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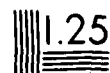
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ORDERING METHODS FOR SPARSE MATRICES

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Boeing Computer Services Company

Six Months Report
December 1981

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The solution of systems of large sparse linear equations is a fundamental computational step in the numerical solution of many scientific and engineering problems. These problems arise in such diverse areas as electromagnetic pulse (EMP) analysis, structural analysis, linear programming, network analysis, chemical process design, optimization, steady state analysis, and policy planning. When direct solution methods are used to solve these equations one of the major difficulties is choosing a reordering of the rows and columns (CONTINUED)		

ITEM #20, CONTINUED: of the sparse matrix to reduce some measure of solution cost.

Because sparse matrix research has grown independently out of many disciplines, there are many heuristic methods (band, profile, Markowitz, tearing, P^4 , and variations) presently used to accomplish this reordering. The challenge in building standard software is to determine if one heuristic works adequately across a broad class of problems, or if several heuristics must be available in a general purpose code. If several heuristics are needed, matrix classes must be identified as a basis for matching a given matrix with the proper ordering method. In either case it must also be determined how much performance will improve for particular problem classes if specialized sparse matrix code rather than general purpose code is used.

This research project is concerned with answering these questions. This report describes the current status of the project. Section 2 describes the project by task. Section 3 reports on the current status of each task. Section 4 contains summaries of related sparse matrix activities at BCS. A list of recent sparse matrix publications by the people working on this project appears at the end of the report.

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1. INTRODUCTION

The solution of systems of large sparse linear equations is a fundamental computational step in the numerical solution of many scientific and engineering problems. These problems arise in such diverse areas as electromagnetic pulse (EMP) analysis, structural analysis, linear programming, network analysis, chemical process design, optimization, steady state analysis, and policy planning. When direct solution methods are used to solve these equations one of the major difficulties is choosing a reordering of the rows and columns of the sparse matrix to reduce some measure of solution cost.

Because sparse matrix research has grown independently out of many disciplines, there are many heuristic methods (band, profile, Markowitz, tearing, P^4 , and variations) presently used to accomplish this reordering. The challenge in building standard software is to determine if one heuristic works adequately across a broad class of problems, or if several heuristics must be available in a general purpose code. If several heuristics are needed, matrix classes must be identified as a basis for matching a given matrix with the proper ordering method. In either case it must also be determined how much performance will improve for particular problem classes if specialized sparse matrix code rather than general purpose code is used.

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Chief, Technical Information Division



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2. PROJECT ORGANIZATION BY TASK

2.1 Task 1: Creation of a Comprehensive Test Matrix Collection

The goal of this task is to assemble a large collection of sparse matrices. These matrices will be representative of realistic problems arising in many different application areas. They should be of varying sizes and structural characteristics.

2.2 Task 2: Analyze the Hellerman-Rarick P⁴ Algorithm

In this task the Hellerman-Rarick ordering algorithm for sparse linear equations and all of its known variations will be studied with the intent of understanding the applicability, stability and effectiveness of it. A precise algorithmic description of the most important version will be produced.

2.3 Task 3: Producing a P⁴ Code

The precise description of the Hellerman-Rarick algorithm from Task 2 will be used to produce a high quality FORTRAN code implementing the algorithm.

2.4 Task 4: Producing a Diagnostic Program

A diagnostic program will be produced which will be capable of monitoring the effectiveness of various ordering algorithms applied to sparse matrices. The diagnostic code will monitor many characteristics such as accuracy, fill-in, storage, run-time and operation counts.

2.5 Task 5: Comparative Analysis

This final task is to utilize the test collection (Task 1) and the diagnostic program (Task 4) to provide detailed comparisons of various ordering algorithms including the Hellerman-Rarick algorithm (Task 3) and the MA28 code from the Harwell library.



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Tasks 1 through 4 will be performed during the first year of the project (June 30, 1981 through June 30, 1982). Task 5, if funded by the AFOSR, will be performed during the period from July 1, 1982 until June 30, 1983.



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3. PROGRESS AND CURRENT STATUS OF TASKS

Considerable progress has been made on Tasks 1 through 4. This section describes those activities.

3.1 Task 1

We began to contact various people from different application areas who have sparse matrix collections and we asked that certain of the matrices be sent to us. Test problems from structural engineering, chemical process design, linear programming and optimization have been identified. We have received some of the test matrices and expect to continue receiving the matrix collections for several more months.

3.2 Task 2

We have collected all of the known written material concerning the Hellerman-Rarick algorithm and have read it. This includes the original material by Hellerman-Rarick, papers by R.S.H. Mah in chemical engineering, papers by M.A. Saunders in the linear programming literature, a paper by Bisschop, Levy and Meeraus, preprint material from a book by A.M. Erisman and J.K. Reid, and several other sources.

Our work on the Hellerman-Rarick algorithm has progressed well. We have arrived at a simple and precise algorithmic description of the original algorithm. Based on that description we have obtained simple necessary conditions under which the algorithm can fail. We have investigated several possible generalizations of the basic algorithm which attempt to remove the flaws in the original. We have proved that the generalization which makes the simplest modifications to the algorithm and which most closely preserves its spirit is not sufficient to remove the potential for structural singularity. On the other hand, we have shown that the generalizations of the algorithm which have been suggested by previous work do



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not preserve the structure of the original algorithm, which they were believed to preserve. We have not yet investigated the efficacy of this latter generalization. This work will continue actively next year.

3.3 Task 3

We have collected several different implementations of the Hellerman-Rarick algorithm but have not started to test them. The testing will occur in early 1982.

3.4 Task 4

We have completed the design of the diagnostic program. This program will collect and analyze data concerning the performance of the different ordering algorithms. This information will be instrumental in deciding which algorithms are most effective for the collection of test matrices. The types of data to be gathered are given in the appendix. The diagnostic program will measure the ordering algorithm's ability in reducing the amount of computer memory required to store the factored matrix as well as reducing the number of operations for the actual factorization. The factorization will be done by a standard sparse matrix factorization module. Additional data on the amount of pivoting required for numerical stability as well as the effect the pivoting tolerance has on the factorization will be collected. Implementation of this program will begin after the beginning of the new year.

3.5 Task 5

This task is scheduled to begin July 1, 1982, assuming that the option for the second year of this project is funded by the AFOSR.



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4. RELATED SPARSE MATRIX ACTIVITIES AT BOEING COMPUTER SERVICES COMPANY

The mathematicians at Boeing Computer Services working on this project also are active in other projects which involve sparse matrix computations. This section briefly describes some of the most recent activities by those people. These projects are not funded by the AFOSR contract but they indicate the significance that sparse matrix research has at BCS.

4.1 Sparse Matrix Computations in Electric Power Problems

A.M. Erisman, R.G. Grimes, J.G. Lewis and W.G. Poole have performed work recently which applied current sparse matrix technology to electric power problems. Two recently completed publications in this area are attached to this report. The papers have appeared in the proceedings of two conferences: the SIAM meeting of Electric Power Problems: The Mathematical Challenge and the IMA conference on Sparse Matrices and their Uses.

4.2 Condition Number Estimation for Sparse Matrices

R.G. Grimes and J.G. Lewis have defined and implemented a condition number estimator for sparse matrices. The estimator has been implemented in a large, sparse eigenvalue program. This paper, which recently appeared in the SIAM Journal on Scientific and Statistical Computing, is attached.

4.3 Band and Envelope Reordering for Sparse Matrices

J.G. Lewis has greatly improved the Gibbs-Poole-Stockmeyer and Gibbs-King algorithm implementations for reducing the bandwidth and profile of a symmetric sparse matrix. A paper (to appear in ACM Transactions on Mathematical Software) is enclosed.



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4.4 CRAY-1 Optimization of SPARSPAK

D.S. Dodson, R.G. Grimes, J.G. Lewis and W.G. Poole have begun work on modifying the sparse matrix package, SPARSPAK, so that it will be optimized to take advantage of the vector capabilities of the CRAY-1 computer. This work is in progress.

4.5 Problems from Structural Engineering

J.G. Lewis has tested several problems from structural engineering by exercising the various ordering algorithms in SPARSPAK. The preliminary results indicate that no single ordering algorithm will suffice for a general code.

4.6 The Necessity of Pivoting

W. Kahan (of the University of California, Berkeley) and W.G. Poole are nearing completion of a paper which discusses the conditions under which matrices do not need some form of pivoting for maintaining numerical stability.



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PUBLICATIONS

1. A. M. Erisman, "Sparse Matrix Problems in Electric Power System Analysis," in Sparse Matrices and their Uses, Iain S. Duff, editor, Academic Press, New York, 1981.
2. R. G. Grimes and John Gregg Lewis, "Condition Number Estimation for Sparse Matrices," SIAM J. Scientific and Statistical Computing, Vol. 2, 1981, pp. 384-388.
3. John Gregg Lewis, "Implementation of the Gibbs-Poole-Stockmeyer Algorithm and the Gibbs-King Algorithm," ACM Transactions on Mathematical Software, to appear.
4. John Gregg Lewis and William G. Poole, Jr., "Ordering Algorithms Applied to Sparse Matrices in Electric Power Problems," in Electric Power Problems: The Mathematical Challenge, A. M. Erisman, K. W. Neves and M. H. Dwarakanath, editors, SIAM, Philadelphia, 1980.



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APPENDIX

Structure of the original matrix A and its factors L and U.

- a. Order of the matrix
- b. No. of nonzeros in the upper triangle
- c. No. of nonzeros in the lower triangle
- d. Distribution of nonzeros per row
- e. Distribution of nonzeros per column
- f. Nearness to symmetric structure
- g. Amount of storage required to represent the original matrix
- h. Presence of dense submatrices, subrows, subcolumns
- i. Storage requirements

Reordering and factorization combination

- a. Fillin
- b. Execution time
- c. Operation counts
- d. Stability bounds
 - i. Erisman and Reid estimate
 - ii. Actual bound based on largest element in the factorization
 - iii. Actual error, $E = A - LU$
- e. Number of pivots for numerical stability
- f. Structure of L and U
- g. Storage requirements
- h. Relative density of the reduced matrix

Reordering only

- a. Execution time
- b. Storage required
- c. Anything else dependent on the reordering module (eg. number of bumps and spikes in P4, optimization steps in HP)



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Symbolic factorization

- a. Execution time
- b. Fillin
- c. Relative density of the reduced matrix
- d. Structure of L and U
- e. Storage requirements

Factorization only (perform using MA28B)

- a. Execution time
- b. Operation counts
- c. Stability bounds
 - i. Erisman and Reid estimate
 - ii. Actual bound based on largest element in the factorization
 - iii. Actual error, $E = A - LU$
- d. Storage requirements

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