\vec{\nabla} P_j - \gamma_j \vec{\nabla} D \right), \qquad (3)$$

where $\vec{\vec{k}}$ is taken to be a diagonal tensor in UTCHEM. By using the definition of capillary pressure,

$P_{c j¢ 1} = P_{j¢} - P_1$ for $j¢ = 2, 3$ we can write the resulting equation in terms of a reference phase (aqueous) pressure:

$$\phi c_t \frac{\partial P_1}{\partial t} + \vec{\nabla} \cdot \vec{\vec{k}} \cdot \lambda_{rTc} \vec{\nabla} P_1 = - \vec{\nabla} \cdot \sum_{j=1}^{n_p} \vec{\vec{k}} \cdot \lambda_{rjc} \vec{\nabla} D +$$

$$+ \vec{\nabla} \cdot \sum_{j=2}^{n_p} \vec{\vec{k}} \cdot \lambda_{rjc} \vec{\nabla} P_{cj1} + \sum_{i=1}^{n_c} Q_i \,, \tag{4}$$

$$\text{where } \lambda_{rjc} = \lambda_{rj} \sum_{i=1}^{n_c} (1 + c_i^{\circ} \Delta P) \, c_{ij} \tag{5}$$

$$\text{and } \lambda_{rTc} = \sum_{j=1}^{n_p} \lambda_{rj} \sum_{i=1}^{n_c} (1 + c_i^{\circ} \Delta P) \, c_{ij} \,. \tag{6}$$

The governing equations are discretized using a third-order finite-difference approximation of the space derivatives and a forward-difference approximation of the time derivatives (Saad, 1989; Saad *et al.*, 1990). The solution scheme used in the simulator is similar to IMPES (implicit pressure/explicit saturation). First, the pressure equation is solved implicitly using explicit dating of saturation-dependent terms. The implicit solution of the pressure equation results in a system of linear equations where the coefficient matrix is a symmetric positive definite banded matrix. The numerical solution of the resulting system is handled using the Jacobi Conjugate Gradient method (Hageman and Young, 1981). The material balance equations are then solved explicitly for overall concentrations. Phase concentrations and saturations are obtained by flash calculations.

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