Highly Parallel Sparse Triangular Solution

Fernando L. Alvarado, Alex Pothen, and Robert Schreiber

The Research Institute of Advanced Computer Science is operated by Universities Space Research Association, The American City Building, Suite 311, Columbia, MD 244, (301)730-2656

Work reported herein was supported in part by the NAS Systems Division of NASA via Cooperative Agreement NCC 2-387 between NASA and the University Space Research Association (USRA). Work was performed at the Research Institute for Advanced Computer Science (RIACS), NASA Ames Research Center, Moffett Field, CA 94035. • •

10.00

-

_

- -

. _--

HIGHLY PARALLEL SPARSE TRIANGULAR SOLUTION *

FERNANDO L. ALVARADO[†], ALEX POTHEN[‡] AND ROBERT SCHREIBER[§]

Abstract. In this paper we survey a recent approach for solving sparse triangular systems of equations on highly parallel computers. This approach employs a partitioned representation of the inverse of the triangular matrix so that the solution can be computed by matrix-vector multiplication. The number of factors in the partitioned inverse is proportional to the number of general communication steps (router steps on a CM-2) required in a highly parallel algorithm. We describe partitioning algorithms that minimize the number of factors in the partitioned inverse over all symmetric permutations of the triangular matrix such that the permuted matrix continues to be triangular. For a Cholesky factor we describe an O(n)time and space algorithm to solve the partitioning problem above, where n is the order of the matrix. Our computational results on a CM-2 demonstrate the potential superiority of the partitioned inverse approach over the conventional substitution algorithm for highly parallel sparse triangular solution. Finally we list a few directions for extending these results.

AMS(MOS) subject classifications: 65F50, 65F25, 68R10.

Keywords. directed acyclic graph, elimination tree, massively parallel computers, partitioned inverse, reordering algorithm, sparse Cholesky factorization, sparse triangular systems.

1. Introduction. We survey some recent developments in the solution of sparse triangular linear systems of equations on a highly parallel computer. For concreteness, we consider a unit lower triangular system $L\underline{x} = \underline{b}$, but the results in the paper apply in a straightforward manner to upper triangular systems as well. We discuss the situation when there are multiple right-hand side vectors \underline{b} , and all these vectors are not necessarily available at once. Such situations occur in finite element applications, preconditioned iterative solvers for linear systems, solution of initial value problems by implicit methods, variants of Newton's method for the solution of nonlinear equations, and in numerical optimization.

There are two possible approaches to the parallel solution of triangular systems of equations. The usual approach is to exploit whatever limited parallelism is available in the usual substitution algorithm [4, 8]. The second approach requires preprocessing, and works with a partitioned representation of L^{-1} .

To begin we review the partitioned inverse approach to parallel triangular solution. Any unit lower triangular matrix L can be expressed as a product of elementary matrices: $L = \prod_{i=1}^{n} L_i$, where the elementary matrix L_i is unit lower triangular and nonzero below the diagonal only in column *i*. Hence it has the representation $L_i = I + \underline{m}_i \underline{e}_i^T$, where \underline{m}_i has its

^{*} Written May 1992. A part of this work was done while the authors were visiting the Institute for Mathematics and its Applications (IMA) at the University of Minnesota. We thank the IMA for its support.

[†] Electrical and Computer Engineering Department, 1425 Johnson Drive, The University of Wisconsin, Madison, WI 53706 (alvarado@ece.wisc.edu). The work of this author was supported in part under NSF Contracts ECS-8822654 and ECS-8907391.

¹ Department of Computer Science, Whitmore Lab, The Pennsylvania State University, University Park, PA 16802 (pothen@cs.psu.edu, na.pothen@na-net.ornl.gov). The research of this author was supported by NSF grant CCR-9024954 and by U. S. Department of Energy grant DE-FG02-91ER25095.

[§] RIACS, MS T045-1, NASA Ames Research Center, Moffett Field, CA 94035 (schreiber@riacs.edu). The work of this author was supported by the NAS Systems Division under Cooperative Agreement NCC 2-387 between NASA and the University Space Research Association (USRA).

first *i* components zero, and \underline{e}_i is the *i*-th coordinate vector. (Here it will be convenient to include $L_n \equiv I$ among the elementary matrices.) The elementary lower triangular matrices can be grouped together to form *m* unit lower triangular factors $L = \prod_{i=1}^{m} P_i$, where each factor P_i has the property that P_i^{-1} can be represented in the same space as P_i . (Here $m \leq n$ is a number to be determined.) Each factor $P_i = \prod_{k=e_i}^{e_{i+1}-1} L_k$, with $e_1 \equiv 1 < e_2 < \ldots < e_m < e_{m+1} \equiv n+1$. The factor P_i is lower triangular and is zero below its diagonal in all columns except columns e_i through $e_{i+1} - 1$. This leads to a partitioned representation of the inverse of L of the form $L^{-1} = \prod_{i=m}^{1} P_i^{-1}$ (each P_i^{-1} is explicitly stored) that can be stored in just the space required for L.

It follows that the solution to $L\underline{x} = \underline{b}$ can be computed by means of m matrix-vector products

$$\underline{x} = L^{-1}\underline{b} = \prod_{i=m}^{1} P_i^{-1}\underline{b}.$$

By using as many virtual processors as there are nonzeros in P_i and summing the products $\{(P_i^{-1})_{k\ell}b_{\ell} \mid (P_i^{-1})_{k\ell} \neq 0\}$ in logarithmic time, we may exploit parallelism fully in computing the matrix-vector products.

We consider the problem of computing partitioned inverses with the fewest factors in this paper, since in practice the complexity of highly parallel triangular solution is determined by the number of factors. There are two variations of this problem, and we describe them next after introducing some notation.

The matrix X is invertible in place if $x_{ij} \neq 0 \Leftrightarrow (X^{-1})_{ij} \neq 0$. Since the elementary lower triangular matrices are invertible in place, there is always at least one partition of L with factors that invert in place. A partition in which the factors P_i are invertible in place is called a *no-fill partition*. A no-fill partition of L with the fewest factors is a best no-fill partition. An admissible permutation Π of L is a symmetric permutation of the rows and columns of L such that the permuted matrix $\Pi L \Pi^T$ is lower triangular. A best reordered partition of L is a best no-fill partition of $\Pi L \Pi^T$ with the fewest factors over all admissible permutations of L.

An overview of this survey is as follows. We shall outline a theory of efficient algorithms for computing best no-fill and best reordered partitions of lower triangular matrices. Then we shall show that if L is restricted to be the unit lower triangular matrix from an LDL^T (Cholesky) factorization, there is an even more efficient algorithm for computing these partitions that makes use of the elimination tree. Next we demonstrate the usefulness of these ideas in practice by comparing the partitioned inverse approach with a conventional triangular solution algorithm on a Connection Machine CM-2. We conclude by summarizing our findings and describing ways in which this work can be extended.

2. Two partitioning problems. We begin by providing formal statements anf graph models of the best no-fill and best reordered partitioning problems, and then describe algorithms for computing the partitions when L is obtained from unsymmetric, symmetric indefinite, or incomplete factorizations.

2.1. Graph models. A formal statement of the best no-fill partitioning problem is as follows:



FIG. 1. A directed acyclic graph G(L) corresponding to a Cholesky factor L. The numbers outside the vertices represent a reordering.

- (P1) Given a unit lower triangular matrix $L = \prod_{i=1}^{n-1} L_i$, find a partition into factors $L = \prod_{i=1}^{m} P_i, \text{ where} \\ 1. \text{ each } P_i = \prod_{k=e_i}^{e_{i+1}-1} L_k, \text{ with } e_1 = 1 < e_2 < \cdots < e_m < e_{m+1} = n,$

 - 2. each P_i inverts in place, and
 - 3. m is minimum over all partitions satisfying the given conditions.

It is helpful to consider a graph model of (P1) and the other partitioning problems. Let G(L) denote a directed graph with vertices $V = \{1, \ldots, n\}$ corresponding to the columns of L and edges $E = \{(j,i) : i > j \text{ and } l_{ij} \neq 0\}$. The edge (j,i) is directed from the lowernumbered vertex j to the higher-numbered vertex i. It follows that G(L) is a directed acyclic graph (DAG). If there is a directed path from a vertex j to a vertex i in G(L), we will say that j is a predecessor of i, and that i is a successor of j. In particular, if $(j,i) \in E$, then j is a predecessor of i and i is a successor of j.

Given a subset P of the columns of L, the column subgraph of G(L) induced by P is the graph which contains all edges that are directed from vertices in P to all vertices in G(L), and all the vertices which are the endpoints of such edges. Thus the column subgraph of P contains all edges corresponding to nonzeros in the column set P.

In what follows, we identify a subset of columns P with the factor formed by multiplying, in order of increasing column number, the elementary matrices corresponding to columns in P. The condition that the nonzero structure of a factor P should be the same as the structure of its inverse corresponds in the graph model to the requirement that the column subgraph of P should be transitively closed [7]. (A DAG G is *transitively closed* if for every pair of vertices j and i such that there is a directed path in G from j to i, the edge (j, i) is present in G.)

Hence a graph model of (P1) is as follows:

- (P1') Find an ordered partition $P_1 \prec P_2 \prec \cdots \prec P_m$ of the vertices of G(L) such that
 - 1. for every $v \in V$, if $v \in P_i$ then all vertices numbered less than v belong to P_1 , ..., P_i ,
 - 2. the column subgraph of each P_i is transitively closed, and
 - 3. m is minimum over all partitions satisfying the given conditions.

We illustrate these concepts by means of an example. Consider the matrix L with graph G(L) illustrated in Fig. 1. L has a best no-fill partition with six factors:

$$L = (L_1)(L_2L_3L_4)(L_5)(L_6\cdots L_9)(L_{10})(L_{11}L_{12}).$$

It is possible to symmetrically permute the rows and columns of L such that L remains lower triangular; this corresponds to a permutation of the vertices of G(L). If in Fig. 1 we reorder the vertices with the numbers shown outside the vertices, then the best no-fill partition of the permuted L is

$$L = (L_1 \cdots L_6)(L_7 L_8 L_9)(L_{10} L_{11} L_{12}),$$

which has only three factors.

A formal statement of the best reordered partitioning problem is as follows:

- (P2) Given a unit lower triangular matrix $L = \prod_{i=1}^{n-1} L_i$, find an admissible permutation
 - $L_{\Pi} = \Pi L \Pi^T$ and a partition $L_{\Pi} = \prod_{i=1}^m P_i$, where

1. each $P_i = \prod_{k=e_i}^{e_{i+1}-1} L_k$, with $e_1 = 1 < e_2 < \cdots < e_m < e_{m+1} = n$,

- 2. each P_i is invertible in place, and
- 3. m is minimum over all permutations Π such that L_{Π} is lower triangular.

In (P2), the action of the permutation Π on L is to reorder the elementary matrices whose product is L; however, these elementary matrices cannot be arbitrarily reordered, since we require the resulting matrix L_{Π} to be lower triangular. From the equation $L_i = I + \underline{m}_i \underline{e_i}^T$ it can be verified that the elementary matrices L_i and L_{i+1} can be permuted if and only if $l_{i+1,i} = 0$. These precedence constraints on the order in which the elementary matrices may appear is nicely captured in a graph model of (P2).

A topological ordering of G(L) is an ordering of its vertices in which predecessors are numbered lower than successors; i.e., for every edge $(j,i) \in E$, i > j. By construction, the original vertex numbering of G(L) is a topological ordering. A permutation Π that leaves L_{Π} lower triangular corresponds to a topological reordering of the vertices of G(L).

The graph model of (P2) is:

- (P2') Find an ordered partition $P_1 \prec P_2 \prec \cdots \prec P_m$ of the vertices of G(L) numbered in a topological ordering such that
 - 1. for every $v \in \{1, 2, ..., n-1\}$, if $v \in P_i$ then all predecessors of v belong to P_1 , ..., P_i ,
 - 2. the column subgraph of each P_i is transitively closed, and
 - 3. m is minimum over all topological orderings of G(L).

The permutation Π in (P2) can be obtained by renumbering the vertices in the ordered partition P_1 to P_m in increasing order, and in topological order within each subset P_i .

2.2. Partitioning algorithms. We now describe "greedy" algorithms for solving the best no-fill and best reordered partitioning problems.

Input: A unit lower triangular matrix $L = L_1 L_2 \cdots L_n$ and its DAG G(L). Output: A best no-fill partition of L. $i \leftarrow 1$; { L_i is the highest-numbered elementary matrix not included in a factor yet} $k \leftarrow 1$; { P_k is the factor being computed} while $(i \le n)$ do {Find the largest integer $r \ge i$ such that $L_i \cdots L_r$ is invertible in place.} $r \leftarrow i$; while r < n and every successor of the vertex r is a successor of all predecessors of r in G(L) do $r \leftarrow r+1$; od $P_k \leftarrow L_i \cdots L_r$; $k \leftarrow k+1$; $i \leftarrow r+1$; od



Best no-fill partitions. Algorithm P1, shown in Fig. 2, was proposed by Alvarado, Yu and Betancourt [3]. This algorithm greedily tries to include as many elementary matrices in the current factor as possible, while maintaining the property that a factor should invert in place, and obeying the 'left-to-right' precedence constraint in problem (P1). The condition that in the graph G(L) every successor of a vertex r is also a successor of every predecessor of r ensures that inclusion of L_r in the current factor P_k will continue to make $G(P_k)$ transitively closed, and thus P_k will be invertible in place. Alvarado, Yu, and Betancourt did not consider the issue of optimality, but later it was proved by Alvarado and Schreiber [2] that Algorithm P1 solves problem (P1).

Best reordered partitions. Now we describe Algorithm RP1 that solves the reordered partitioning problem (P2). A vertex v in the DAG G(L) is a source if there are no edges directed into v: i.e., there are no edges (u, v). The level of a vertex v is the length of a longest directed path into v. It follows that if v is a source, then level(v) = 0; furthermore, if v is not a source, then level(v) is the length of a longest path from a source to v. The level

values of all the vertices of G(L) can be computed in $\mathcal{O}(e)$ time. We define the set hadj(v) to be the set of all vertices adjacent to v and numbered higher than v.

Input: A lower triangular matrix $L = L_1 \cdots L_n$ and its DAG G(L). <u>Output</u>: A permutation $\Pi: V \longrightarrow \{1, \ldots, n\}$ and a partition of the permuted matrix L_{Π} into factors. Compute level(v) for all $v \in V$; $max_level \leftarrow \max_{v \in V}(level(v));$ $\{i \text{ elementary matrices have been included in factors}\}$ $i \leftarrow 0;$ $k \leftarrow 1;$ $\{P_k \text{ is the factor being computed}\}$ $e_0 \leftarrow 0;$ while i < n do $P_k \leftarrow \emptyset;$ $\ell \leftarrow min\{j | \text{ there is an unnumbered vertex at level } j\};$ $e_k \leftarrow i;$ repeat for every vertex v at level ℓ do if (([Condition 1a] v is unnumbered) and ([Condition 1b] Every predecessor of v has been numbered) and ([Condition 2] Every successor of v is a successor of all $u \in P_k$ such that u is a predecessor of v)) then $i \leftarrow i + 1; \quad \Pi(v) \leftarrow i;$ $P_k \leftarrow P_k \cup \{v\}; \quad e_k \leftarrow e_k + 1;$ fi od $\ell \leftarrow \ell + 1;$ until $\ell > max_level$ or no vertices at level $\ell - 1$ were included in P_k ; $k \leftarrow k+1;$ od

FIG. 3. Algorithm RP1.

Algorithm RP1, shown in Fig. 3, renumbers the elementary matrices during the course of its execution since it computes an appropriate symmetric permutation Π to minimize the number of factors.

Conditions 1a and 1b in the algorithm ensure that the first condition of problem (P2) is satisfied; similarly condition 2 ensures that the column subgraphs of the factors are transitively closed

Alvarado and Schreiber [2] proved that Algorithm RP1 finds a best reordered partition. The time complexity of the algorithm is dominated by the checking of condition 2: in the worst-case, this cost is $\sum_{v \in V} d_I(v)d_O(v)$, where $d_I(v)$ is the indegree and $d_O(v)$ is the outdegree of v. Since $d_I(v) \leq n-1$, and $\sum_{v \in V} d_O(v) = e$, the time complexity of the algorithm is $\mathcal{O}(ne)$. If we assume that the indegrees and outdegrees are bounded by d, then the complexity is $\mathcal{O}(d^2n)$. The space complexity is $\mathcal{O}(e)$.

₹

At the expense of additional space, in most cases we can reduce the running time required by Algorithm RP1 by incorporating two enhancements.

The first improvement is that a vertex need not be tested for inclusion into a factor P_k until all of its predecessors have been numbered. To accomplish this, in count(v) we count the number of unnumbered predecessors of each vertex v; initially, this is its indegree, and when the count reaches zero, we include it in a set \mathcal{E} of vertices eligible for inclusion in a factor.

The second improvement is to reduce the cost of checking condition 2 in Algorithm RP1. If u and v are both numbered vertices which have been included in the current factor P_k , and v is a successor of u, then $hadj(v) \subseteq hadj(u)$, otherwise v would have failed condition 2. Thus we need not consider vertex u when applying the requirements of condition 2 to a vertex that is also a successor of v. We make use of this in the faster implementation by keeping track in pred(v) the set of predecessors of each vertex v that may need to be examined in checking condition 2. In the situation above, when v is included in P_k we remove u from the predecessor sets of v's successors, thus avoiding the unnecessary checking.

Fig. 4 contains a description of Algorithm RP2 that incorporates these improvements.

The worst-case time complexity of Algorithm RP2 is $\mathcal{O}(ne)$ as well (and there are DAGs which attain this bound), though practically the above improvements should reduce the running times in many cases.

3. Cholesky factorization. Now we consider the restriction of (P2) to Cholesky factors. Then the graph G(L) viewed as an undirected graph is *chordal*; i.e., every cycle with more than three edges has a *chord*, an edge joining two nonconsecutive vertices on the cycle. The chordality of G(L) simplifies the problem a great deal since it suffices to consider the transitive reduction of G(L), the elimination tree, instead of G(L). This simplification enables the design of an $\mathcal{O}(n)$ -time and space algorithm for computing the partition.

The elimination tree of L (equivalently G(L)) is a directed tree $T = (V, E_T)$, whose vertices are the columns of L, with a directed edge $(j,i) \in E_T$ if and only if the lowestnumbered row index of a subdiagonal nonzero in the *j*-th column of L is *i*. (The edge is directed from *j* to *i*.) The vertex *i* is the *parent* of *j*, and *j* is a *child* of *i*. If (j,i) is an edge in the elimination tree, the lowest-numbered vertex in hadj(j) is *i*. A comprehensive survey of the role of elimination trees in sparse Cholesky factorization has been provided by Liu [10].

Our partitioning algorithm will require as input the elimination tree with vertices numbered in a topological ordering. It also requires the subdiagonal nonzero counts of each column v of L, stored in an array hd(v) (the higher degree of v). The algorithm uses a variable member to partition the vertices; $member(v) = \ell$ implies that v belongs to the set P_{ℓ} .

Unlike Algorithms RP1 and RP2 which compute the factors P_1, \ldots, P_m in that sequence by examining vertices according to their *level* values, Algorithm RPtree examines the vertices of the elimination tree in increasing order of their numbers. If a vertex v is a leaf of the tree, then it is included in the first *member* (the vertices in P_1). Otherwise, it divides the children of v into two sets: C_1 is the subset of the children u such that the column subgraph of G(L) induced by u and v is transitively closed, and C_2 denotes the subset of the remaining children. Let m_1 denote the maximum member value of a child in C_1 and m_2 denote the maximum member value of a child in C_2 . Set $m_i = 0$ if $C_i = \emptyset$. If C_1 is empty, or if $m_1 \leq m_2$, then we will show that v cannot be included in the same member as any of its children, and hence v begins a new member (m_2+1) . Otherwise, $m_1 > m_2$, and v can be included together with some child $u \in C_1$ such that member $(u) = m_1$.

We now describe the details of an implementation. The vertices of the elimination tree are numbered in a topological ordering from 1 to n. The descendant relationships in the elimination tree are represented by two arrays of length n, child and sibling. child(v) represents the first child of v, and sibling(v) represents the right sibling of v, where the children of each vertex are ordered arbitrarily. If child(v) = 0, then v has no child and is a leaf of the elimination tree; if sibling(v) = 0, then v has no right sibling. Algorithm RPtree is shown in Fig. 5.

The reader can verify that $P_1 = \{1, 3, 4, 7, 8, 9\}$, $P_2 = \{2, 5, 10\}$, and $P_3 = \{6, 11, 12\}$ for the graph in Fig. 1. The time and space complexities of the algorithm are easily shown to be $\mathcal{O}(n)$. We turn to a discussion of the the correctness of the algorithm.

Condition 1 of problem (P2) requires that if a vertex v belongs to P_{ℓ} , then all predecessors of v must belong to P_1, \ldots, P_{ℓ} . The elimination tree T, being the transitive reduction of the DAG G(L), preserves path structure: i.e., there exists a directed path from v to w in G(L)if and only if there is a (possibly some other) directed path from v to w in the elimination tree T. Hence the predecessors of a vertex in G(L) remain its predecessors in the elimination tree. Further, since we assign *member* values in a topological ordering of the vertices in the elimination tree, to satisfy Condition 1 we need consider only the children of a vertex v among its predecessors. Now since Algorithm RPtree assigns *member* values such that *member*(v) is greater than or equal to *member*(u) for any child u, the condition is satisfied.

Condition 2 requires that each factor P_{ℓ} be transitively closed. An important property of the elimination tree [10] is that if v is the parent of a vertex u in the elimination tree, then $hadj(u) \subseteq v + hadj(v)$. Hence $hd(u) \leq 1 + hd(v)$. On the other hand, if u and v can be included in the same transitively closed column subgraph, then $hadj(u) \supseteq v + hadj(v)$. It then follows that u and v can be possibly included in the same column subgraph only if $hadj(u) = \{v\} \cup hadj(v)$, or equivalently, hd(u) = 1 + hd(v). Furthermore, if v has a child u not satisfying the degree condition, then v but not u is adjacent to some higher numbered vertex x, and hence v cannot belong to the same member as u. Thus we partition the children of v into two subsets: C_1 consists of children u such that u and v can be included in the same column subgraph; C_2 includes the rest of its children. It follows that if m_i is the maximum member value among vertices in C_i , then the inclusion of v into a column subgraph containing a child preserves transitivity only if $m_1 > m_2$.

It can be established by induction that Algorithm RPtree solves (P2) by partitioning G(L) into the minimum number of factors over all topological orderings [12].

4. Experimental Results. In this Section we provide experimental results to demonstrate the superiority of the partitioned inverse approach over the conventional substitution algorithm for highly parallel triangular solution. First we describe the performance of the various partitioning algorithms, and then we report results for triangular solution on a CM-2. 4.1. Partitioning algorithms. We implemented Algorithms RP1, RP2, and RPtree and compared their performances on eleven problems from the Boeing-Harwell collection [6]. All the algorithms were implemented in C, within Alvarado's Sparse Matrix Manipulation System [1]. Each problem was initially ordered using the Multiple-Minimum-Degree ordering of Liu [9], and the structure of the resulting lower triangular factor L was computed. We call this the primary ordering step. Then Algorithms RP1, RP2, or RPtree were used in a secondary ordering step to reorder the structure of L to obtain the minimum number of partitions over reorderings that preserve the DAG G(L). All three algorithms lead to the same number of factors in the partition since they solve the same problem.

3

The experiments were performed on a Sun SPARC station IPC with 24 Mbytes of main memory and a 100 Mbyte swap space running the SunOS 4.1 version of the Unix operating system. The unoptimized standard system compiler was used to compile the code. Let $\tau(A)$ denote the number of nonzeros in the strict lower triangle of A; $\tau(L)$ is then e, the number of edges in G(L). We scale these numbers by a thousand for convenience. In Table 1, we report the scaled values of $\tau(A)$ and $\tau(L)$, the CPU times taken by the primary and secondary ordering algorithms (in seconds), and the height of the elimination tree obtained from the primary ordering.

Table 1 also reports the number of factors in the partitioned inverse of L. The number in the column 'Factors(P1)' corresponds to the number of factors in the solution of problem (P1), i.e., the best no-fill partition problem. The number in the column 'Factors(P2)' indicates the number of factors in the solution of problem (P2), i.e., the best reordered partitioning problem. Note the substantial decrease in the number of factors obtained by the permutation.

	Original Data		MMD		etree	CPU time (sec)		Factors		
Problem	n	$\tau(A)$	time	$\tau(L)$	height	RP1	RP2	RPtree	(P1)	(P2)
BCSPWR10	5,300	8.27	1.72	23.2	128	1.07	1.26	0.10	70	32
BCSSTK13	2,003	40.9	4.74	264	654	61.1	22.1	0.05	53	24
BCSSTM13	2,003	9.97	1.12	42.6	261	5.08	2.63	0.03	25	16
BLCKHOLE	2,132	6.37	0.73	53.8	224	3.15	2.58	0.05	24	15
CAN1072	1,072	5.69	0.72	19.4	151	0.78	0.92	0.02	21	16
DWT2680	2,680	11.2	1.82	49.9	371	2.43	2.45	0.05	50	36
LSHP3466	3,466	10.2	1.03	81.2	341	4.48	4.14	0.07	37	25
NASA1824	1,824	18.7	1.42	72.2	259	6.01	3.88	0.03	34	16
NASA4704	4,704	50.0	3.92	275	553	33.8	16.1	0.12	41	17
39x39 9pt	1,521	10.9	0.50	31.6	185	1.35	1.50	0.02	19	15
79x79 9pt	6,241	45.9	2.17	190	429	12.7	11.4	0.12	30	23

TABLE 1

Comparison of execution times on a Sun SPARC station IPC for three secondary reordering schemes with the MMD primary ordering. The parameters $\tau(A)$ and $\tau(L)$ have been scaled by a thousand for convenience.

Later results in this section will show that when the partitioned inverse is employed on a highly parallel computer, the number of factors in the partitioned inverse determines the

9

complexity of parallel triangular solution. On the other hand, the complexity of a conventional triangular solution algorithm is governed by the height of the elimination tree. Table 1 shows both these quantities, and it is seen that the number of factors in the partitioned inverse is several fold smaller (by a factor of sixteen on the average) than the elimination tree height. Hence the use of the partitioned inverse potentially leads to much faster parallel triangular system solution on massively parallel computers.

For the $k \times k$ model grid problem ordered by the optimal nested dissection ordering, the height of the elimination tree is $3k + \Theta(1)$, while the number of factors (in (P1) and (P2)) is $2\log_2 k + \Theta(1)$. The results in Table 1 show that the number of factors for these irregular problems is only weakly dependent on the order of A, compatible with logarithmic growth.

The RPtree algorithm has $\mathcal{O}(n)$ time complexity while RP1 and RP2 are both $\mathcal{O}(n\tau(L))$ algorithms. This is confirmed by the experiments: on the average problem in this test set, RPtree is more than a hundred times faster than RP1 or RP2, and the advantage increases with increasing problem size. From a practical perspective, the time needed by the RPtree algorithm is quite small when compared to the cost of computing the initial MMD ordering. An equally important advantage of the RPtree algorithm is that it requires only $\mathcal{O}(n)$ additional space, whereas both RP1 and RP2 require $\mathcal{O}(\tau(L))$ additional space. However, Algorithms RP1 and RP2 can be used to partition triangular factors arising from approximate or incomplete Cholesky factorizations as well as unsymmetric and symmetric indefinite factorizations.

We have also experimented with a variant of the Minimum-Length-Minimum-Degree (MLMD) ordering [5] as the primary ordering, but we do not report detailed results here. The MLMD ordering incurs a great deal more fill in L than the MMD algorithm, and its current, fairly straightforward implementation is quite slow compared to the MMD algorithm. We believe an implementation comparable in sophistication to the MMD algorithm should not be significantly slower than MMD, and may also reduce fill. In spite of the greater fill, the MLMD ordering is more effective in almost all cases than MMD in reducing the number of factors in the partition of both L and L_{Π} . In some cases, the initial number of factors obtained when MLMD is used as the primary ordering is lower than the final number of *levels* obtained with MMD after the secondary reordering (II in problem (P2)). However, because of the increased fill, choosing between MMD and MLMD as the primary ordering is not straightforward.

4.2. Triangular solution on a CM-2. Now we compare the performance of the partitioned inverse approach with the conventional substitution algorithm for triangular solution on a CM-2.

An efficient parallel substitution algorithm was implemented in CM Fortran, a dialect of Fortran 90. The data structure consists of several arrays of length equal to $\tau(L)$. We associate, at least conceptually, a set of $\tau(L)$ virtual processors, one with each position in these arrays. We store the factors \hat{L} and D where $L = \hat{L}D$ and \hat{L} is unit triangular, and solve $L\underline{x} = \underline{b}$ via $\hat{L}\underline{x} = D^{-1}\underline{b}$, since this removes a multiplication from the inner loop. The matrix \hat{L} is stored as a one-dimensional array containing its nonzeros in column-major order. In addition, the *level* of vertex j in G(L) is stored along with \hat{L}_{ij} . The elements of \underline{b} are stored at the processors containing the corresponding diagonal elements of \hat{L} . The solution \underline{x} overwrites \underline{b} . Finally, a Boolean vector indicates the location of the diagonal elements in the arrays. This vector thus segments the arrays into columns of differing lengths—in other words, the matrix is stored as a ragged array of columns of nonzeros. The Connection Machine software provides some operations for such data structures. It allows broadcast of values from diagonal elements to all elements of the corresponding column (called a segmented copy scan) and summation of the values in a column (with a segmented add scan). Also, the Connection Machine router allows processors to send data to any other processor or read from any other processor; this is expressed using a vector-valued subscript in CM Fortran. Calls to utility library routines were used for the scan operations, which are not part of CM Fortran.

The substitution algorithm for triangular solution loops sequentially over levels of G(L)starting with the source vertices (level zero). At the beginning of step ℓ , those elements x_j for which $level(j) = \ell$ are known. Recall that x_j is stored in the processor holding \hat{L}_{jj} . These known values of \underline{x} are sent to the processors holding the corresponding column of \hat{L} by a segmented copy scan. These processors then multiply their \hat{L} value by the element of \underline{x} they receive. The router is then used to permute all these products into row-major order, so that the elements of each set $R_i \equiv \{\hat{L}_{ij}x_j \mid L_{ij} \neq 0 \text{ and } level(j) = \ell\}$ are stored in consecutive locations. The vector-valued subscript used to accomplish this permutation is computed in a preprocessing step. The rows R_i now form a ragged array. A segmented add scan forms the sums of these partial results within rows. Finally, the router is used to send the sum of the elements of R_i to the processor holding \hat{L}_{ii} and b_i where it can be subtracted from b_i . (In fact, our code avoids this last subtraction entirely, doing it as part of the add scan above.)

Thus an iteration of the loop involves one parallel multiplication, one copy scan and one add scan, and two uses of the router for permutation of data. The time required to set up and load the data structure, including the computation of the permutation used, the loading of \underline{b} and extraction of \underline{x} , was not timed.

The sequential algorithm for solving a triangular system is quite similar to the algorithm for computing a matrix-vector product involving a triangular matrix. Hence the code for triangular solution using the partitioned inverse approach is nearly identical to that for our substitution method in that the inner loop involves the same operations. But the number of executions of the loop in the partitioned inverse approach is equal to the number of factors in the partition of L rather than the number of *levels* in its graph.

We report the CM performance of these two methods for an $n \times n$, dense, unit lowertriangular matrix L. Our results are obtained with CM Fortran in the 'slice-wise' execution model, which treats each Weitek chip of the CM-2 as a processor. For this experiment we used 256 Weitek processors on the Connection Machine at NASA Ames. Results are given in Table 2. Clearly, the partitioned method is superior, by a factor roughly equal to the ratio of the number of *levels* in G(L) (which is n in this case) to the number of factors (one) in the partition of L.

Next, we performed an experiment using a sparse matrix A of order 4037 obtained from a triangular mesh in the region around a three-element airfoil. Three unit lower triangular matrices L_1 , L_2 , and L_3 were obtained by approximate factorization. L_1 is obtained by an incomplete LU factorization of A; we carry out the Gaussian elimination process, but we

n	$\tau(L)$	Levels	Substitution	Factors	Partitioned		
		in $G(L)$	Time		soln. time		
256	32,896	256	7.34	1	0.04		
512	131,328	512	50.22	1	0.21		
TABLE 2							

CM-2 times (seconds) for full matrix substitution and partitioned solution.

Matrix	Ordering	Factor-	$\tau(L)$	Levels	Substitution	Factors	Partitioned
	0	ization		in $G(L)$	Time		soln. time
L	RCM	ILU	23,526	823	19.22	816	11.66
	MLMD	ILU	26,793	78	1.38	66	1.20
La	MLMD	exact	118,504	311	16.78	16	0.87
13			I			· · · · · · · · · · · · · · · · · · ·	

TABLE 3

CM-2 times (seconds) for sparse triangular substitution and partitioned solution.

allow nonzeros in L (and U) only where there is a nonzero in A^2 . The ordering of A is obtained from a lexicographic sort of the (x, y) coordinates of the grid which leads to the matrix; this ordering produces a large number of *levels* in G(L). L_2 is the incomplete LU factor obtained when a variant of MLMD is used as the primary ordering of A. L_3 is the exact lower-triangular factor of A, with the same primary ordering as for L_2 .

In Table 3 we give the size of these factors, the number of *levels* (this is proportional to the time required for our parallel substitution algorithm), and the number of factors, which is in practice proportional to the time required by the partitioned inverse approach.

These results confirm that the time required to solve a triangular system by partitioning of the inverse is quite well predicted by the number of factors in the partition. It also shows that the number of *levels* in G(L) is a good predictor of the time required for solution by substitution methods. We see that when L has a fairly rich structure the partitioned inverse approach is much better than the substitution method, but when L is very sparse there is little gained. The use of an MLMD primary ordering improves both substitution and partitioned methods. However, with the introduction of the additional fill in the exact factor L_3 (compared with L_2), the number of *levels* in G(L) increases sharply (as does the time for substitution) while the number of factors in the best reordered partition drops dramatically. The difference in the solution time, even for this problem of modest size, is about a factor of twenty. Thus we conclude that the method can be quite useful in highly parallel machines when the matrix L has a rich enough structure, as happens when it is an exact triangular factor.

5. Concluding remarks. We have considered several issues associated with highly parallel sparse triangular solution. We have described algorithms for minimizing the number of factors in the partitioned inverse over symmetric permutations of a lower triangular matrix L. When L is obtained from unsymmetric, symmetric indefinite, or incomplete factorization, Algorithms RP1 and RP2 may be used to compute the partitions. When L is a Cholesky factor, Algorithm RPtree is an extremely efficient $\mathcal{O}(n)$ time and space algorithm for com-

puting the partitions. We believe that the results in this paper demonstrate the potential superiority of the partitioned inverse approach over the conventional substitution algorithm for sparse triangular solution on highly parallel computers.

There are several directions to explore in future work.

3

One issue is to reduce the number of factors in the partitioned inverse further by permitting some fill. Another is to partition the original matrix A into a block triangular matrix ensuring only that the diagonal blocks incur no fill upon inversion. Then the subdiagonal blocks of A need not be inverted, since the solution to the triangular system can be decomposed in the usual way into the solution of several subsystems. The solution vector associated with each subsystem can be computed using the partitioned inverse of its diagonal block, and then by block back-substitution the contribution this solution vector makes to higher numbered subsystems can be eliminated. Thirdly, it may be possible to design partitioning algorithms which are more efficient in practice by using the transitive reduction of the DAG G(L).

A fourth issue concerns sparse Cholesky factors. Given the factorization $A = LDL^{T}$ of a symmetric, positive definite matrix, consider the filled matrix $F = L + L^{T}$ and the corresponding undirected graph G(F) which is chordal. In problem (P3) we ask for the minimum number of factors m in the partitioned inverse representation of L over all vertex orderings that preserve the structure of the filled graph G(F) (rather than preserving the structure of the DAG G(L) as (P2) does). Such an ordering would have to be applied to the original matrix A, before the computation of the factorization. This problem turns out to be much harder than (P2), but can be solved by developing a theory of transitive perfect elimination orderings: i.e., perfect elimination orderings of subgraphs of chordal graphs which make them transitively closed subgraphs as well. An efficient algorithm to solve (P3) by means of the clique tree data structure will be reported in [11].

REFERENCES

- F. L. ALVARADO, Manipulation and visualization of sparse matrices, ORSA J. Comput., 2 (1990), pp. 180-207.
- [2] F. L. ALVARADO AND R. SCHREIBER, Optimal parallel solution of sparse triangular systems. SIAM J. Sci. Stat. Comput., to appear, 1992.
- [3] F. L. ALVARADO, D. C. YU, AND R. BETANCOURT, Partitioned sparse A⁻¹ methods, IEEE Trans. Power Systems, 5 (1990), pp. 452-459.
- [4] E. ANDERSON AND Y. SAAD, Solving sparse triangular systems on parallel computers, International Journal of High Speed Computing, 1 (1989), pp. 73–95.
- [5] R. BETANCOURT, An efficient heuristic ordering algorithm for partial matrix refactorization, IEEE Trans. Power Systems, 3 (1988), pp. 1181–1187.
- [6] I. S. DUFF, R. G. GRIMES, AND J. G. LEWIS, Sparse matrix test problems, ACM Trans. Math. Softw., 15 (1989), pp. 1-14.
- [7] J. R. GILBERT, Predicting structure in sparse matrix computations, Tech. Report 86-750, Computer Science, Cornell University, 1986.
- [8] S. W. HAMMOND AND R. SCHREIBER, Efficient ICCG on a shared memory multiprocessor. International Journal of High-Speed Computing, to appear, 1992.
- J. W. H. LIU, Modification of the minimum-degree algorithm by multiple elimination, ACM Trans. Math. Softw., 11 (1985), pp. 141–153.

- [10] —, The role of elimination trees in sparse factorization, SIAM J. Mat. Anal. Appl., 11 (1990), pp. 134-172.
- [11] B. W. PEYTON, A. POTHEN, AND X. YUAN, Transitive perfect elimination of chordal graphs and sparse triangular solution. Work in preparation, 1992.
- [12] A. POTHEN AND F. L. ALVARADO, A fast reordering algorithm for parallel sparse triangular solution, SIAM J. Sci. Stat. Comput., 13 (1992), pp. 645-653.

1

Ŧ

Input: A lower triangular matrix $L = L_1 \cdots L_n$ and its DAG G(L). <u>Output</u>: permutation $\Pi: V \longrightarrow \{1, \ldots, n\}$ and a partition of L into factors. forall $v \in V$ do $pred(v) \leftarrow \{u : L_{vu} \neq 0\}; \quad count(v) \leftarrow indegree(v);$ compute level(v); od $max_level \leftarrow max_{v \in V}(level(v));$ $i \leftarrow 0; \{i \text{ elementary matrices have been included in factors}\}$ $k \leftarrow 1; \{ P_k \text{ is the factor being computed} \}$ $e_0 \leftarrow 0;$ $\mathcal{E} \leftarrow \{v \in V : count(v) = 0\}; \{vertices with no unnumbered predecessors\}$ while i < n do $P_k \leftarrow \emptyset; \quad e_k \leftarrow i;$ $\ell \leftarrow min\{j \mid \text{there is an unnumbered vertex at level } j\};$ repeat for every vertex $v \in \mathcal{E}$ at level ℓ do if ([Condition 2'] Every successor of v is a successor of all $u \in pred(v)$) then $i \leftarrow i+1; \quad \Pi(v) \leftarrow i;$ $P_k \leftarrow P_k \cup \{v\}; \quad e_k \leftarrow e_k + 1;$ for every successor w of v do $pred(w) \leftarrow pred(w) \setminus pred(v);$ $count(w) \leftarrow count(w) - 1;$ if count(w) = 0 then $\mathcal{E} \leftarrow \mathcal{E} \cup \{w\}$; fi od fi od $\ell \leftarrow \ell + 1;$ until $\ell > max_level$ or no vertices at level $\ell - 1$ were included in P_k ; $k \leftarrow k+1;$ od

7

FIG. 4. Algorithm RP2.

```
Input: The elimination tree of a DAG G(L) and the higher degrees of the vertices.
<u>Output</u>: A mapping of the vertices such that member(v) = \ell implies that v \in P_{\ell}.
for v := 1 to n \rightarrow 
     if child(v) = 0 then \{v \text{ is a leaf}\}
            member(v) := 1;
      else \{v \text{ is not a leaf}\}
            u := child(v); m_1 := 0; m_2 := 0;
            while u \neq 0 do
                  if hd(u) = 1 + hd(v) then
                        m_1 := \max\{m_1, member(u)\};
                         \{hd(u) < 1 + hd(v)\}
                  else
                        m_2 := \max\{m_2, member(u)\};
                  fi
                  u := sibling(u);
            od
            if m_1 \leq m_2 then \{v \text{ begins a new factor}\}
                  member(v) := m_2 + 1;
            else \{m_1 > m_2, v \text{ can be included in a factor which includes a child}\}
                  member(v) := m_1;
            fi
      fi
rof
```



3