

IAIN S. DUFF^{†‡} AND KAMER KAYA^{†§}

Abstract. This paper proposes an approach for obtaining block diagonal and block triangular preconditioners that can be used for solving a linear system $\mathbf{Ax} = \mathbf{b}$, where \mathbf{A} is a large, nonsingular, real, $n \times n$ sparse matrix. The proposed approach uses Tarjan's algorithm for hierarchically decomposing a digraph into its strong subgraphs. To the best of our knowledge, this is the first work that uses this algorithm for preconditioning purposes. We describe the method, analyse its performance, and compare it with preconditioners from the literature such as ILUT and XPABLO and show that it is highly competitive with them in terms of both memory and iteration count. In addition, our approach shares with XPABLO the benefit of being able to exploit parallelism through a version that uses a block diagonal preconditioner.

Key words. sparse matrices, strong subgraphs, strong components, preconditioners

AMS subject classifications. 05C50, 05C70, 65F50

1. Introduction. Given a linear system

$$(1.1) Ax = b$$

where A is a real, large, sparse square matrix of order n, we propose a method to construct a preconditioning matrix M to accelerate the solution of the system when using Krylov methods. The proposed method is based on a hierarchical decomposition of the associated digraph into its strong subgraphs. This decomposition can be used to find a permutation of the matrix to produce a block form that can be used to build either a block diagonal matrix for use as a block Jacobi preconditioner or a block tridiagonal matrix for use as a block Gauss-Seidel preconditioner.

The algorithm we use to create the blocks on the diagonal of M is a modified version of Tarjan's algorithm HD that decomposes a digraph into its strong subgraphs hierarchically [26]. Tarjan assumed that the edges of the digraph are weighted and HD uses this weight information to create the hierarchical decomposition. However, HD requires distinct edge weights if it is implemented as given in [26]. In this paper, we propose a slight modification of HD which allows us to handle digraphs whose edge weights are not necessarily distinct. We make further modifications to the algorithm to use it for preconditioning purposes. The strong subgraphs formed by the modified version of HD correspond to the blocks on the diagonal of M. To the best of our knowledge, this is the first work that uses Tarjan's hierarchical decomposition algorithm for preconditioning purposes. We call our modified version HDPRE.

We should emphasize at this point that this algorithm of Tarjan is different from the much better known algorithm for obtaining the strong components of a reducible matrix. This earlier algorithm [24], which we call SCC, is used widely in the solution of reducible systems and is also called by HD and HDPRE, which can be viewed as extending the earlier work to irreducible matrices. We use the output from HDPRE to determine our preconditioners. This is done by SCPRE that can generate a block diagonal preconditioner or a block upper-triangular one.

^{*} Received January 29, 2012. Accepted March 20, 2013. Published online on July 15, 2013. Recommended by D. Szyld.

[†]CERFACS, 42 Avenue Gaspard Coriolis, 31057, Toulouse, Cedex 01, France

^{({}duff, Kamer.Kaya}@cerfacs.fr).

[‡]Building R 18, RAL, Oxon, OX11 0QX, England (iain.duff@stfc.ac.uk).

[§]Current address: Department of Biomedical Informatics, The Ohio State University, Columbus, OH, USA.

We have conducted several experiments to see the efficiency of the SCPRE algorithm. We compare the number of iterations for convergence and the memory requirement of the GMRES [23] iterative solver when the proposed approach and a set of ILUT preconditioners [21, 22] are used. We are aware that block based preconditioning techniques have been studied before and successful preconditioners such as PABLO and its derivatives have been proposed [14, 15]. These preconditioners were successfully used for several matrices [3, 5, 10]. In this paper, we compare our results also with XPABLO [14, 15].

Section 2 gives the notation used in the paper and background on Tarjan's algorithm HD. The proposed algorithm is described in Section 3 and the implementation details are given in Section 4. Section 5 gives the experimental results and Section 6 concludes the paper.

2. Background. Let **A** be a large, nonsingular, $n \times n$ sparse matrix with m off-diagonal nonzeros. The digraph G = (V, E) associated with **A** has n vertices, $v_i, i = 1, ..., n$, in its vertex set V where v_i corresponds to the *i*th row/column of **A** for $1 \le i \le n$, and $v_i v_j$ is in the edge set E if and only if \mathbf{A}_{ij} is nonzero for $1 \le i \ne j \le n$. Note that we do not consider self-loops of the form $v_i v_i$ corresponding to diagonal entries in the matrix. Figure 2.1 shows a simple 6×6 matrix with 13 nonzeros and its associated digraph.



FIG. 2.1. A 6×6 matrix **A** with 13 off-diagonal nonzeros on the left and its associated digraph *G* on the right. The nonzeros on the diagonal of **A** are shown with \times . Except for these entries, there is an edge in the associated digraph *G* for each nonzero of **A**.

A path is a sequence of vertices such that there exists an edge between every two consecutive vertices. A path is called *closed* if its first and last vertex are the same. A vertex u is *connected* to v if there is a path from u to v in G. A directed graph G is *strongly connected* if uis connected to v for all $u, v \in V$. Note that a digraph with a single vertex u is strongly connected. A digraph G' = (V', E') is a subgraph of G if $V' \subset V$ and $E' \subseteq E \cap (V' \times V')$. If G'is strongly connected, it is called a strong subgraph (or a strongly connected subgraph) of G. Furthermore, if G' is *maximally* strongly connected, i.e., if there is no strong subgraph G''of G such that G' is a subgraph of G'', it is called a strong component (or a strongly connected component) of G. If the matrix \mathbf{A} cannot be permuted into a block triangular form (BTF) by simultaneous row and column permutations, i.e., if the associated digraph is strongly connected, we say that \mathbf{A} is irreducible. Otherwise, we call it reducible.

Let G = (V, E) be a digraph and $\mathcal{P}(V) = \{V_1, V_2, \dots, V_k\}$ define a partition of V into disjoint sets, i.e., $V_i \cap V_j = \emptyset$ for $i \neq j$ and $\bigcup_{i=1}^k V_i = V$. Let $\mathcal{V} = \{\mathcal{V}_1, \mathcal{V}_2\}$ be a set of two vertex partitions such that $\mathcal{V}_1 = \mathcal{P}(V)$ and

$$\mathcal{V}_2 = \bigcup_{V_i \in \mathcal{V}_1} \mathcal{P}(V_i),$$

i.e., \mathcal{V}_2 is a finer partition obtained from partitioning the parts in \mathcal{V}_1 . Hence, for instance, if $\mathcal{V}_1 = \{\{1, 2, 3\}, \{4, 5, 6\}\}$ then \mathcal{V}_2 can be $\{\{1\}, \{2, 3\}, \{4, 5\}, \{6\}\}$ but cannot be the partition $\{\{1, 2\}, \{3, 4\}, \{5, 6\}\}$. Let $no_1(v)$ and $no_2(v)$ denote the index of the part containing the vertex $v \in V$ for \mathcal{V}_1 and \mathcal{V}_2 , respectively.

Let condense be an operation which takes G and \mathcal{V} as inputs and returns a condensed digraph condense $(G, \mathcal{V}) = G^{\mathcal{V}} = (V^{\mathcal{V}_2}, E^{\mathcal{V}_1})$ where each vertex set $V_i \in \mathcal{V}_2$ is condensed into a single vertex $\nu_i \in V^{\mathcal{V}_2}$. For all $uv \in E$, with $no_2(u) = i$ and $no_2(v) = j$, there exists an edge $\nu_i \nu_j \in E^{\mathcal{V}_1}$ if and only if $no_1(u) \neq no_1(v)$, i.e., u and v are in different coarse parts. Note that even though G is a simple digraph, $G^{\mathcal{V}}$ can be a directed multigraph, i.e., there can be multiple edges between two vertices. The definitions of connectivity and strong connectivity in directed multigraphs are the same as those in digraphs. An example for the condense operation is given in Figure 2.2.



FIG. 2.2. An example for the condense operation on the digraph in Figure 2.1(b). The vertex partitions $\mathcal{V}_1 = \{\{1, 2, 3\}, \{4, 5, 6\}\}$ and $\mathcal{V}_2 = \{\{1\}, \{2, 3\}, \{4, 5\}, \{6\}\}$ are shown in (a). The condensed graph is shown in (b).

3. A strong subgraph based preconditioner. Our proposed algorithm, SCPRE, generates a preconditioner M with a block diagonal or block upper-triangular structure where the size of each block is smaller than a requested maximum block size mbs. For the experiments, we scale and permute A from (1.1) by Duff and Koster's MC64 with the option that uses the maximum product transversal [11]. The idea used by MC64 is due to Olschowska and Neumaier [20], who propose an algorithm which permutes and scales the matrix in such a way that the magnitudes of the diagonal entries are one and the magnitudes of the off-diagonal entries are all less than or equal to one. Such a matrix is called an *I-matrix*. For direct methods, it has been observed that the more dominant the diagonal of a matrix, the higher the chance that diagonal entries are stable enough to serve as pivots for elimination. For iterative methods, as previous experiments have shown, such a scaling is also of interest [4, 11]. We observed a similar behaviour in our preliminary experiments and used MC64 for scaling and permuting the original matrix. From now on, we will assume that the diagonal of A is nonzero since this is the case after this permutation.

SCPRE uses the block structure from HDPRE to determine the diagonal blocks of the preconditioner **M**. We then combine some of these blocks if the combination has fewer than *mbs* rows/columns and the combination is not block diagonal. The diagonal blocks of the resulting matrix can then be used to precondition the iterative solver using the block Jacobi algorithm and can exploit parallel architectures as the blocks are independent. If we

ETNA Kent State University http://etna.math.kent.edu

require a block diagonal preconditioner, then we are finished. Otherwise, SCPRE permutes the blocks and builds a block upper-triangular preconditioner.

If **A** is reducible and the maximum block size in the BTF of **A** is less than or equal to *mbs*, then SCPRE will find this form or will return the diagonal blocks of it if a block diagonal preconditioner is desired. The permutation of a matrix into its block triangular form is a well-known technique that has been recently and successfully used by direct and iterative solvers for circuit simulation matrices [9, 27], which can often be permuted to a non-trivial BTF. For some applications, such as DC operating point analysis, the block triangular form has many but small blocks [27]. Such a matrix is usually easy to factorize if we initially permute it to BTF, so that a direct solver like KLU [9] only needs to factorize the diagonal blocks. Note that Tarjan's SCC algorithm that has linear complexity in the matrix order and the number of nonzeros has been widely and successfully used by the computational linear algebra community for obtaining a BTF that is then exploited by subsequent solvers. A code implementing this algorithm is available as MC13 from HSL [19] and it is also an algorithm in ACM TOMS [12, 13].

However, when the matrix is irreducible, the SCC algorithm is not applicable. Furthermore, even if the matrix is reducible, we may have little gain from using the BTF because this form may have one or more very large blocks. This is the case for applications like transient simulation or for circuit matrices with feedbacks. For this reason we propose using Tarjan's HD algorithm [26] as an additional tool to SCC. SCPRE uses HDPRE and further decomposes blocks larger than *mbs* to make the resulting preconditioner practical. For these reasons, in our experiments, we only use matrices that are irreducible or have a large block in their BTF. The details of SCPRE and the algorithms it uses are given in the next section. Note that since we use a combinatorial algorithm from graph theory for preconditioning purposes, we will use terms from graph theory in the following text so that *row/column* and *vertex* are used interchangeably as well as *nonzero* and *edge*.

3.1. SCPRE: obtaining the block diagonal preconditioner. To obtain a block diagonal preconditioner, SCPRE uses HDPRE and then combines some of these blocks if the size of the combined block is at most *mbs* and the combined block is not block diagonal. In this section, we present the details of these algorithms. First, we describe Tarjan's hierarchical decomposition algorithm more precisely.

3.1.1. Tarjan's algorithm for hierarchical clustering. Let G = (V, E) be the digraph associated with A. The weight of an edge $uv \in E$ is denoted by w(uv) and is set to the absolute value of the corresponding off-diagonal nonzero. Hence, there are m edges and all of the edges have positive weights. A hierarchical decomposition of G into its strong subgraphs can be defined in the following way. Let σ_0 be a permutation of the edges. For $1 \le i \le m$, let $\sigma_0(i)$ be the *i*th edge in σ_0 and $\sigma_0^{-1}(uv)$ be the index of the edge uvin the permutation for all $uv \in E$. Let $G_0 = (V, \emptyset)$ be the graph obtained by removing all the edges from G. We then add edges one by one to G_0 in the order determined by σ_0 . Let $G_i = (V, \{\sigma(j) : 1 \le j \le i\})$ be the digraph obtained after the addition of the first i edges. Initially in G_0 , there are n strong components, one for each vertex, and during the edge addition process, the strong components gradually coalesce until there is only one, as we are assuming that \mathbf{A} is irreducible. Note that if this is not the case, the algorithm will be used for the large irreducible blocks in \mathbf{A} . The hierarchical decomposition of G into its strong subgraphs with respect to the edge permutation σ_0 shows which strong components are formed in this process hierarchically. Note that a strong component formed in this edge addition process is indeed a strong component of some digraph G_i but not of G. For G, all except the last are just strong subgraphs.



FIG. 3.1. The hierarchical decomposition tree for the digraph G and the permutation given by the edge ordering in Figure 2.1(b).

A hierarchical decomposition can be represented by a hierarchical decomposition tree T, whose leaf nodes correspond to the vertices in V, non-leaf nodes correspond to edges in E, and subtrees correspond to the decomposition trees of the strong components that form as the process proceeds. Note that only the edges that create strong components during the process have corresponding internal nodes in T. If σ_0 is the ordering determined by the edge numbers, the hierarchical decomposition tree for the digraph in Figure 2.1(b) is given in Figure 3.1. As the figure shows, during the edge addition process, after the addition of the 3rd and 6th edges in σ_0 , the sets of vertices $\{1, 2, 3\}$ and $\{4, 5\}$ form a strong component of G_3 and G_6 , respectively. These strong components are then combined and form a larger one after the addition of the 11th edge. In Figure 3.1, the root of the tree is labelled with 12. Hence the first 12 edges in σ_0 are sufficient to construct a strongly connected digraph. For the figures in this paper, we use the labels of the corresponding vertices and the σ_0^{-1} -values of the corresponding edges to label each leaf and non-leaf node of a hierarchical decomposition tree, respectively.

Given a digraph G = (V, E) with n vertices and m edges and a permutation σ_0 , the hierarchical decomposition tree T can be obtained by first constructing G_0 and executing SCC for each internal digraph G_i obtained during the edge addition process. Note that this is an $\mathcal{O}(mn+m^2)$ algorithm since $1 \leq i \leq m$ and the cost of SCC is $\mathcal{O}(n+m)$ due to the strong component algorithm of Tarjan [24]. To obtain T in a more efficient way, Tarjan first proposed an $\mathcal{O}(m\log^2 n)$ recursive algorithm [25] and later improved his algorithm and reduced the complexity to $\mathcal{O}(m \log n)$ [26]. He assumed that the weights of the edges in the digraph are distinct, i.e., $w(uv) \neq w(u'v')$ for two distinct edges uv and u'v'. Here we modify the description of the algorithm so that it also works for the case when some edges have equal weights. Note that the connectivity of the digraph is purely structural and is independent of the edge weights. The only role that they play in Tarjan's algorithm HD is in the preprocessing step that defines a permutation σ_0 of the edges and in determining the ordering of the edges during the course of the algorithm. We eliminate the necessity of this latter use by avoiding numerical comparisons through just using the indices of the edges with respect to σ_0 . With this slight modification, the algorithm remains correct even when some edges have the same weight, which is very important as many matrices have several or many nonzeros with the same numerical value.

HD uses a recursive approach and for every recursive call, it gets a digraph G = (V, E), a permutation σ of the edges, and a parameter *i* as inputs such that *G* is strongly connected and G_i is known to be acyclic, i.e., every vertex is a separate strong component [26]. For the initial call, *i* is set to 0 and the initial permutation is set to σ_0 which is a permutation of all the edges in the original digraph.

For a call of $HD(G = (V, E), \sigma, i)$, the size of the subproblem is set to |E| - i, the number of edges that remain to be investigated (Tarjan used the term rank to denote the size of a subproblem). Note that in the first step, HD knows that G_i (that is G_0) is acyclic, that is, there are |V| strong components of G_0 , one for each vertex. If the subproblem size is one, since G

Algorithm 1 $T = HD(G = (V, E), \sigma, i)$. For the initial call, $\sigma = \sigma_0$ and i = 0.

1: if |E| - i = 1 then Let T be a tree with V leaves. Root is labelled with $\sigma_0^{-1}(\sigma(|E|))$ 2: 3: return T 4: **end if** 5: j = [(i + |E|)/2]6: if $G_j = (V, \{\sigma(k) : 1 \le k \le j\})$ is strongly connected then return $T = HD(G_j, \sigma, i)$ 7: 8: else for each strong component $SC_{\ell} = (V_{\ell}, E_{\ell})$ of G_j do 9: if $|V_\ell| > 1$ then 10: σ_{ℓ} = the permutation of E_{ℓ} ordered with respect to σ 11: if i = 0 or $(\sigma^{-1}(uv) > i, \forall uv \in E_{\ell})$ then 12: 13: $i_{\ell} = 0$ else 14: $i_{\ell} = \max\{k : \sigma^{-1}(\sigma_{\ell}(k)) \le i\}$ 15: end if 16: $T_{\ell} = \operatorname{HD}(SC_{\ell}, \sigma_{\ell}, i_{\ell})$ 17: 18: else 19: $T_{\ell} = (V_l, \emptyset)$ end if 20: end for 21: $\mathcal{V}_1 = \mathcal{V}_2 = \{V_\ell : SC_\ell \text{ is a strong component of } G_i\}$ 22: $\mathcal{V} = \{\mathcal{V}_1, \mathcal{V}_2\}$ 23: $G^{\mathcal{V}} = \texttt{condense}(G, \mathcal{V}) = (V^{\mathcal{V}_2}, E^{\mathcal{V}_1})$ 24: $\sigma^{\mathcal{V}}$ = the permutation of $E^{\mathcal{V}_1}$ ordered with respect to σ 25: if $(\sigma^{-1}(uv) > j, \forall uv \in E^{\mathcal{V}_1})$ then $i^{\mathcal{V}} = 0$ 26: 27: 28: else $i^{\mathcal{V}} = \max\{k : \sigma^{-1}(\sigma^{\mathcal{V}}(k)) \le j\}$ 29: end if 30: $T^{\mathcal{V}} = \mathrm{HD}(G^{\mathcal{V}}, \sigma^{\mathcal{V}}, i^{\mathcal{V}})$ 31: replace the leaves of $T^{\mathcal{V}}$ with the corresponding trees T_{ℓ} 32: return $T^{\mathcal{V}}$ 33: 34: end if

is strongly connected and G_i is acyclic, the vertices in V are combined with the addition of the |E|th edge in σ . Hence HD returns a tree T having a root labelled with $\sigma_0^{-1}(\sigma(|E|))$ and |V| leaves. If the subproblem size is not one, HD performs a binary chop and checks if G_j , $j = \lceil (i + |E|)/2 \rceil$, is strongly connected. If G_j is strongly connected, then all of the strong components will be combined before the addition of the (j + 1)th edge. Hence the algorithm calls HD(G_j , σ , i). Otherwise, a recursive call is made for each strong component of size larger than one. A detailed pseudo-code of HD is given in Algorithm 1.

By the definition of i, G_i , the subgraph containing the first i edges of G in σ , is known to be acyclic. Let i_ℓ be the number of these edges in the ℓ th strong subgraph $SC_\ell = (V_\ell, E_\ell)$ of G_j , i.e., $i_\ell = |\{uv \in E_\ell : \sigma^{-1}(uv) \leq i\}|$. Since SC_ℓ is a subgraph of G_i , G_i being acyclic implies that the subgraph of SC_ℓ containing only these i_ℓ edges is also acyclic. In Algorithm 1, lines 12–16, the number i_ℓ is found for each strong component SC_ℓ . This value is then used in the recursive call for SC_ℓ at line 17.

ETNA Kent State University http://etna.math.kent.edu

PRECONDITIONERS BASED ON STRONG SUBGRAPHS

Since G_j has more than one strong component and G is known to be strongly connected, with the addition of some edge(s) after the *j*th one, at least two strong components of G_j will be combined. To find this edge, another recursive call, $\text{HD}(G^{\mathcal{V}}, \sigma^{\mathcal{V}}, i^{\mathcal{V}})$, is made for the condensed graph $G^{\mathcal{V}} = (V^{\mathcal{V}_2}, E^{\mathcal{V}_1})$. Since each strong component of G_j is reduced to one vertex in $G^{\mathcal{V}}$, a subgraph of the condensed graph which contains only the edges from G_j must be acyclic. Hence we can find the value $i^{\mathcal{V}}$ in a similar fashion to i_{ℓ} . But this time instead of *i* we use *j* and set $i^{\mathcal{V}} = |\{uv \in E^{\mathcal{V}_1} : \sigma^{-1}(uv) \leq j\}|$ for the corresponding recursive call at line 31.

We investigate the size of each new subproblem for the complexity analysis of HD. At line 7 of Algorithm 1, the size of the subproblem becomes at most j - i and for the lines 17 and 31, there will be smaller subproblems with sizes at most j-i and |E|-j, respectively. By definition of j, every subproblem has a size at most $\frac{2}{3}$ of the original problem size (consider the case when i = 0 and |E| = 3). Note that every edge in the original problem corresponds to an edge in at most one subproblem and, if we do not count the recursive calls, the rest of the algorithm takes $\mathcal{O}(|E|)$. Let t(m, r) be the total complexity of a problem with m edges and problem size r, and k be the number of recursive calls. Then

$$\mathsf{t}(m,r) = \mathcal{O}(m) + \sum_{i=1}^{k} \mathsf{t}(m_i, r_i).$$

Since $\sum_{i=1}^{k} m_i \leq m$ and $r_i \leq 2r/3$, for $1 \leq i \leq k$, a simple induction argument shows that $t(m, r) = \mathcal{O}(m \log r)$. Hence the total complexity of the algorithm is $\mathcal{O}(m \log m)$ which is actually $\mathcal{O}(m \log n)$ since the original graph is a simple digraph (not a directed multigraph).

Let us sketch the algorithm for the digraph G = (V, E) in Figure 2.1(b). Assume that σ_0 is the ordering described in that figure. In the initial call, line 5 of Algorithm 1, the value j = 7 is computed and it is checked if G_7 is strongly connected. As Figure 3.2 shows, G_7 has three strong components where the first and second are the new subproblems, which are solved recursively. Since the third strong component contains only one vertex, HD does not make a recursive call for it. An additional recursive call is made for the condensed graph. Figure 3.3 displays the graphs for the recursive calls and the returned trees. The number of edges in the Figures 3.3(a), 3.3(b), and 3.3(c) are 4, 2, and 7, whereas the corresponding problem sizes are 4, 2, and 6 respectively. Note that i_1 and i_2 are 0 for the first two calls and $i^{\mathcal{V}} = 1$ for the last one with $G^{\mathcal{V}}$ since $G_1^{\mathcal{V}}$ is known to be acyclic because j = 7 and $\sigma^{\mathcal{V}}(1) = \sigma(7)$.



FIG. 3.2. Strong components of G_7 for the digraph G given in Figure 2.1(b).

Because of the multiple edges between two vertices, the condensed graph in Figure 3.3(c) has 7 edges. However, the algorithm still works if we sparsify the edges of $G^{\mathcal{V}} = (V^{\mathcal{V}_2}, E^{\mathcal{V}_1})$ and obtain a simple digraph as follows: for an edge $uv \in E$ such that $u \in V_i$ and $v \in V_j$ and $i \neq j$, there exists $v_i v_j \in E^{\mathcal{V}_1}$ if no other $u'v' \in E$ exists such that $u' \in V_i$ and $v' \in V_j$ and $\sigma^{-1}(u'v') < \sigma^{-1}(uv)$. That is, for multiple edges between u and v, we delete all but the first in the permutation σ . In Figure 3.3(c), these edges, $\sigma(7)$ and $\sigma(8)$, are shown in bold. In [26], Tarjan states that although having less edges in the condensed graphs with this modification is desirable, in practice the added simplicity does not compensate for the cost of the reduction of multigraphs to simple digraphs. This is also validated by our preliminary experiments.



FIG. 3.3. Three recursive calls for the digraph G and σ_0 in Figure 2.1(b). Internal nodes in trees are labelled with the σ_0^{-1} -value of the corresponding edge. Note that the overall hierarchical decomposition tree is already given in Figure 3.1.

3.1.2. HDPRE: obtaining the initial block structure. As mentioned in Section 3.1.1, Tarjan proposed HD for hierarchical clustering purposes and sorted the edges with respect to increasing edge weights. Thus, if σ_0 is the permutation used for a hierarchical clustering, it holds that $w(\sigma_0(i)) \leq w(\sigma_0(j))$, for i < j. In this work, we propose using two different approaches to obtain the permutation: the first solely depends on the weights of the edges and sorts them in the order of decreasing edge weights, i.e., we define the permutation σ such that $w(\sigma(i)) \geq w(\sigma(j))$ if i < j. The second uses the sparsity pattern of the matrix. The reverse Cuthill-McKee (RCM) ordering [6, 18] is used to find a symmetric row/column permutation. Then the edges are ordered in a natural, row-wise order. That is, an edge ijalways comes before $k\ell$ if i < k or, i = k and $j < \ell$.

The decomposition tree T obtained from the output from Tarjan's HD algorithm could be used for preconditioning without modification, but we postprocess this tree to ensure that all leaf nodes are as large as they can be but still have fewer than mbs nodes. For the decomposition tree T in Figure 3.1, the cases for mbs = 2 and mbs = 3 are given in Figure 3.4. In T, for the case mbs = 2, the vertices 1, 2, and 3 cannot be combined since the number of vertices in the combined component will be 3, which is greater than mbs. Hence, there will be 5 blocks after this phase. However, the vertices 1, 2, and 3 can be combined for the case mbs = 3 and the number of blocks will be 3. Note that for preconditioning, we do not need to construct the whole tree of HD. We only need to continue hierarchically decomposing the blocks until they contain at most mbs vertices. Hence, for efficiency we modify line 10 of HD to check if the current strong component has more than mbs vertices (instead of a single vertex). Hence the modified algorithm will make a recursive call for a strong component if and only if the component has more than mbs vertices.



FIG. 3.4. Using the output of the HD algorithm. Two cases, mbs = 2 and mbs = 3, are shown for the decomposition tree in Figure 3.1.

To obtain denser and larger blocks, we incorporate some more modifications to HD as follows: first, we modify the definition of \mathcal{V} . Note that $\mathcal{V} = \{\mathcal{V}_1, \mathcal{V}_2\}$ for HD, where the parts in $\mathcal{V}_1 = \mathcal{V}_2$ are the vertex sets of the strong components of G_j . For preconditioning, we keep the definition of \mathcal{V}_1 but use a finer partition \mathcal{V}_2 that contains the vertex sets of strong components obtained by hierarchically decomposing the strong components of size larger than *mbs*. For example, in Figure 3.2, we have 3 strong components of sizes 3, 2, and 1, respectively. Hence, $\mathcal{V}_1 = \{\{1, 2, 3\}, \{4, 5\}, \{6\}\}$. If mbs = 2, SC_1 will be further divided so that $\mathcal{V}_2 = \{\{1\}, \{2\}, \{3\}, \{4, 5\}, \{6\}\}$. However, if mbs = 3, no more decomposition will occur and \mathcal{V}_1 will be equal to \mathcal{V}_2 . With this modification, the algorithm will try to combine the smaller strong components and obtain larger ones with at most *mbs* vertices. Note that setting $\mathcal{V} = \{\mathcal{V}_2, \mathcal{V}_2\}$ tries to do the same but will fail since the only components that can be formed by this approach will be the same as those in \mathcal{V}_1 . Hence, by deleting the edges within the vertex sets in \mathcal{V}_1 , we eliminate the possibility of obtaining the same components.

A second modification is applied to the condense operation by deleting the edges between two vertices $\nu_i, \nu_j \in V^{\nu_1}$ in the condensed graph G^{ν} if the total size of the corresponding parts $V_i, V_j \in \mathcal{V}_2$ is larger than *mbs*. Note that if we were to retain these edges, they would only be used to form blocks of size more than *mbs*. We call this modified condense operation pcondense. An example of the difference between condense and pcondense is given in Figure 3.5.

As Figure 3.5 shows, with this last modification, some of the graphs for the recursive calls may not be strongly connected. Hence, instead of a whole decomposition tree, we may obtain a forest such that each tree in the forest, which corresponds to a strong subgraph in the hierarchical decomposition, has less than *mbs* leaves. The modified algorithm HDPRE, described in Algorithm 2, also handles digraphs which are not strongly connected. Note that for preconditioning, the only information we need is the block structure information. That is, we need to know which vertex is in which tree in the forest after the modified hierarchical decomposition algorithm is performed. Instead of a tree (or a forest), HDPRE returns this information in the *scomp* array.

The structure of the algorithm HDPRE is similar to that of HD. In addition to G, σ , and i, HDPRE requires an additional input array vsize which stores the number of vertices condensed into each vertex of V. For the initial call with G = (V, E), vsize is an array containing |V| ones. On the other hand, for the condensed vertices, this value will be equal to the sum of the vsize-values condensed into that vertex. For the condensed digraph in Figure 3.3(c), $vsize = \{3, 2, 1\}$ when its vertices are ordered from left to right. To be precise, for a recursive call with G = (V, E), the total number of simple vertices is $\sum_{v \in V} vsize(v)$



FIG. 3.5. Difference between condense and pcondense operations for the strong components of G_7 given in Figure 3.2. Let mbs = 3, so that all of the components have a desired number of vertices and $\mathcal{V}_1 = \mathcal{V}_2 = \{\{1, 2, 3\}, \{4, 5\}, \{6\}\}$. Note that the condensed graphs obtained by condense and pcondense are the same except that the latter does not have some of the edges that the former has. For this example, the edges 7, 10, 11, and 13 are missing since the total size size of SC_1 and SC_2 is 5, which is greater than mbs. As a result, for the condense graph, we obtain 3 blocks of sizes 3, 2, and 1, respectively, whereas for the pcondense graph, we have 2 blocks of size 3.

and this number is larger than mbs for all recursive calls because of the size check in line 17 of Algorithm 2.

For each call, HDPRE checks if the problem size |E| - i is equal to one. If this is the case, it finds the strong components $SC_{\ell} = (V_{\ell}, E_{\ell})$ of G. If a strong component SC_{ℓ} has $\sum_{v \in V_{\ell}} vsize(v) > mbs$ vertices, then HDPRE considers each vertex in V_{ℓ} as a different strong component. Otherwise, i.e., if the size of a strong component is less than or equal to mbs, this component is considered as a whole. Following this logic, HDPRE constructs the scomp array and returns. If the problem size |E| - i is greater than 1, as it was done for HD, HDPRE constructs G_j for $j = \lceil (i+|E|)/2 \rceil$ and, if it is strongly connected, the search for the combining edge among the first j edges starts with the call HDPRE($G_j, \sigma, i, vsize$). If not, then for every strong component $SC_{\ell} = (V_{\ell}, E_{\ell})$ of G_j with $\sum_{v \in V_{\ell}} vsize(v) > mbs$, it makes a recursive call HDPRE($SC_{\ell}, \sigma_{\ell}, i_{\ell}, vsize_{\ell}$) and updates the strong component information for the vertices in V_{ℓ} . This update operation can be considered as further dividing the strong component SC_{ℓ} hierarchically until all of the strong components obtained during this process contain at most mbs vertices.

Similarly to HD, at line 33, HDPRE makes one more recursive call for the condensed graph $G^{\mathcal{V}}$, where the definition of the vertex partition \mathcal{V} (in line 27) is modified as in Figure 3.5. In HD, each vertex in the condensed graph corresponds to a strong component of G_j which defines a partition \mathcal{V}_1 . In HDPRE, these components are further divided until all of them have a size no larger than *mbs*. A second partition, \mathcal{V}_2 , is obtained from these smaller strong components and $\mathcal{V} = {\mathcal{V}_1, \mathcal{V}_2}$ is defined. After obtaining the condensed graph $G^{\mathcal{V}}$, in the algorithm HDPRE it is checked if $G^{\mathcal{V}}$ is acyclic. Note that if $i^{\mathcal{V}} = |E^{\mathcal{V}_1}|$, no strong component with two or more vertices exists in $G^{\mathcal{V}}$, and hence it is acyclic. If $i^{\mathcal{V}} \neq |E^{\mathcal{V}_1}|$, after obtaining $scomp^{\mathcal{V}}$, HDPRE updates scomp if a larger strong component is obtained.

For the matrix given in Figure 2.1(a), HDPRE generates the blocks for the cases mbs = 2 and mbs = 3 as shown in Figure 3.6(a) and Figure 3.6(b), respectively. For mbs = 2, the condensed graph has 5 vertices and no edges, hence no combination will occur. For mbs = 3, as shown in Figure 3.6(b), the condensed graph has 3 vertices, where 2 of them will combine with the 12th edge in σ_0 .

235

Algorithm 2 scomp = HDPRE($G = (V, E), \sigma, i, vsize$) (mbs is global, i = 0 for the initial call).

1: if |E| - i = 1 then find strong components of G2: 3: for each strong component $SC_{\ell} = (V_{\ell}, E_{\ell})$ of G do if $\sum_{v \in V_{\ell}} vsize(v) > mbs$ then 4: consider each $v \in V_{\ell}$ as a strong component 5: else 6: $\forall v \in V_{\ell}, scomp(v) = \ell$ 7: 8: end if 9: end for return scomp 10: 11: end if 12: j = [(i + |E|)/2]13: if $G_j = (V, \{\sigma(k) : 1 \le k \le j\})$ is strongly connected then **return** scomp = HDPRE($G_i, \sigma, i, vsize$) 14: 15: else for each strong component $SC_{\ell} = (V_{\ell}, E_{\ell})$ of G_{j} do 16: if $\sum_{v \in V_{\ell}} vsize(v) > mbs$ then 17: 18: σ_{ℓ} = the permutation of E_{ℓ} ordered with respect to σ 19: compute i_{ℓ} as in Algorithm 1 $vsize_{\ell}(v) = vsize(v), \forall v \in V_{\ell}$ 20: $scomp_{\ell} = \text{HDPRE}(SC_{\ell}, \sigma_{\ell}, i_{\ell}, vsize_{\ell})$ 21: update scomp according to $scomp_{\ell}$ 22: end if 23: 24: end for $\mathcal{V}_1 = \{V_\ell : SC_\ell \text{ is a strong component of } G_i\}$ 25: $\mathcal{V}_2 = \{ V_{\ell'} : SC_{\ell'} = (V_{\ell'}, E_{\ell'}) \text{ is a strong component in } scomp \}$ 26: 27: $\mathcal{V} = \{\mathcal{V}_1, \mathcal{V}_2\}$ $G^{\mathcal{V}} = \texttt{pcondense}(G, \mathcal{V}, mbs) = (V^{\mathcal{V}_2}, E^{\mathcal{V}_1})$ 28: $\sigma^{\mathcal{V}}$ = the permutation of $E^{\mathcal{V}_1}$ ordered with respect to σ 29: compute $i^{\mathcal{V}}$ as in Algorithm 1 30: if $i^{\mathcal{V}} \neq |E^{\mathcal{V}_1}|$ then 31: $vsize^{\mathcal{V}}(v_{\ell'}) = \sum_{v \in V_{\ell'}} vsize(v), \forall V_{\ell'} \in \mathcal{V}_2$ 32: $scomp^{\mathcal{V}} = \text{HDPRE}(G^{\mathcal{V}}, \sigma^{\mathcal{V}}, i^{\mathcal{V}}, vsize^{\mathcal{V}})$ 33: update scomp with respect to $scomp^{\mathcal{V}}$ 34. end if 35: return scomp 36. 37: end if

3.1.3. Combining the blocks. After HDPRE obtains a block diagonal partition, SCPRE performs a loop on the nonzeros which are not contained in a block on the diagonal to see if it is possible to put more into the block diagonal by combining original blocks. To do this, SCPRE first constructs a condensed simple graph H where the vertices of H correspond to the diagonal blocks and the inter-block edges of G in both directions are combined as a single edge with a weight that is the sum of the weights of the combined edges.

After H is obtained, its edges are visited in an order corresponding to a permutation σ_H . This permutation is consistent with the original permutation σ_0 . That is, if the edges of



FIG. 3.6. Initial block structure of the preconditioner after the HDPRE algorithm. Two cases, mbs = 2 and mbs = 3, are investigated for the matrix in Figure 2.1(a).

the original digraph are sorted in descending order with respect to the edge weights, σ_H permutes the edges of H with respect to descending edge weights. On the other hand, if the initial permutation is based on the RCM ordering, we compute the RCM ordering of H, relabel the vertices of H accordingly, and order the edges with respect to this RCM ordering. Let vsize(u) be the number of rows/columns in a block corresponding to the vertex u.

Assume that SCPRE constructs σ_0 by sorting the edges with respect to decreasing weights. For the matrix given in Figure 3.6(a), if w(2) + w(4) > w(1), then the vertices 2 and 3 are combined or if $w(2) + w(4) \le w(1)$, then the vertices 1 and 2 are combined. Since mbs = 2 and there is no edge between the vertices 1 and 6, no further combinations are performed.

3.2. SCPRE: extending to a BTF preconditioner. If the desired structure of M is block diagonal, SCPRE stops. Otherwise, while preserving the blocks, it tries to extend the block diagonal preconditioner to a block upper-triangular one. Note that in this case, the order of the blocks is important since it changes depending on which nonzeros are in the upper-triangular part of M. By permuting the blocks, SCPRE tries to put entries that are larger in magnitude into the block upper-triangular part. Our preliminary experiments confirmed that having larger and more nonzeros in a SCPRE preconditioner increases its effectiveness. Since the nonzeros in the diagonal blocks stay the same while extending a block diagonal preconditioner to a block triangular one, we focus on improving the nonzeros in the block upper-triangular part.

Let G = (V, E) be the digraph associated with the matrix and k be the number of diagonal blocks. Let $\mathcal{V}_1 = \{V_1, V_2, \dots, V_k\}$ be a partition of V such that the vertices in V_i correspond to the rows/columns of the *i*th block. Let $\mathcal{V} = \{\mathcal{V}_1, \mathcal{V}_1\}$ and $G^{\mathcal{V}} = \text{condense}(G, \mathcal{V})$ be the condensed multigraph. Note that if $G^{\mathcal{V}}$ is acyclic, a topological sort in $G^{\mathcal{V}}$ gives a symmetric block permutation such that all of the nonzeros in the matrix will be in the uppertriangular part of the permuted matrix. However, this only happens for a reducible matrix with blocks having no more than *mbs* rows/columns.

The problem of finding a good block permutation which maximizes the number of nonzeros in the upper part of \mathbf{M} can be reduced to the problem of finding the smallest edge set E' such that $\overline{G}^{\mathcal{V}} = (V^{\mathcal{V}_1}, E^{\mathcal{V}_1} \setminus E')$ is acyclic. For the weighted version of the problem, i.e., to maximize the total magnitude in the upper part, we need to find an edge set E' where $\overline{G}^{\mathcal{V}}$ is acyclic and the sum $\sum_{uv \in E'} |w(uv)|$ is minimal. In the literature, the first problem is called the *directed feedback arc set* problem and the second one is called the *directed weighted feedback arc set* problem. Both problems are NP-complete [16, 17].

Our simple heuristic proposed for this problem is a greedy algorithm: we first choose the block row with the largest entries in the off-diagonal blocks and remove the corresponding rows/columns in this block. We then do the same with the remaining block matrix to obtain the second block row and continue in this way until a single block remains. More

formally, we let $G^{\mathcal{V}}$ be the condensed graph described above. For each vertex $u \in V^{\mathcal{V}}$, let $tweight(u) = \sum_{uv \in E^{\mathcal{V}}} w(uv)$. The main body of the algorithm is a for-loop where at the *i*th iteration, the vertex *u* with maximal tweight is chosen, and this is assigned as the *i*th vertex in the permutation. Then *u* is removed from $V^{\mathcal{V}}$, its edges are removed from $E^{\mathcal{V}}$, and the algorithm continues with the next iteration. After permuting the matrix with SCPRE, we expect that nonzeros with larger magnitudes are mostly placed in the diagonal blocks and some in the upper-triangular part. We display in Figures 3.7(a) and 3.7(b) the matrix $ckt11752_tr_0$ after scaling using MC64 and after the reordering from SCPRE, respectively. In the reordered matrix of Figure 3.7(b), it is clear that the larger entries are in the diagonal blocks.

4. Using SCPRE with an iterative solver. The iterative solver we use in our experiments is the right-preconditioned GMRES [23] with restarts. A template for this can be found in [2]. Let A = D + U + L be the scaled and permuted matrix such that D, U, and L are the block diagonal, upper, and lower parts, respectively.

If the desired structure is block diagonal, which is suitable for the exploitation of parallelism, $\mathbf{M} = \mathbf{D}$ is the preconditioner. If this is not the case, $\mathbf{M} = \mathbf{D} + \mathbf{U}$ is the preconditioner for \mathbf{A} . For the latter case, the computation $\mathbf{A}\mathbf{M}^{-1}\mathbf{x}$ becomes

$$\mathbf{A}\mathbf{M}^{-1}\mathbf{x} = (\mathbf{D} + \mathbf{U} + \mathbf{L})(\mathbf{D} + \mathbf{U})^{-1}\mathbf{x} = \mathbf{x} + \mathbf{L}((\mathbf{D} + \mathbf{U})^{-1}\mathbf{x}).$$

Note that SCPRE tries to maximize the total magnitude in **D** and **U**. As a consequence and as experiments not included here show, **L** usually contains much fewer nonzeros than **A**. Hence computing the vector $\mathbf{z} = \mathbf{L}\mathbf{y}$ usually takes very little time and the main operation is to compute $\mathbf{y} = (\mathbf{D} + \mathbf{U})^{-1}\mathbf{x} = \mathbf{M}^{-1}\mathbf{x}$. In our implementation, in addition to **A**, we store the **LU** factors of the diagonal blocks, i.e., the factors \mathbf{L}_i and \mathbf{U}_i such that $\mathbf{D}_i = \mathbf{L}_i \mathbf{U}_i$ where \mathbf{D}_i is the *i*th diagonal block. We reduce the memory requirements for these factors by ordering the blocks using the approximate minimum degree (AMD) heuristic [1, 7] before using the MATLAB sparse factorization. We then solve the upper block triangular system $\mathbf{M}\mathbf{y} = \mathbf{x}$ using these factors, starting with the last block, so that the off-diagonal part **U** is only used to multiply vectors.

4.1. Robustness. The use of the *I*-matrix scaling via MC64 helps to reduce the possibility of a singular preconditioner M obtained by SCPRE because all the submatrices on the diagonal will also be *I*-matrices. But, although it is very rare, these *I*-matrices can be singular and we still find cases in which some of the blocks on the diagonal of M are singular.

When using the MATLAB factorization, we guard against this potential problem by using the simple and cheap stability check proposed and used by XPABLO [14, 15]. That is, if n_i is the dimension of D_i , after computing L_i and U_i , we check whether

(4.1)
$$\left|1 - \frac{||\mathbf{U}_{\mathbf{i}}^{-1}\mathbf{L}_{\mathbf{i}}^{-1}\mathbf{x}||}{||\mathbf{e}||}\right| < \sqrt{\epsilon_{M}},$$

where $\mathbf{e} = (1, ..., 1)^T$ is an $n_i \times 1$ column vector, $\mathbf{x} = \mathbf{D}_i \mathbf{e}$, and ϵ_M is the machine epsilon. If a block does not satisfy (4.1), XPABLO replaces \mathbf{D}_i either by \mathbf{U}_i or \mathbf{L}_i according to whether it is solving a block upper- or lower-triangular system, respectively. For SCPRE, we use the same test as XPABLO but always use the factor having the largest Frobenius norm to replace \mathbf{D}_i , where the Frobenius norm of an $n \times n$ matrix **B** is given by

$$||\mathbf{B}||_F = \sqrt{\sum_{1 \le i,j \le n} |\mathbf{B}_{ij}|^2}.$$



FIG. 3.7. The matrix $ckt11752_tr_0$ after scaling (a) and after SCPRE (b), respectively. The nonzeros are coloured with respect to their magnitudes; mbs is set to 5000.

5. Experiments. All of the experiments are conducted on an Intel 2.4Ghz Quad Core computer, equipped with 24GB RAM with a Fedora Linux operating system. For the experiments, we use matrices from the University of Florida Sparse Matrix Collection [8]. The matrices we use come from circuit simulation problems (CSP), semiconductor device problems (SDP), electromagnetics problems (EMP), and optimization problems (OPT). We run three sets of comparisons using these matrices. The first set contains 45 matrices with $m \le 2 \times 10^6$ nonzeros. For this set, we use mbs = 2000 in the experiments. The second set contains 13 relatively large matrices with $m \ge 2 \times 10^6$ nonzeros. For this set, we use mbs = 5000 since they are larger. The third set contains 12 average-size optimization matrices with $10^6 \le m \le 2.5 \times 10^6$ nonzeros. In constructing the sets, we do not use matrices whose largest blocks in their BTF form have less than mbs rows/columns. We also exclude from the tables any matrices on which none of our preconditioned iterative solvers converged. The lists of the remaining 37 matrices in the first set, 12 matrices in the second set, and 6 matrices in the third set are given in Table 5.1.

In our experiments, we restarted GMRES [23] after every 50 iterations. The desired error tolerance for GMRES(50) is set to $\epsilon = 10^{-8}$ and the stopping criterion we use for GMRES is

$$\frac{||\mathbf{A}\mathbf{M}^{-1}\overline{\mathbf{z}} - \mathbf{b}||}{||\mathbf{b}||} < \epsilon$$

where $\overline{\mathbf{z}} = \mathbf{M}\overline{\mathbf{x}}$, with $\overline{\mathbf{z}}$ the computed solution of the preconditioned system and $\overline{\mathbf{x}}$ the computed solution of the original system. After obtaining the solution $\overline{\mathbf{x}}$ to the original system, we compute the relative error $||\mathbf{A}\overline{\mathbf{x}} - \mathbf{b}||/||\mathbf{b}||$ to the unpreconditioned system. For all cases, this error is smaller than 10^{-7} and indeed, for most of the cases it is also smaller than ϵ .

The maximum number of outer iterations is set to 20, hence the maximum number of inner iterations is 1000. In the tables, we give the inner iteration counts when the stopping criterion is satisfied. Otherwise, if the criterion is not satisfied, we put "-" in the table to denote that GMRES did not converge. Also, we put the lowest iteration count for each matrix in bold font.

To compare the efficiency of the preconditioner, we used a generic preconditioner, ILUT, c.f. [21, 22], from MATLAB 7.11 with two drop tolerances, $dtol = 10^{-3}$ and 10^{-4} . In addition to ILUT, we also compared our results with those of XPABLO [14, 15]. For all of the preconditioners, we use MC64 and obtain a maximum product transversal by scaling and permuting the matrix as a preprocessing step.

In the MATLAB implementation of ILUT, for the *j*th column of the incomplete L and U, entries smaller in magnitude than $dtol \times ||\mathbf{A}_{*j}||$ are deleted from the factor where $||\mathbf{A}_{*j}||$ is the norm of the *j*th column of A. However, the diagonal entries of U are always kept to avoid a singular factor. For the ILUT based preconditioners, we use AMD before computing the incomplete factorization of the matrix. For XPABLO preconditioners, we use the J variant for the block Jacobi iterations and LX and UX variants for the forward and backward block Gauss-Seidel iterations, respectively, with the parameters given in [14, 15]. For the maximum block size of XPABLO, we used the same *mbs* as for SCPRE. We note that the authors of XPABLO recommend a value for *mbs* of 1000 [14], but in our experiments we found the value 2000 to work better and found that it was necessary for our larger problems to avoid failure in XPABLO.

SCPRE will automatically find the BTF for a reducible matrix. To be fair to the other algorithms that do not detect this form, we use this reducibility information also for the ILUT and XPABLO preconditioners. That is, when using ILUT (XPABLO) for reducible matrices, we first compute the BTF form and apply ILUT (XPABLO) only to the blocks on the diagonal. For smaller blocks, we compute the complete factors. We then use these complete and

TABLE 5.1 Properties of the matrices used for the experiments. n is the dimension of the matrix, m is the number of nonzeros, and n_1 and n_2 are the sizes of the largest and second largest blocks in the BTF form. Note that $n_2 = 0$ means that the matrix is irreducible, i.e., $n_1 = n$. The column Type shows the application from which the matrix arises. The sets are sorted first according to the type of the problem and then their n_1 values.

	Matrix	Group	n	m	n_1	n_2	Туре
	Hamrle2	Hamrle	5952	22162	5952	0	
	raiat03	Rajat	7602	32653	7500	1	
	circuit_3	Bomhof	12127	48137	7607	1	
	coupled	IBM_Austin	11341	97193	11293	1	
	memplus	Hamm	17758	99147	17736	1	
	rajat??	Rajat	39899	195429	26316	7672	
	onetone?	ATandT	36057	222596	32211	2	
	onetonel	ATandT	36057	335552	32211	2	
	rajat15	Daiat	37261	143573	37243	1	
	$a_{l+11752}$ += 0	IDM EDA	40702	222907	40271	1	
	ckill/J2_ll_0	DWI_EDA Domhof	80200	307604	52005	-++	
	h oinouit	Domm	60209	275559	52005	0	
	DCIFCUII		08902	373338	08902	50	CCD
	rajatis	Kajat	94294	4/9151	84507	52	CSP
	hcircuit	Hamm	1056/6	513072	92144	4927	
	ASIC_100ks	Sandia	99190	5/8890	98843	2	
	ASIC_100k	Sandia	99340	940621	98843	2	
	ASIC_680ks	Sandia	682712	1693767	98843	2	
	rajat23	Rajat	110355	555441	103024	216	
SET	twotone	ATandT	120750	1206265	105740	6	
1	trans5	IBM_EDA	116835	749800	116817	1	
	dc2	IBM_EDA	116835	766396	116817	1	
	G2_circuit	AMD	150102	726674	150102	0	
	scircuit	Hamm	170998	958936	170493	216	
	transient	Freescale	178866	961368	178823	11	
	Raj1	Rajat	263743	1300261	263571	5	
	AŠIC_320ks	Sandia	321671	1316085	320926	6	
	ASIC_320k	Sandia	321821	1931828	320926	6	
	utm5940	ТОКАМАК	5940	83842	5794	1	
	dw4096	Bai	8192	41746	8192	0	EMP
	Zhao1	Zhao	33861	166453	33861	Õ	
	iaht3	Schenk ISEI	10038	130500	10038	0	
	wana 3	Wang	26064	177168	26064	0	
	wangs wang	Wang	26069	177106	26068	0	
	wung4	Songhovi	51003	280/15	42241	1	SDD
	ihan matuin 2	Saligliavi	51449	527029	42341	1	SDF
	10m_matrix_2	Schenk_IDMSDS	125220	202084	44022	1	
	mairix-new_S	Schenk IDMSDS	123329	093904	18072	1	
	mairix_9	SCHERK_IDIVISUS	103430	1203318	99512	1	
	ASIC_680k	Sandia	682862	2638997	98843	2	
	G3_circuit	AMD	1585478	7660826	181343	0	
	rajat29	Rajat	643994	3760246	629328	71	CSP
	rajat30	Rajat	643994	6175244	632151	0	
	Hamrle3	Hamrle	1447360	5514242	1447360	0	
SET	memchip	Freescale	2707524	13343948	2706851	0	
2	offshore	Um	259789	4242673	259789	0	
	tmt_svm	CEMW	726713	5080961	726713	0	EMP
	t2em	CEMW	921632	4590832	917300	1	
	tmt unsym	CEMW	917825	4584801	917825	0	
	nava A	Schopk ISEI	152026	2020882	152026	0	SDD
	ohne?	Schenk ISEI	181343	6869939	181343	0	501
		CHR : 1 C		22/27/20			
	ex_data1	GHS_indef	6001	2269500	6001	0	
0 D T	Doyal	GHS_indef	93279	1211231	93279	0	
SET 3	majorbasis	QLI	160000	1750416	160000	0	0.00
	c-/3b	Schenk_IBMNA	169422	1279274	169422	0	OPT
	c-big	Schenk_IBMNA	345241	2340859	345089	2	
	boyd2	GHS_indef	466316	1500397	466316	0	

incomplete factors together while computing a matrix vector product using M^{-1} . Our experiments show that this approach is almost always better than using ILUT (XPABLO) in a straightforward manner in terms of the iteration count. We also tried this approach while using the J variant of the XPABLO preconditioner. Surprisingly, even for the block Jacobi case, this approach helps to reduce the iteration counts slightly for most of the reducible matrices. We call this variant J-red in the tables below. Note that for the block Gauss-Seidel case, when we apply XPABLO (or ILUT) only to the large blocks in the BTF form of a reducible matrix, we keep all of the nonzeros in the preconditioner from the off-diagonal blocks. However, for block Jacobi iterations, we automatically drop them from the preconditioning matrix M since its desired structure is block diagonal, not block triangular.

In addition to the number of iterations required for convergence, we compare the performance of the preconditioners according to the relative memory requirement with respect to the number of nonzeros in **A**. Let $nz(\mathbf{B})$ be the number of nonzeros in a matrix **B**. For ILUT, the relative memory requirement is equal to

$$mem_{\text{ILUT}} = \frac{nz(\mathbf{L}) + nz(\mathbf{U})}{nz(\mathbf{A})},$$

where L and U are the incomplete triangular factors of A. On the other hand, the relative memory requirement for SCPRE and XPABLO is equal to

$$mem_{\text{SCPRE}} = mem_{\text{XPABLO}} = \frac{\sum_{i=1}^{k} \left(nz(\mathbf{L}_{i}) + nz(\mathbf{U}_{i}) \right)}{nz(\mathbf{A})},$$

where k is the number of blocks in the block diagonal **D**, and **L**_i and **U**_i are the lowerand upper-triangular factors of the LU-factorization of the *i*th block in **D**. Note that the relative memory requirements of the preconditioners can give an idea for the cost of computing $\mathbf{M}^{-1}\mathbf{x}$. Assuming that x is a dense vector, a preconditioned GMRES iteration will require approximately $nz(\mathbf{A})(1 + mem_{\mathbf{X}})$ operations for the preconditioner generated by the algorithm X.

There are two parameters for the proposed algorithm: the first is the maximum block size mbs, the second is the permutation for the nonzeros denoted by σ_0 . As expected, our experiments (not reported here) show that increasing the number mbs usually reduces the iteration counts and increases the relative memory requirements of the solver.

We conduct some experiments to show the effect of our choice of σ_0 on the performance of our algorithm. Note that in HD, the edges are sorted in increasing order with respect to their weights. In our implementation, we define the weight of an edge as the magnitude of the corresponding nonzero and sort the edges in decreasing order. We test our decision by comparing its effect with that of a random permutation. As Table 5.2 shows, our decision to sort the edges in decreasing order with respect to the edge weights makes the solver converge more quickly.

5.1. Experiments with block Gauss-Seidel iterations. Table **5.3** shows the performance of SCPRE and XPABLO for block Gauss-Seidel iterations and their comparison with ILUT. Note that both SCPRE(*dec*) and SCPRE(RCM) are robust, that is, the solvers converge for most of the matrices. Although there are a few matrices for which the SCPRE(RCM) preconditioned solver converges more quickly than that preconditioned with SCPRE(*dec*) (such as *ASIC_680k*) and, amongst all preconditioners, only SCPRE(RCM) converges for matrices *onetone1* and *onetone2*, SCPRE(*dec*) is almost always better and is our preferred preconditioner.

In general, all the preconditioners work well for the matrices in the first set. However, SCPRE(dec) is the most robust since the preconditioned solver fails to converge only

TABLE 5.2

Effect of the permutation σ_0 on the number of iterations. Two options are compared: a decreasing order with respect to the edge weights and a random order. The maximum block size for SCPRE is set to 2000 where the structure of **M** is block upper-triangular. For each case, the ratio of the total magnitude in **M** to the total magnitude in **A**, the relative memory requirement, and the number of inner iterations for preconditioned GMRES are given.

		Decreasing		Random			
Matrix	$\frac{\sum \left \mathbf{M}_{ij}\right }{\sum \left \mathbf{A}_{ij}\right }$	mem _{SCPRE}	iters	$\frac{\sum \mathbf{M}_{ij} }{\sum \mathbf{A}_{ij} }$	$mem_{\mathtt{SCPRE}}$	iters	
Hamrle2	0.998	2.03	16	0.993	2.05	157	
rajat03	0.999	1.07	2	0.997	1.02	5	
circuit_3	0.996	1.45	9	0.987	1.23	445	
coupled	0.998	1.57	11	0.992	1.58	34	
memplus	0.999	1.03	5	0.998	1.03	7	
rajat22	0.973	1.20	21	0.962	1.15	-	

for 3 out of 37 matrices, whereas the next best result is 9 by the XPABLO variants. Thus, SCPRE(*dec*) is the best block preconditioner on this set of matrices. When comparing SCPRE(*dec*) to ILUT(10^{-4}) on this set, we see that they are comparable in terms of the number of best performances, but ILUT(10^{-4}) is less robust, failing to converge for 10 matrices in this set and requiring more memory than SCPRE(*dec*).

For the second set, $ILUT(10^{-4})$ is the best preconditioner in terms of robustness and iteration count. For the matrices in this set, the $ILUT(10^{-4})$ preconditioned solver fails to converge in only 2 out of 12 matrices, whereas SCPRE(dec) does not converge on 4. Although $ILUT(10^{-4})$ is better than SCPRE(dec) for 10 out of 12 matrices in the second set, its average relative memory usage is 9.39 which is almost 3 times as much as the relative memory requirement of SCPRE(dec). Note that for the second set, even $ILUT(10^{-3})$ uses slightly more memory than SCPRE(dec). However, it fails to converge on 7 matrices. Hence, if memory is the bottleneck, SCPRE(dec) may be a suitable choice for preconditioning.

The performance of the SCPRE-based preconditioners depends on the application. For example, as Table 5.3 shows, SCPRE(*dec*) preconditioned GMRES fails to converge in 3 out of 7 matrices from electromagnetics applications. On the other hand, it fails to converge on only 4 of the remaining 42 matrices. Hence its performance is much better for circuit and device simulation applications. Note that even though some of these matrices are reducible, they have a large reducible block with a size much larger than *mbs*. That is, we still have a large subproblem to deal with. On the circuit simulation and semiconductor device matrices, SCPRE works better than XPABLO, which is another block based preconditioner with a promising performance in practice for several matrix classes [3, 5, 10]. Note that we used the BTF forms of the reducible matrices for both the XPABLO and ILUT preconditioners. Hence, reducibility alone is not a reason for the good performance of SCPRE-based preconditioners.

5.1.1. Memory usage. As Table 5.3 shows, the memory usage of $ILUT(10^{-4})$ is much higher than that of XPABLO and SCPRE. Table 5.4 shows the results of additional experiments conducted to further compare the memory usage of SCPRE and ILUT preconditioners. There are 6 optimization matrices in the set. SCPRE-based preconditioned solvers converged for 5 of them. For ILUT-based solvers with drop tolerance 10^{-3} and 10^{-4} , the numbers of matrices for which the solver converged are 4 and 5, respectively. Hence, on this matrix set, SCPRE is as robust as ILUT. With respect to the number of iterations, ILUT is much better with 7–8 iterations on the average instead of 36 for SCPRE. The main reason for such a big difference is the matrix *c*-73*b*, where the SCPRE preconditioned solver requires 127 inner iterations. On the other hand, the average relative memory usage of ILUT is 11–18 times more than that of SCPRE. This difference is due to the matrices *c*-73*b* and *c*-*big*, where ILUT's relative memory requirements are 28.47 and 61.89, respectively. Additionally, for the matrices the matrices are 28.47 and 61.89.

243

TABLE 5.3

Number of inner iterations for GMRES using XPABLO, ILUT, and SCPRE preconditioners and block Gauss-Seidel iterations. For SCPRE and XPABLO, mbs is set to 2000 and 5000 for the first and second sets, respectively. For SCPRE, we give the results using two permutations for σ_0 , based on descending order and RCM. For SCPRELO, we give the results for both the UX and LX variants. For ILUT, the drop tolerance is set to 10^{-3} and 10^{-4} . A '-' sign indicates that the preconditioned solver did not converge. Average relative memory requirements are computed by taking the averages over the cases when the solvers converge.

	l	XPABLO		SCPRE		ILUT	
	Matrix	UX	LX	dec	RCM	10^{-3}	10^{-4}
	Hamrle?	31	31	16	28	6	4
	raiat03	2	2	2	20	2	2
	circuit_3	135	137	9	61	_	-
	coupled	12	12	11	13	6	4
	memplus	9	9	5	18	15	9
	rajat22	36	37	21	61	36	16
	onetone2	-	-	-	248	-	-
	onetone1	-	-	-	297	-	-
	rajat15	-	-	120	467	-	33
	ckt11752_tr_0	197	188	19	323	-	-
	circuit_4	100	81	39	346	-	-
	bcircuit	-	-	40	620	568	93
	rajat18	-	-	11	-	393	54
	hcircuit	8	9	9	21	9	5
	ASIC_100ks	9	10	9	10	4	4
	ASIC_100k	9	9	10	10	4	4
	ASIC_680ks	3	4	3	4	4	4
	rajat23	40	41	16	88	47	18
mbs =	twotone	-	-	25	128	_	48
2000	trans5	9	9	5	7	7	6
	dc2	13	12	12	11	10	6
	G2_circuit	-	-	444	834	124	30
	scircuit	/41	/64	317	9//	-	-
	transient	-	-	33	-	-	
	Kaji	1/5	/89	636	-	269	39
	ASIC_320KS	4	4		4	2	2
	ASIC_520K	3	3		3	3	
	utm5940	-	-	- 10	-	-	29
	dw4096	881	798	13	141	24	10
	Zhao1	/	/	4	9	4	3
	igbt3	29	29	20	17	94	12
	wang3	107	105	54	58	18	9
	wang4	39	38	21	36	11	6
	ecl32	99	99	30	32	32	13
	1bm_matrix_2	-	249	10	10	-	-
	matrix-new_5	85	80	30	41	-	-
	matrix_9	140	90	98	66	-	-
Avg. re	lative memory	2.95	3.04	3.36	3.19	2.12	4.02
	ASIC_680k	2	2	27	2	3	3
	G3_circuit	-	-	357	422	212	81
	rajat29	-	-	11	-	-	-
	rajat30	12	12	14	15	7	5
-	Hamrle3	-	-	-	-	-	17
mbs =	memchip	26	27	10	20	8	5
5000	offshore	330	327	488	451	-	15
	tmt_sym	-	-	-	-	-	69
	t2em	-	-	876	-	132	38
	tmt_unsym	-	-	-	-	-	136
	para-4	-	-	-	-	-	433
	ohne2	-	-	196	-	-	-
Avg. re	lative memory	3.58	3.58	3.23	2.51	3.36	9.39
		0.00	0.00	0.20		0.00	

ETNA Kent State University http://etna.math.kent.edu

TABLE 5.4

Number of inner iterations and relative memory usage of GMRES using SCPRE or ILUT preconditioners with block Gauss-Seidel iterations for optimization matrices. For SCPRE, mbs is set to 2000, and σ_0 is obtained by using the descending order. For ILUT, the drop tolerance is set to 10^{-3} and 10^{-4} . The '*' sign indicates that the memory of our machine (24 GBytes) is not sufficient to obtain the preconditioner. The '-' sign indicates that the preconditioner is obtained, but the solver did not converge in fewer than 1000 iterations. The average number of iterations and relative memory requirements are computed by taking the averages over the cases when the solvers converge.

	SCPR	E(dec)	ILUT	-10^{-3}	$ $ ILUT- 10^{-4}		
Matrix	Matrix iters mem		iters	mem	iters	mem	
ex_data1	14	0.60	-	-	23	0.47	
boyd1	18	0.19	7	0.77	5	1.03	
majorbasis	10	2.50	4	1.20	3	1.87	
c-73b	127	0.72	10	14.19	5	28.47	
c-big	-	-	6	30.39	4	61.89	
boyd2	13	1.17	*	*	*	*	
Avg.	36	1.04	7	11.64	8	18.75	

trix *boyd2*, ILUT could not generate a preconditioner since the maximum memory available in the system, 24GB, is exceeded. Given that only 28MB is used to store *boyd2*, the relative memory requirement of ILUT is excessive. This shows that although SCPRE-preconditioned solvers require more iterations than ILUT-preconditioned ones, SCPRE can still be a good replacement for some matrix classes if the matrices are big and memory is the main bottleneck.

5.2. Experiments with block Jacobi iterations. The Table 5.5 shows the performance of SCPRE and XPABLO preconditioners for block Jacobi iterations. ILUT is not included here since it does not explicitly give a block diagonal structure. Similar to the experiments with block Gauss-Seidel iterations, the performance of SCPRE(dec) is better than that of SCPRE(RCM) for the matrices in our sets. For XPABLO, applying the preconditioner only to the blocks in the BTF form, the variant J-red reduces the number of iterations on 11 matrices. Furthermore, for 5 of the matrices, J-red converges, whereas J does not. Note that there are 32 reducible matrices in the sets and J-red differs from J only for these matrices. Although J-red required more iterations for convergence for the matrices *matrix_new_3* and *matrix_9*, for the matrices in our experiments, J-red generally performs better than J.

As Table 5.5 shows, SCPRE(*dec*) preconditioned GMRES converges for 36 matrices, whereas XPABLO's J-red variant converges for only 24 matrices. The XPABLO based preconditioner has the least number of iterations in only 8 cases, whereas the SCPRE variants are better on 35 matrices. The difference in the performance is not due to the relative memory usage of the SCPRE variants. For the first set, SCPRE(*dec*) uses only 8% more memory than XPABLO(J-red) on average, and for the second set its memory usage is much less.

On the right-hand side of Table 5.5, the execution times of the GMRES solver are given. As the table shows, for most of the cases the best solver in terms of iteration count has also the best execution time. Note that there are some exceptions such as the *matrix_9*, for which the solver preconditioned by XPABLO(J) requires 49 iterations fewer than when preconditioned by SCPRE, but its execution time is slightly more. This is because for this matrix, $mem_{XPABLO(J)} = 8.43$ and $mem_{SCPRE(dec)} = 3.69$, and the cheaper cost of computing $M^{-1}x$ more than compensates for the difference in iteration counts. For 39 matrices, a SCPRE variant has the best or very close to the best time. In summary, SCPRE(*dec*) performs better than the XPABLO variants in our block Jacobi experiments.

5.3. Cost of generating the preconditioner. It has been the aim of this paper to establish the viability of using hierarchical decompositions to obtain a block preconditioning

TABLE 5.5

Number of inner iterations and solver times (in seconds) for GMRES using XPABLO and SCPRE preconditioners and block Jacobi iterations. The maximum block size mbs is set to 2000 and 5000 for the first and second sets, respectively. For SCPRE, we give the results using two permutations for σ_0 , based on descending order and RCM. For XPABLO, we give the results for the J variant, which is used with the parameters suggested in [14]. The J-red variant described in the text, also uses the same parameters. A '-' sign indicates that the preconditioned solver did not converge. Average relative memory requirements are computed by taking the averages over the cases when the solver converges.

		# iterations		solver time (in secs.)					
		XP	ABLO	SCPRE		XPABLO		SCPRE	
	Matrix	J	J-red	dec	RCM	J	J-red	dec	RCM
	Hamrle2	99	99	31	96	0.32	0.32	0.08	0.30
	rajat03	7	3	4	4	0.03	0.01	0.01	0.01
	circuit_3	680	327	19	179	3.72	1.81	0.07	0.93
	coupled	43	22	21	25	0.22	0.09	0.08	0.11
	memplus	17	17	8	33	0.08	0.08	0.03	0.19
	rajat22	190	77	42	124	3.03	1.61	0.63	1.88
	onetone2	-	-	-	627	-	-	-	9.62
	onetone1	-	-	-	622	-	-	-	14.95
	rajat15	-	-	265	-	-	-	4.85	-
	ckt11752_tr_0	-	776	36	-	-	20.28	0.83	-
	circuit_4	-	864	112	-	-	27.48	3.33	-
	bcircuit	-	-	107	-	-	-	3.06	-
	rajat18	-	-	16	-	-	-	0.39	-
	hcircuit	16	15	16	40	0.43	0.47	0.43	1.55
	ASIC_100ks	17	17	16	18	0.46	0.50	0.44	0.50
	ASIC_100k	17	16	17	18	0.48	0.52	0.49	0.51
	ASIC_680ks	-	8	-	8	-	0.72	-	0.74
	rajat23	203	140	32	208	9.29	7.65	1.17	9.09
	twotone	-	-	49	322	-	-	2.70	17.11
	trans5	23	16	9	13	0.75	0.47	0.24	0.36
	dc2	76	21	20	20	3.32	0.67	0.64	0.64
	G2_circuit	-	-	833	-	-	-	56.55	-
	scircuit	-	-	682	-	-	-	49.25	-
	transient	-	-	186	-	-	-	13.60	-
	Raj1	-	-	-	-	-	-	-	-
	ASIC_320ks	5	6	1	7	0.43	0.70	0.19	0.54
	ASIC_320k	11	9	3	10	0.91	0.85	0.42	0.61
	utm5940	-	-	-	-	-	-	-	-
	dw4096	-	-	24	-	-	-	0.11	-
	Zhao1	12	12	7	16	0.12	0.12	0.08	0.19
	igbt3	60	60	32	26	0.52	0.52	0.21	0.17
	wang3	263	263	140	138	3.26	3.26	1.96	1.78
	wang4	91	91	39	79	1.24	1.24	0.54	1.02
	ecl32	-	-	79	90	-	-	2.50	3.08
	ibm_matrix_2	-	344	22	30	-	12.29	0.65	1.09
	matrix-new_3	184	248	71	95	13.21	20.20	4.64	6.79
	matrix_9	208	240	257	346	14.85	18.80	14.41	21.83
Avg	g. relative memory	2.67	3.10	3.35	3.32				
	ASIC_680k	-	3	-	3	-	0.54	-	0.54
	G3_circuit	-	-	674	-	-	-	516.38	-
	rajat29	-	-	18	-	-	-	3.03	-
	rajat30	43	22	24	27	11.84	4.59	5.12	6.12
	Hamrle3	-	-	-	-	-	-	-	-
	memchip	41	50	17	38	53.39	74.55	14.60	38.82
	offshore	883	883	-	-	189.98	189.98	-	-
	tmt_sym	-	-	-	-	- 1	-	-	-
	t2em	-	-	-	-	-	-	-	-
	tmt_unsym	-	-	-	-	-	-	-	-
	para-4	-	-	-	-	-	-	-	-
	ohne2	_	-	_	_	-	_	_	-
						1			

 Avg. relative memory
 3.58
 2.84
 1.81
 0.92

245

ETNA Kent State University http://etna.math.kent.edu

TABLE 5.6

Preconditioner generation times for 10 CSP matrices from the first matrix set in seconds. For SCPRE and XPABLO, mbs is set to 2000. For XPABLO, the UX variant is used, and for SCPRE, σ_0 is obtained by using the descending order. For ILUT, the drop tolerance is set to 10^{-3} . Results are the averages of 5 executions.

Matrix	XPABLO	SCPRE(dec)	$ILUT-10^{-3}$
rajat15	0.23	5.92	0.71
ckt11752_tr_0	0.45	3.97	0.23
circuit_4	0.15	8.13	0.11
bcircuit	0.21	3.95	0.12
rajat18	0.23	7.31	0.08
hcircuit	0.28	5.03	0.09
ASIC_100ks	0.35	9.65	0.24
ASIC_100k	0.43	9.50	0.19
ASIC_680ks	1.40	9.96	0.28
rajat23	0.29	7.64	0.08
twotone	1.02	9.09	12.41

matrix that greatly reduces the number of iterations of Krylov solvers without requiring too much additional memory.

However, the cost of obtaining the preconditioning matrix is also important, especially if it is being generated for the solution of a single system. The analysis presented in Section 3.1.1 shows that the complexity of the HD algorithm is $\mathcal{O}(m \log n)$ which means that it scales well as the problem sizes increase. However, we note that the complexity of XPABLO is $\mathcal{O}(m+n)$, which is thus linear in the order and number of entries in the matrix and could be expected to have smaller generation execution times than SCPRE.

A straight comparison of the generation times is not meaningful as our implementation is fully in MATLAB without any low-level optimization, whereas for XPABLO we used the available implementation in C, for which the compiler directly optimizes the code for the machine. It is the intention in future work to develop and optimize the implementation, but it is certainly outside the scope of this present work.

However, there is no doubt that although our algorithm has good complexity bounds, it is quite complicated, so we did time the generation of the SCPRE preconditioner on some of our test matrices. For example, for the CSP matrices of Table 5.1, we found that SCPRE took between 2.5 and 9.5 seconds, whereas XPABLO required between 0.25 and 1.40 seconds. Thus, although our algorithm takes much longer and would still be slower with an efficient C implementation (which we estimate would be about 5 times faster), the times are not unreasonable and indicate that our approach is feasible even for one-off solutions. Indeed, if we look at the total cost, we are still faster than XPABLO on several problems in the one-off case, and of course the greater robustness of our more costly preconditioner compensates for this extra cost.

6. Conclusions and future work. Given a linear system Ax = b, we have proposed a method to construct generic block diagonal and block triangular preconditioners. The proposed approach is based on Tarjan's algorithm HD for hierarchical decomposition of a digraph into its strong subgraphs. Although our preconditioner SCPRE is outperformed by ILUT for electromagnetics matrices, we obtain promising results for many device and circuit simulation matrices, and we suggest using it with these types of problems. In future research, the structure of graphs for different classes of matrices can be analysed to try to understand the reason for the difference in performance.

There are two main parameters for the algorithm: the permutation σ_0 of the edges and the maximum block size *mbs*. For σ_0 we used two approaches: the first sorts the edges in the order of decreasing weights. With this approach, we wanted to include nonzeros with large magnitudes in our preconditioner. The second approach uses the well known reverse Cuthill-

McKee ordering. We tested this approach since a sparsity structure with a small bandwidth may be useful for putting more nonzeros into the preconditioner. The permutation decisions are validated by the experiments which also show that the first approach is usually better than the second. In future work, other ways to generate σ_0 can be investigated.

The second parameter, *mbs*, affects the memory requirement of the matrix significantly and hence the number of iterations required for convergence. The experiments show that for the preconditioners ILUT, SCPRE, and XPABLO, the memory requirement and the number of iterations are inversely correlated. For the proposed preconditioner SCPRE, *mbs* needs to be set by the user without knowing how much memory will be required by the solver. In future work, we will look for a self-tuning mechanism which enables SCPRE to determine *mbs* automatically given the memory available to store the preconditioner. A straightforward tuning mechanism, which combines the blocks only when sufficient memory for the factors is available, can be easily implemented and integrated into SCPRE. However, this simple idea still needs to be enhanced to optimize the execution time of SCPRE and further reduce the number of iterations required for convergence.

Acknowledgments. The authors thank Dr. Philip Knight of the University of Strathclyde for bringing the elegant hierarchical decomposition algorithm of Tarjan to our attention. They also thank Dr. Mikko Byckling of CERFACS for valuable discussions and his GMRES implementation. Finally, we would like to thank the referees for their comments that have significantly improved our manuscript.

REFERENCES

- P. AMESTOY, T. A. DAVIS, AND I. S. DUFF, Algorithm 837: AMD, An approximate minimum degree ordering algorithm, ACM Trans. Math. Software, 30 (2004), pp. 381–388.
- [2] R. BARRETT, M. BERRY, T. F. CHAN, J. DEMMEL, J. DONATO, J. DONGARRA, V. EIJKHOUT, R. POZO, C. ROMINE, AND H. V. DER VORST, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, 2nd ed., SIAM, Philadelphia, 1994.
- [3] M. BENZI, H. CHOI, AND D. B. SZYLD, *Threshold ordering for preconditioning nonsymmetric problems*, in Proceedings of the Workshop on Scientific Computing '97 – Hong Kong, G. Golub, S. Lui, F. Luk, and R. Plemmons, eds., Springer, Singapore, 1997, pp. 159–165.
- M. BENZI, J. C. HAWS, AND M. TŮMA, Preconditioning highly indefinite and nonsymmetric matrices, SIAM J. Sci. Comput., 22 (2000), pp. 1333–1353.
- [5] H. CHOI AND D. B. SZYLD, Application of threshold partitioning of sparse matrices to Markov chains, in Proceedings of the IEEE International Computer Performance and Dependability Symposium, IPDS'96, Urbana-Champaign, Illinois, September 4–6, 1996, IEEE Computer Society Press, Los Alamitos, CA, 1996, pp. 158–165.
- [6] E. CUTHILL AND J. MCKEE, *Reducing the bandwidth of sparse symmetric matrices*, in ACM Proceedings of the 24th National Conference, ACM, New York, 1969, pp. 157–172.
- [7] T. A. DAVIS, Direct Methods for Sparse Linear Systems, SIAM, Philadelphia, 2006.
- [8] T. A. DAVIS AND Y. HU, *The University of Florida sparse matrix collection*, ACM Trans. Math. Software, 38 (2011), Art. 1 (25 pages).
- [9] T. A. DAVIS AND E. P. NATARAJAN, Algorithm 907: KLU, A direct sparse solver for circuit simulation problems, ACM Trans. Math. Software, 37 (2010), Art. 36 (17 pages).
- [10] T. DAYAR AND W. J. STEWART, Comparison of partitioning techniques for two-level iterative solvers on large, sparse markov chains, SIAM J. Sci. Comput., 21 (2000), pp. 1691–1705.
- [11] I. S. DUFF AND J. KOSTER, On algorithms for permuting large entries to the diagonal of a sparse matrix, SIAM J. Matrix Anal. Appl., 22 (2001), pp. 973–996.
- [12] I. S. DUFF AND J. K. REID, An implementation of Tarjan's algorithm for the block triangularization of a matrix, ACM Trans. Math. Software, 4 (1978), pp. 137–147.
- [13] —, Algorithm 529: Permutations to block triangular form [F1], ACM Trans. Math. Software, 4 (1978), pp. 189–192.
- [14] D. FRITZSCHE, Overlapping and Nonoverlapping Orderings for Preconditioning, PhD Thesis, Dept. of Mathematics, Temple University, Philadelphia, 2010.
- [15] D. FRITZSCHE, A. FROMMER, AND D. B. SZYLD, Extensions of certain graph-based algorithms for preconditioning, SIAM J. Sci. Comput., 29 (2007), pp. 2144–2161.

247

ETNA Kent State University http://etna.math.kent.edu

- [16] M. R. GAREY AND D. S. JOHNSON, Computers and Intractability: A Guide to the Theory of NP-Completeness, W. H. Freeman, San Francisco, 1979.
- [17] F. GAVRIL, Some NP-complete problems on graphs, in Proceedings of the 11th Conference on Information Sciences and Systems, Johns Hopkins University, Baltimore, 1977, pp. 91–95.
- [18] A. GEORGE, Computer implementation of the finite-element method, PhD Thesis, Department of Computer Science, University of Ilinois at Urbana-Champaign, Urbana-Champaign, IL, 1971.
- [19] HSL, HSL 2011: A collection of Fortran codes for large scale scientific computation, 2011. http://www.hsl.rl.ac.uk.
- [20] M. OLSCHOWKA AND A. NEUMAIER, A new pivoting strategy for Gaussian elimination, Linear Algebra Appl., 240 (1996), pp. 131–151.
- [21] Y. SAAD, ILUT: A dual threshold incomplete ILU factorization, Numer. Linear Algebra Appl., 1 (1994), pp. 387–402.
- [22] _____, Iterative Methods for Sparse Linear Systems, 2nd ed., SIAM, Philadelphia, 2003.
- [23] Y. SAAD AND M. H. SCHULTZ, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 856–869.
- [24] R. E. TARJAN, Depth-first search and linear graph algorithms, SIAM J. Comput., 1 (1972), pp. 146–160.
- [25] —, A hierarchical clustering algorithm using strong components, Inform. Process. Lett., 14 (1982), pp. 26–29.
- [26] ——, An improved algorithm for hierarchical clustering using strong components, Inform. Process. Lett., 17 (1983), pp. 37–41.
- [27] H. THORNQUIST, E. R. KEITER, R. J. HOEKSTRA, D. M. DAY, AND E. G. BOMAN, A parallel preconditioning strategy for efficient transistor-level circuit simulation, in Proceedings of the 2009 International Conference on Computer-Aided Design (ICCAD'09), ACM, New York, 2009, pp. 410–417.