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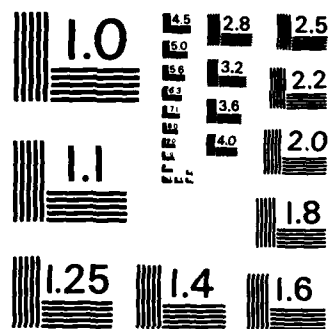   UNIV AT RALEIGH R J PLEMMONS 19 JUL 85
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FAST ALGORITHMS FOR STRUCTURAL OPTIMIZATION, LEAST SQUARES AND OTHER COMPUTATIONS

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FIELD	GROUP	SUB. GR.	Constrained minimization, least squares, numerical linear algebra, parallel processing, structural optimization

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Fast algorithms for solving large-scale structural optimization and least squares problems are being investigated. An especially significant aspect of this work is the development and testing of parallel algorithms for alternatives to the often ill-conditioned stiffness equations approach in structural analysis on machines such as the Cray X-MP, the Denelcor HEP and the Intel Hypercube. The principal thrusts in this project on least squares methods have been in developing techniques for the solution of superlarge problems in a stable way, i.e., employing orthogonal factorization techniques, on multiprocessors. These computations involve various levels of parallelism, including domain decomposition as well as pipelining type schemes for orthogonal factorization.

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I. RESEARCH OBJECTIVES

It is now generally recognized that to achieve the computation speeds necessary to solve the new complex scientific problems of significant impact to the DOD community requires radical reorganization of traditional algorithms in numerical linear algebra. It is not sufficient to implement old algorithms in a parallel processing environment. New fast algorithms for the next generation of supercomputers, currently being previewed by, e.g., the Cray X-MP, the Denelcor HEP and the Intel Hypercube, are essential. In order to meet the challenges of this emerging new generation of machines, it is the goal of this project to develop techniques in numerical linear algebra for efficient implementation on advanced multiprocessors. Significantly, applications of our work to the practical real world problems of structural optimization and least squares estimation methods are being developed.

In the area of structural optimization we have been concerned with the fundamental problem of linear elastic analysis - that of finding the stresses and strains, given a finite element model of a complex structure and a set of external loads. To obtain the solution of this constrained minimization problem a variety of algorithms such as the displacement method, the force method, the natural factor method and the weighted least squares method can be applied. While the advantages of implementing one of these methods over another on serial computers have been widely studied, the effects of parallelism in performing the linear algebra computations have not.

Over the past year we have written several reports on our studies of fast algorithms for large-scale structural optimization problems, including comprehensive papers to appear in the <u>SIAM Journal on Algebraic and Discrete Methods</u>, <u>Linear Algebra and Its Applications</u> and <u>Numerische Mathematik</u>. Our goals over the next 2-5 years continue to be the development and testing of complete sparse matrix finite element structural optimization packages on machines such as the Cray X-MP with up to 4 processors and its comparison with traditional serial methods in packages such as NASTRAN. We also intend to test highly parallel segments of these algorithms on a Hypercube with up to 128 processors, in order to obtain a better understanding of the possible ramifications of applying massive parallelism to structural analysis computations.

The principal thrusts in our work on least squares methods and applications to constrained minimization, to linear estimation and to geodetic adjustment, have been on developing techniques for the solution of superlarge problems in a stable way, i.e., employing orthogonal factorization techniques, on multi-processors. A paper on a parallel block iterative scheme developed for these purposes will appear in <u>Linear Algebra and Its Applications</u>. Another approach using domain decomposition techniques is part of some joint work between our project and

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one by A. Sameh at the University of Illinois. A paper on our
results will be presented at the forthcoming SIAM Conference on
Parallel Processing in Norfolk, Virginia. Our short term goals
in this area include testing of these schemes using large-scale
practical least squares data on the Cray X-MP at the BSC this
fall, to be followed by implementation on the Cedar machine
being constructed at the University of Illinois. Our longer
range goals are to investigate stable methods for least squares
computations which involve various levels of parallelism inc-
luding domain decomposition as well as pipelining type schemes
for orthogonal reduction.

Thus there are two areas of particular excitement in this
project. We are close to the establishment of a framework for
testing and comparing parallel algorithms for structural
optimization against the more traditional approaches in
commercial software. In addition, we are developing new tools
for large-scale least squares computations necessary to meet the
challenges of solving data-massive problems in a stable way on
the new generation of supercomputers.

Some major results obtained during the past year of this project
are outlined in the next section.

II. SUMMARY OF MAJOR RESULTS

The most important reserach accomplishments by the principal
investigator and co-workers are described below. These results
have been obtained on four specific problems in computational
mathematics and applications.

1. Parallel Algorithms for Finite Element Structural Analysis
    on the HEP Multiprocessor.

    A fundamental problem of linear elastic analysis is that of
    finding the vectors of stresses and strains, given a finite
    element model of a structure and a set of external applied
    loads. To obtain the solution to this linearly constrained
    quadratic minimization problem a variety of methods
    involving the force method or the displacemment method may
    be used. The primary consideration in using the force
    method is the computation of a basis matrix Z for the null
    space of the equilibrium matrix E for the structure, whereas
    the primary consideration in using the displacement method
    is the solution of the stiffness equations with coefficient
    matrix $K = EkE^T$ where k is the element flexibility matrix.

    One purpose of this paper is to report on the design and
    testing of a parallel version of a highly effective but
    computation intensive algorithm for computing a banded basis
    matrix Z for the null space associated with the force
    method. FORTRAN codes for both the serial and parallel
    versions of the algorithm have been implemented on the
    Denelcor HEP computer at the Argonne National Laboratory.

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Performance results using data from some practical
structural problems indicates that the parallel version
executes significantly faster on the HEP than the serial
version, which has also been run on a CYBER 205 and a Cray
1S.   Secondly, a preliminary report on the use of a
pipelined Givens orthogonal factorization scheme in
conjunction with a weighted least squares approach in
avoiding the often ill-conditioned stiffness equations in
the displacement method is given. The scheme is based upon
a method recently proposed by Dongarra, Sameh and Sorensen.
The effectiveness of this orthogonal factorization scheme on
structural analysis problems is currently being investigated
on the HEP.

2. Convergent Iterations for Computing Stationary Distributions
    of Markov Chains

    Classical iterative schemes such as the Gauss-Seidel method
    and its variations constitute powerful tools for ocmputing
    stationary distribution vectors for large-scale Markov
    process, such as those arising in queueing network analysis.
    The coefficient matrix A in these processes in a Q-matrix,
    i.e., a singular irreducible M-matrix with zero column sums
    and, unlike the nonsingular case, the classical iterations
    for A do not always converge. The purpose of this paper is
    to survey the recent literature and to analyze the behavior
    of these methods completely in terms of the graph structure
    of A. The results given here hold under somewhat weaker
    assumptions or A.

3. Updating LU Factorizations for Computing Stationary
    Distributions

    The computation of stationary probability distributions for
    Markov chains is important in the analysis of many models in
    the mathematical sciences, such a queueing network models,
    input-output economic models and compartmental tracer
    analysis models. These computations often involve the
    solution of large-scale homogeneous linear equations by
    Gaussian elimination, where A is a Q-matrix, i.e., $A = (a_{ij})$
    is irreducible, $a_{ij} \leq 0$ for all $i \neq j$ and has zero column
    sums. The stationary distributions are the components of
    the unique solution vector x of positive components whose
    sum is one. Stable direct methods for computing x by
    triangular factorization $A = LU$ have received considerable
    attention recently and the purpose of this paper is to
    provide a stable method for updating the factors L and U in
    $O(n^2)$ flops in the case where a column of A is modified.
    Updating formulas are derived here using an approach similar
    to that for updating the Cholesky factor of a symmetric
    positive definite matrix after the addition of a rank one
    matrix. The algorithm is effective more generally for any
    matrix that has a stable LU factorization and for which the
    updated matrix has a stable LU factorization.   An error

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analysis for the LU update algorithm is outlined along the lines of that given for the Cholesky update by Fletcher and Powell. Details of the algorithm based on the error analysis and other considerations are given.

4. **A Parallel Block Iterative Scheme Applied to Computations in Structural Analysis**

In this paper it is shown how a block cyclic successive over-relaxation direct-iterative method can be applied to the parallel solution of certain large-scale linear equality-constrained quadratic programming problems. The scheme is similar in nature to those studied recently by de Pillis, Niethammer and Varga and by Markham, Neumann and Plemmons for solving large sparse least squares problems. It is based upon a partitioning strategy of the fundamental matrix into a block consistently ordered 2-cyclic form where the nonzero eigenvalues of the Jacobi matrix are all pure imaginary. The method is shown to be globally convergent and convergence rates are established.

Applications of the algorithm are discussed for large-scale structural analysis computations where it is shown how the algorithm can be adapted to the simultaneous computation of the system forces and the nodal displacements. Here, advantage can be taken of the special forms of the matrices involved. In particular, it is shown that much of the algorithm lends itself to efficient implementation on pipelined vector machines and on multiprocessors.

III. RESEARCH IN PROGRESS

The research projects in support of this grant which are currently underway are briefly described below. A more complete description of the results of this current work will be given in next year's annual scientific report.

1. **Parallel Version of the Golub/Plemmons Algorithm for the Orthogonal Factorization of Least Squares Observation Matrices in Block Angular Form.**

The Golub/Plemmons block orthogonal factorization algorithm was designed for the stable least squares adjustment of large amounts of geodetic data which is assembled so that the observation matrix has a bordered block diagonal form. The algorithm can also be applied to more general substructuring or domain decomposition methods. In this work we are investigating how a parallel version of the algorithm can be applied not only to the factorization scheme but also to the back substitution phase of the least squares method. The algorithm has been programmed for testing on the Denelcor HEP multiprocessing computer at the Argonne National Laboratory and will be implemented later on the Cedar multiprocessor. This is joint work with A. Sameh

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in the Computer Science Department at the University of Illinois.

2. <u>Multi-Splitting Iterative Methods on a Hypercube Multiprocessor</u>.

This research is concerned with parallel algorithms for the iterative solution of systems of linear equations $Ax = b$, where A is nonsingular. Our attention on this project is restricted to the implementation on a 64 processor Intel Hypercube of a multi-splitting type algorithm. Here, overlapping sets of rows of A are assigned to seperate processors which in turn perform seperate iterations. Using the message passing communication scheme between processors, the iterations are weighted in such a way that convergence results whenever A is either symmetric positive definite or an M-matrix. The communication complexity of our algorithm is $O(2\log_2 p)$ where p is the number of processors being used. The algorithm has previously been implemented by R. White on the shared memory Denelcor HEP system at Argonne. This is current work with R. Funderlic at the Oak Ridge National Laboratory.

3. <u>Finite Element Calculations for Structural Analysis on a Hypercube Multiprocessor</u>.

A new approach to calculating the vector f of internal forces and the associated stresses, given a finite element model of a structure and an external load vector p, is being developed for implementation on a hypercube multiprocessing system. This joint work with M. T. Heath at the Oak Ridge National Laboratory is based upon solving the fundamental problem of linear elastic analysis

$$\min f^T F f \text{ subject to } Ef = p,$$

where F denotes the element flexibility matrix and E the equilibrium matrix, by the weighting method for linearly constrained least squares, thus avoiding the often ill-conditioned stiffness equations. The particular formulation of this problem, based upon earlier work of Berry and Plemmons for the Denelcor HEP shared memory system, lends itself to the solution on a hypercube configured into a ring type topology, with a central host node. A significant advantage of our scheme will be that the matrix factors are distributed throughout the processors.

This work is part of our continuing efforts to test highly parallel segments of alternative algorithms to the displacement method in order to obtain a better understand of the possible ramifications of applying massive parallelism to structural analysis computations.

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IV. TECHNICAL PUBLICATIONS

1. "Parallel Algorithms for Finite Element Structural Analysis on the HEP Multiprocessor," _Proceedings of the Workshop on Parallel Processing Using the HEP_, Norman, Oklahoma, March 1985, pp. 157-180 (with M. Berry).

2. "Updating LU Factorizations for Computing Stationary Distributions," _SIAM Journal of Algebraic and Discrete Methods_, 6(1985), to appear (with R. Funderlic).

3. "Convergent Iterations for Computing Stationary Distribution of Markov Chains," _SIAM Journal on Algebraic and Discrete Methods_, to appear (with G. P. Barker).

4. "A Parallel Block Iterative Scheme Applied to Computations in Structural Analysis," _SIAM Journal on Algebraic and Discrete Methods_, to appear.

5. "A Parallel Algirithm for Orthogonal Factorization of Least Squares Observation Matrices in Dual Angular Form," in preparation (with D. Pierce and A. Sameh).

6. "Multisplitting Iterative Methods on a Hypercube Multiprocessor," in preparation (with R. Funderlic).

7. "Finite Element Calculation for Structural Analysis on a Hypercube Multiprocessor," in preparation (with M. Heath).

V. PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

R. J. Plemmons, Principal Investigator

M. W. Berry, Graduate Research Assistant
D. J. Pierce, Graduate Research Assistant
            (part-time, starting 7/15/85)
R. B. Mattingly, Graduate Research Assistant
            (part-time, starting 7/15/85)

VI. CONFERENCE AND COLLOQUIUM LECTURES

1. Invited Lecture - "Computing a Banded Basis of the Null Space on the Denelcor HEP Multiprocessor," NSF-SIAM _Workshop on Linear Algebra and Systems Theory_, Bowdoin, Maine, August 1984.

2. Contributed Lecture - "Parallel Algorithms for Finite Element Structural Analysis on the HEP Multiprocessor," _Workshop on the Denelcor HEP_, Norman, Oklahoma, March 1985 (given by M. Berry).

3. Contributed Lecture - "Parallel Matrix Algorithms for

Structural Analysis," <u>SIAM Conference on Applied Linear
Algebra</u>, Raleigh, North Carolina, April 1985
(given by M. Berry).

4. Colloquium Lecture - "Accurate Finite Element Computation in
   Structural Analysis," <u>Ohio University</u>, Athens, Ohio,
   October 1984.

5. Colloquium Lecture - "Some Parallel Processing Algorithms
   for Structural Optimization," <u>Penn State University</u>,
   University Park, Pennsylvania, December 1984.

6. Colloquium Lecture - "Accurate Least Squares Computations
   for Large-Scale Structures and Geodetic Adjustments,"
   <u>University of Illinois</u>, Urbana, Illinois, June 1985.

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