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## Department of Computer Science and Engineering University of Minnesota, Twin Cities

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# A HIERARCHICAL LOW RANK SCHUR COMPLEMENT PRECONDITIONER FOR INDEFINITE LINEAR SYSTEMS\*

5 GEOFFREY DILLON<sup>†</sup>, VASSILIS KALANTZIS<sup>†</sup>, YUANZHE XI<sup>†</sup>, AND YOUSEF SAAD<sup>†</sup>

Abstract. Nonsymmetric and highly indefinite linear systems can be quite difficult to solve 6 by iterative methods. This paper combines ideas from the multilevel Schur low rank preconditioner 7 developed by Y. Xi, R. Li, and Y. Saad [SIAM J. Matrix Anal., 37 (2016), pp. 235–259] with 8 classic block preconditioning strategies in order to handle this case. The method to be described 9 generates a tree structure  $\overline{T}$  that represents a hierarchical decomposition of the original matrix. 10 This decomposition gives rise to a block structured matrix at each level of  $\mathcal{T}$ . An approximate 11 12 inverse of the original matrix based on its block LU factorization is computed at each level via a low rank property that characterizes the difference between the inverses of the Schur complement and 13 14 another block of the reordered matrix. The low rank correction matrix is computed by several steps of the Arnoldi process. Numerical results illustrate the robustness of the proposed preconditioner 15 with respect to indefiniteness for a few discretized partial differential equations (PDEs) and publicly 16 available test problems. 17

Key words. block preconditioner, Schur complements, multilevel, low rank approximation,
 Krylov subspace methods, domain decomposition, nested dissection ordering

20 AMS subject classifications. 65F08, 65F10, 65F50, 65N55, 65Y05

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1. Introduction. This paper focuses on the solution of large nonsymmetric sparse linear systems

24 (1.1) Ax = b

via Krylov subspace methods where  $A \in \mathbb{C}^{n \times n}$  and  $b \in \mathbb{C}^n$ . When solving (1.1), it is often necessary to combine one of these Krylov methods with some form of preconditioning. For example, a *right-preconditioning* method would solve the system  $AM^{-1}u = b, M^{-1}u = x$  in place of (1.1). Other variants include left and two-sided preconditioners. Ideally, M is an approximation to A such that it is significantly easier to solve linear systems with it than with the original A.

A commonly used preconditioner is the incomplete LU (ILU) factorization of A, 31 where  $A \approx LU = M$ . ILU preconditioners can be very effective for certain types 32 of linear systems. However, if the original matrix A is poorly conditioned or highly 33 indefinite (A has eigenvalues on both sides of the imaginary axis), then ILU methods 34 can fail due to very small pivots or unstable factors [12, 42]. Another disadvantage of 35 ILU methods is their poor performance on high-performance computers, e.g., those 36 with graphics processing units [33] or Intel Xeon Phi processors. Algebraic multigrid 37 (AMG) is another popular technique for solving problems arising from discretized 38 PDEs. Multigrid methods are provably optimal for a wide range of SPD matrices 39 and also perform well in parallel. However, without specialization, multigrid will 40 fail on even mildly indefinite problems. Sparse approximate inverses emerged in the 41

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<sup>&</sup>lt;sup>†</sup>Department of Computer Science & Engineering, University of Minnesota, Twin Cities, Minneapolis, MN 55455 (gdillon@umn.edu, kalan019@umn.edu, yxi@umn.edu, saad@umn.edu).

1990s as alternatives to ILU factorizations [9, 13, 22]. These methods were mostly 42 abandoned due to their high cost in terms of both arithmetic and memory usage. A 43 subsequent class of preconditioners were based on rank-structured matrices [10]. Two 44 such types of matrices are  $\mathcal{H}^2$ -matrices [23, 24] and hierarchically semiseparable (HSS) 45 matrices [49, 50, 51]. Both of these forms are the result of a partition of the original 46 matrix where some of the off-diagonal blocks are approximated by low rank matrices. 47 These ideas have been used to develop both sparse direct solvers and preconditioners 48 [52]. Similarly, it is also possible to exploit preconditioners based on hierarchical LU 49 factorizations [4]. 50

In this paper we focus on approximate inverse preconditioners which are based 51 on low rank corrections. Such approaches include the multilevel low rank (MLR) 52 [32], the Schur complement low rank (SLR) preconditioner [34], and the multilevel 53 Schur complement low rank (MSLR) preconditioner [46]. The idea behind the MSLR 54 preconditioner is to combine a multilevel hierarchical interface decomposition (HID) 55 ordering [25] along with an efficient Schur complement approximation. This approach 56 is shown to be much less sensitive to indefiniteness than the classical ILU and domain 57 decomposition based methods. However, MSLR is designed for symmetric problems. 58 This paper presents a preconditioner that incorporates a modified hierarchical low 59 rank approximation of the inverse Schur complement from the MSLR preconditioner 60 into a block preconditioner based on the block LU factorization of A. The resulting 61 method will be called a generalized multilevel Schur complement low rank (GMSLR) 62 preconditioner. Two characteristics of GMSLR are worth highlighting. First, GM-63 SLR is designed to be applicable to a wide range of problems. The preconditioner is 64 nonsymmetric, changes at each iteration, and, since it incorporates inner solves, uses 65 flexible GMRES [40] as the accelerator. The method also performs well for symmetric 66 matrices. As observed in [7, section 10.1.2], the loss of symmetry incurred by appli-67 cation of a nonsymmetric preconditioner is not a major concern provided that good 68 approximations to certain blocks of A are available. The numerical experiments will 69 confirm this observation. Second, a property that is inherited from MSLR is that the 70 GMSLR preconditioner computes a recursive, multilevel approximation to the inverse 71 of the Schur complement. GMSLR is a block preconditioner with inner sub solves re-72 quired at every outer iteration. These inner solves can themselves be preconditioned 73 in order to reduce computational costs. One of these required inner solves is with the 74 Schur complement; i.e., we must solve Sy = g. For most problems, this inverse Schur 75 complement approximation turns out to be an effective preconditioner for these inner 76 solves. Since an important goal of this paper is to deal with indefinite problems, we 77 explored another improvement targeted specifically at such problems. This improve-78 ment consists of a well-established strategy [20, 35, 39, 45, 48] of adding complex shifts 79 to the diagonal prior to performing any of the ILU factorizations required by GMSLR. 80 In the case of GMSLR, this entails modifying the diagonal of coefficient matrix at each 81 level by adding a complex scalar. As is the case for other (standard) preconditioners 82 [39, 48], this strategy also has the effect of improving robustness while decreasing 83 the fill-in required by GMSLR, especially for highly indefinite problems such as those 84 arising from Helmholtz problems. 85

We note at this point that our focus is on a purely algebraic viewpoint where *A* is a general sparse indefinite matrix that does not necessarily originate from the discretization of a partial differential equation. Therefore, we do not consider approaches based on hierarchical matrices.

This paper is organized as follows. In section 2 we briefly review the HID ordering. Section 3 has a brief overview of block preconditioning that motivates the need for the low rank property of the inverse of the Schur complement. The details of the Schur complement approximation are given in section 4. In section 5 we present
the preconditioner construction process. A 2-level analysis of the preconditioned
eigenvalues is presented in section 6. Then, in section 7, we present some numerical

<sup>96</sup> results from test problems and problems from the SuiteSparse Matrix Collection [17].

<sup>97</sup> Concluding remarks and some ideas for future work can be found in section 8.

2. HID ordering. Reordering the original system matrix A is essential for the 98 performance of direct as well as iterative methods [8, 31, 38, 43]. GMSLR uses one 99 such reordering technique known as hierarchical interface decomposition (HID) [25]. 100 This ordering has also been used in the context of hierarchical linear system solvers 101 [5] but is applicable to a wide class of sparse matrices, not just those that originate 102 from PDEs. An HID ordering can be obtained in a number of ways. A particular 103 method for obtaining such an ordering is the well-known nested dissection method 104 [21]. Nested dissection recursively partitions the adjacency graph of A into two disjoint 105 subgraphs and a *vertex separator* in such a way that the removal of the vertices of 106 the separator from the original graph results in two disjoint subgraphs. Each level of 107 bisection produces a new separator and new subgraphs. This level information can 108 be represented by an HID tree  $\mathcal{T}$ . The matrix itself is reordered by levels, starting 109 with level 0 and ending with level L - 1. 110

Since we assume that A is large, sparse, and nonsymmetric, then an HID ordering results in the following multilevel, recursive structure:

(2.1) 
$$A_l = \begin{pmatrix} B_l & F_l \\ E_l & C_l \end{pmatrix}$$
 and  $C_l \equiv A_{l+1}$  for  $l = 0 : L - 1$ .

In this notation,  $A_0$  denotes the original matrix A after HID ordering, whereas  $A_l$  is 114 the submatrix associated with the *l*th-level connector(s). The  $B_l$  block-itself has a 115 block-diagonal structure due to the block independent set ordering [43], making solves 116 with  $B_l$  ideally suited for parallel computation. Figure 2.1 shows an example of the 117 HID ordering for a three-dimensional (3D) convection-diffusion operator discretized 118 with the standard 7-point finite difference stencil. The left subfigure plots the nonzero 119 pattern of the entire matrix while the right subfigure is a close-up view of the nonzero 120 pattern of the matrix  $C_0 \equiv A_1$ . 121

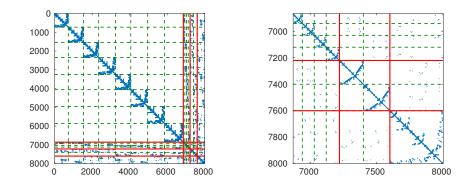


FIG. 2.1. A three-level HID ordered 3D convection-diffusion matrix with zero Dirichlet boundary conditions. The red (solid) lines separate the different levels. The green (dashed) lines separate subdomains located at the same level. Left: The original matrix is discretized on a  $20 \times 20 \times 20$ regular grid with the standard 7-point stencil. Right: Close-up view of the nonzero pattern of the matrix  $C_0 \equiv A_1$ .

Block preconditioning. Domain decomposition reordering gives rise to lin ear systems of the form

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix};$$

see [2, 11]. Similar block structured matrices also arise from the discretization of
systems of partial differential equations. In these coupled systems, the individual
blocks usually correspond to differential/integral operators; however, in this context
they represent different sets of unknowns (interior, interface, coupling) that result
from domain decomposition. There is a large body of work on preconditioning these
systems; mostly from the point of view of saddle point systems; see [6, 7, 28, 36, 37].
For examples of preconditioning other coupled systems of PDEs, see [14, 26, 27].

At the starting level, i.e., l = 0, GMSLR uses a block triangular preconditioner of the form

$$\mathcal{P} = \begin{pmatrix} \widetilde{B}_0 & F_0 \\ 0 & \widetilde{S}_0 \end{pmatrix},$$

where  $\tilde{B}_0$  is an approximation to the (1,1) block of  $A_0$  and  $\tilde{S}_0$  is an approximation to the Schur complement  $S_0 = C_0 - E_0 B_0^{-1} F_0$ .

In the ideal case where  $\tilde{B}_0 = B_0$  and  $\tilde{S}_0 = S_0$ , it is well known that the matrix  $A_0 \mathcal{P}_{\text{ideal}}^{-1}$  has a quadratic minimal polynomial, which means that GMRES will converge in two iterations [28, 37]. Therefore the total cost of the procedure based on the ideal form of (3.2) is two linear solves with  $B_0$  and two linear solves with  $S_0$ , plus additional sparse matrix-vector products. This is made clear by looking at the factored form of  $\mathcal{P}_{\text{ideal}}^{-1}$ :

$$\mathcal{P}_{\text{ideal}}^{-1} = \begin{pmatrix} B_0 & F_0 \\ & S_0 \end{pmatrix}^{-1} = \begin{pmatrix} B_0^{-1} \\ & I \end{pmatrix} \begin{pmatrix} I & -F_0 \\ & I \end{pmatrix} \begin{pmatrix} I \\ & S_0^{-1} \end{pmatrix}.$$

This choice corresponds to using only the upper triangular part of the block LUfactorization of  $A_0$  as a preconditioner. If both parts of this factorization are used, i.e., if our preconditioner is of the form

$$\mathcal{P}^{-1} = \begin{pmatrix} B_0^{-1} \\ I \end{pmatrix} \begin{pmatrix} I & -F_0 \\ I \end{pmatrix} \begin{pmatrix} I & \\ S_0^{-1} \end{pmatrix} \begin{pmatrix} I \\ -E_0 B_0^{-1} & I \end{pmatrix},$$

then in the ideal case we have an exact inverse of  $A_0$  and a Krylov method will converge in a single iteration at the total cost of two solves with  $B_0$  and one solve with  $S_0$ . Thus, in all, using (3.4) saves one  $S_0$  solve over (3.3).

The scenario just described involves ideal preconditioners (3.3) and (3.4), which are, however, not practical since they involve the exact computation of  $S_0^{-1}$ . In practice,  $\tilde{B}_0$  and  $\tilde{S}_0$  are approximated, at the cost of a few extra outer iterations. With these approximations in place, it turns out that there is little difference in practice between these two options, and, based on our experience, we prefer to use (3.2). This issue will be revisited at the end of section 7.1.1.

Similar to [34], we solve linear systems with the B blocks by using ILU factorizations. Approximations to the Schur complement are typically tailored specifically to the problem being studied (e.g., the pressure convection diffusion [19] and leastsquares commutator [18] preconditioners for Navier–Stokes). However, in our framework, the block form of A is the result of a reordering of the unknowns, and so our Schur complement approximation is inherently algebraic and not based on the physics
 of the problem. We base our Schur complement approximation on ideas from [34, 46].

4. Schur complement approximation. GMSLR is an extension of the MSLR preconditioner of [46] based on approximating the block  $\mathcal{LDU}$  factorization of (2.1),

(4.1) 
$$A_l = \begin{pmatrix} I \\ E_l B_l^{-1} & I \end{pmatrix} \begin{pmatrix} B_l \\ S_l \end{pmatrix} \begin{pmatrix} I & B_l^{-1} F_l \\ I \end{pmatrix}$$

at every level  $l = 0, \ldots, L - 1$ . We write the Schur complement as

(4.2) 
$$S_l = \left(I - E_l B_l^{-1} F_l C_l^{-1}\right) C_l \equiv \left(I - G_l\right) C_l.$$

<sup>174</sup> Let the *complex* Schur decomposition<sup>1</sup> of  $G_l$  be

(4.3) 
$$G_l = E_l B_l^{-1} F_l C_l^{-1} = W_l R_l W_l^H,$$

where  $W_l$  is unitary and  $R_l$  is an upper triangular matrix whose diagonal contains the eigenvalues of  $G_l$ . Substituting (4.3) into (4.2) we get that

178 (4.4) 
$$S_l = (I - W_l R_l W_l^H) C_l = W_l (I - R_l) W_l^H C_l.$$

Then, the Sherman–Morrison–Woodbury formula yields the inverse of  $S_l$ ,

(4.5) 
$$S_l^{-1} = C_l^{-1} W_l (I - R_l)^{-1} W_l^H = C_l^{-1} \left[ I + W_l ((I - R_l)^{-1} - I) W_l^H \right],$$

<sup>181</sup> which reduces to

(4.6) 
$$S_l^{-1} = C_l^{-1} + C_l^{-1} W_l \left[ (I - R_l)^{-1} - I \right] W_l^H.$$

Some observations about the matrix  $S_l^{-1} - C_l^{-1}$  will be stated in the next section.

In our algorithm, we do not compute the full Schur decomposition of  $G_l$ , just the  $k_l \times k_l$  leading submatrix of  $R_l$  and the first  $k_l$  Schur vectors. These choices give rise to the following inverse Schur complement approximation.

DEFINITION 4.1. Let  $G_l = E_l B_l^{-1} F_l C_l^{-1}$ ,  $l = 0 \dots L - 1$ , and  $G_l = W_l R_l W_l^H$  be its Schur decomposition at level l. In addition, let  $W_{l,k_l}$  be the matrix of the first  $k_l$ Schur vectors,  $k_l \leq s_l$ , of  $W_l$ , where  $s_l$  denotes the size of the matrix  $C_l$ . If we define  $R_{l,k_l}$  to be the  $k_l \times k_l$  leading principal submatrix of  $R_l$ , then the approximate lth-level inverse Schur complement  $\tilde{S}_{l,k_l}^{-1}$  is given by

<sup>192</sup> (4.7) 
$$\widetilde{S}_{l,k_l}^{-1} = C_l^{-1} (I + W_{l,k_l} H_{l,k_l} W_{l,k_l}^H),$$

193 where

<sup>194</sup> (4.8) 
$$H_{l,k_l} = [(I - R_{l,k_l})^{-1} - I].$$

The inverse Schur complement approximation in (4.7) will be used at every level l = 0, ..., L - 1. Due to the potential large size of the  $C_l$  blocks, we can only afford to factor  $C_{L-1}$  since it is the smallest of all the  $C_l$  blocks. For  $l \neq L - 1$  we use a slightly modified version of the recursive scheme of [46] for approximating the action of  $C_l^{-1}$  on a vector. The details of this approximation will be shown in section 5.

<sup>&</sup>lt;sup>1</sup>Throughout the rest of this paper we use the superscript "H" to denote the conjugate transpose.

4.1. Low rank property of  $S_l^{-1} - C_l^{-1}$ . Consider the inverse Schur complement formula given by (4.6). In this section we claim that for certain problems, the matrix  $S_l^{-1} - C_l^{-1}$  is of low rank. If this is the case, then (4.7) will be a good approximation to (4.6). The only assumption we make on the blocks  $B_l, C_l$  is that they have *LU* factorizations, i.e.,

205 (4.9) 
$$B_l = L_{B_l} U_{B_l}, \ C_l = L_{C_l} U_{C_l}$$

 $_{206}$  In practice we will use incomplete LU factorizations, so instead

$$B_l \approx L_{B_l} U_{B_l}, \ C_l \approx L_{C_l} U_{C_l}.$$

Note that for 3D problems the number of interface points (i.e., the size of the  $C_l$ block) can be quite large, making this factorization too costly. This is part of the motivation for the multilevel decomposition.

To see that  $S_l^{-1} - C_l^{-1}$  is usually of low rank, again define the matrix  $G_l$  by

(4.10) 
$$G_l = E_l B_l^{-1} F_l C_l^{-1} = (C_l - S_l) C_l^{-1}$$

Let  $\gamma_i, i = 1, \ldots, s$ , be the eigenvalues of  $G_l$  (and also  $R_l$ ) and define  $X_l \equiv C_l(S_l^{-1} - C_l^{-1})$ . By (4.6) the eigenvalues  $\theta_1, \theta_2, \cdots, \theta_{s-1}, \theta_s$  of  $X_l$  are given explicitly by

215 (4.11) 
$$\theta_i = \frac{\gamma_i}{1 - \gamma_i}, \quad i = 1, \dots, s,$$

since  $(I - G_l)^{-1} - I = G_l (I - G_l)^{-1}$ .

As long as the eigenvalues  $\gamma_i$  of  $G_l$  are not clustered at 1, the eigenvalues  $\theta_i$  of  $X_l$  will be well separated. This in turn means that  $S_l^{-1} - C_l^{-1}$  can be approximated by a low rank matrix. This was studied in detail in [46, section 2] for the symmetric case, where a theoretical bound for the numerical rank was established.

4.2. Building the low rank correction. We use Arnoldi's method [1] to build the low rank correction matrices in (4.7). This approximation can be efficient if the desired eigenpairs of  $G_l$  are on the periphery of the spectrum. However, as we shall see in the numerical results, this is simply not the case for some of the more indefinite problems. A particular remedy is to take more steps of Arnoldi's method.

Taking m steps of Arnoldi's method on  $G_l$  yields the Krylov factorizations,

227 
$$G_l U_m = U_m H_m + h_{m+1,m} u_{m+1} e_m^T$$
228 
$$U_m^H G_l U_m = H_m,$$

where  $U_m$  is an orthonormal matrix and  $H_m$  is a Hessenberg matrix whose eigenvalues (also called *Ritz values*) are good estimates to the extreme eigenvalues of  $G_l$ . We then take the complex Schur factorization of  $H_m$ 

232 (4.12) 
$$Q^H H_m Q = T.$$

We can reorder the  $k_l$  eigenvalues closest to 1 we wish to deflate so that they appear as the first  $k_l$  diagonal entries of T [3, 44]. The low rank matrices in (4.7) are approximated by

(4.13) 
$$R_{l,k_l} \approx T_{1:k_l,1:k_l} \text{ and } W_{l,k_l} \approx U_m Q_{:,1:k_l}.$$

5. Preconditioner construction process. In this section we show how the low rank property discussed in the previous section is used to build an efficient preconditioner. The only assumption we make is that each of the  $B_l$ ,  $C_l$  blocks is nonsingular. This assumption is typically satisfied unless the original matrix has a block of all zeros (e.g., a saddle point system). At the end of this section we also present an analysis of the computational and memory costs of the proposed preconditioner.

5.1. 3-level scheme. We illustrate the steps taken to solve Ax = b with a 3-level example.

Step 0: Apply a 3-level HID ordering to the original matrix A and right-hand side b. Call the resulting reordered matrix and right-hand side  $A_0$  and  $b_0$ , respectively.

248 Step 1: At this level (only) we use the block triangular matrix

$$\mathcal{U}_0^{-1} = \begin{pmatrix} B_0 & F_0 \\ & S_0 \end{pmatrix}^{-1} = \begin{pmatrix} B_0^{-1} & \\ & I \end{pmatrix} \begin{pmatrix} I & -F_0 \\ & I \end{pmatrix} \begin{pmatrix} I & \\ & S_0^{-1} \end{pmatrix}$$

as a right preconditioner for  $A_0$ ; i.e., we solve  $A_0 \mathcal{U}_0^{-1} u = b_0$ . Here we approximately factor  $B_0$  by ILU and approximate the Schur complement by

252 
$$S_0^{-1} \approx \widetilde{S}_0^{-1} = C_0^{-1} (I + W_0 H_0 W_0^H)$$

where  $H_0$  and  $W_0$  are taken from (4.8) and (4.13), respectively. To solve with  $C_0$ , we refer to (2.1) and move from level 0 to level 1.

<sup>255</sup> Step 2: At level 1, we have

249

256

262

265

$$C_0^{-1} = A_1^{-1} = \begin{pmatrix} I & -B_1^{-1}F_1 \\ I \end{pmatrix} \begin{pmatrix} B_1^{-1} & \\ & S_1^{-1} \end{pmatrix} \begin{pmatrix} I & \\ -E_1B_1^{-1} & I \end{pmatrix},$$

where  $S_1^{-1}$  is approximated by  $C_1^{-1}$  plus a low rank correction,

258  $S_1^{-1} \approx \widetilde{S}_1^{-1} = C_1^{-1} (I + W_1 H_1 W_1^H).$ 

- Next we move up a level again to define an approximate inverse for  $C_1$ , referring again to (2.1).
- <sup>261</sup> Step 3: At level 2 we have

$$C_1^{-1} = A_2^{-1} = \begin{pmatrix} I & -B_2^{-1}F_2 \\ & I \end{pmatrix} \begin{pmatrix} B_2^{-1} & \\ & S_2^{-1} \end{pmatrix} \begin{pmatrix} I & \\ -E_2B_2^{-1} & I \end{pmatrix}.$$

Similarly to Step 2, we now approximate  $S_2^{-1}$  by  $C_2^{-1}$  plus a low rank correction term, i.e.,

$$S_2^{-1} \approx \widetilde{S}_2^{-1} = C_2^{-1} (I + W_2 H_2 W_2^H)$$

As this is the last level, we compute the ILU factorization  $C_2 \approx L_{C_2} U_{C_2}$ .

In order to apply the preconditioner  $\mathcal{U}_0^{-1}$ , the actual algorithm starts at level 2 and proceeds up to level 0. For this particular example, that means we start forwardbackward solving with the ILU factorization of  $C_2$  since  $C_2^{-1}$  is needed in order to apply  $S_2^{-1}$ . Now that the action of  $S_2^{-1}$  is available, we can then approximate  $A_2^{-1}$ , and the pattern continues until we hit level 0, i.e.,

$$L_{C_2}U_{C_2} \to C_2^{-1} \to \widetilde{S}_2^{-1} \to A_2^{-1} \to \widetilde{S}_1^{-1} \to A_1^{-1} \to \widetilde{S}_0^{-1} \to \mathcal{U}_0^{-1}.$$

Once  $C_l^{-1}$  (or its action on a vector) is available, the low rank correction matrices  $W_l, H_l$  can be computed.

**5.2.** General case. When computing the partial Schur decomposition of the 275 matrix  $G_l$ , we need to be able to compute matrix vector products with the matrix 276  $E_l B_l^{-1} F_l C_l^{-1}$  at each level l. We already have the factors of  $B_l$ , so any matrix-vector 277 product with  $B_l^{-1}$  can be computed with one forward and one backward substitution. 278 The same does not hold true for  $C_l$ , since we only compute its factorization at level 279 L-1. However, we already have an approximate factorization of  $A_{l+1}^{-1}$ , and since 280  $C_l^{-1} = A_{l+1}^{-1}$  we can use this approximation to apply  $C_l^{-1}$  to a vector. The construction of the preconditioner is summarized in Algorithm 1. The details of the recursively 281 282 defined product of  $C_l^{-1}$  with a vector b are given in Algorithm 2. 283

Algorithm 1. Generalized multilevel Schur low rank (construction phase).

1: procedure GMSLR Apply an *L*-level reordering to A ( $A_0$  = reordered matrix). 2: for level l from L - 1 to 0 do 3: if l = L - 1 then 4: Compute ILU factorization of  $C_{L-1}$ ,  $C_{L-1} \approx L_{C_{L-1}} U_{C_{L-1}}$ 5: 6: end if 7: Compute ILU factorization of  $B_l$ ,  $B_l \approx L_{B_l} U_{B_l}$ . Perform  $k_l$  steps of the Arnoldi process  $\triangleright$  Call Algorithm 2 to apply  $C_l^{-1}$ 8:  $[V_l, K_l] = \text{Arnoldi}(E_l U_{B_l}^{-1} L_{B_l}^{-1} F_l C_l^{-1}, k_l)$ Compute the complex Schur decomposition  $K_l = WTW^H$ . 9: Compute  $W_{l,k_l} = V_l W$  and set  $R_{l,k_l} = T_{1:k_l,1:k_l}$ . Compute  $H_l = (I - R_{l,k_l})^{-1} - I = R_{l,k_l}(I - R_{k_l})^{-1}$ . 10: 11:

12: end for

13: end procedure

Algorithm 2. Approximation of  $y = C_l^{-1}b$  for  $l \ge 1$  and  $y = \mathcal{U}_0^{-1}b$ .

1: procedure RecursiveSolve(l, b)if l = L - 1 then 2: return  $y = U_{C_L}^{-1} L_{C_L}^{-1} b$ 3: 4: else Split  $b = (b_1^H, b_2^H)^H$  conformingly with the blocking of  $C_l$ Compute  $z_1 = U_{B_{l+1}}^{-1} L_{B_{l+1}}^{-1} b_1$ Compute  $z_1 = b_{B_{l+1}} L_{B_{l+1}}^{-1} b_1$ 5: 6: Compute  $z_2 = b_2 - E_{l+1} z_1$ 7: if  $1 \leq l < L - 1$  then 8: Compute  $w_2 = W_{l+1,k_{l+1}}H_{l+1}W_{l+1,k_{l+1}}^H z_2$ Compute  $y_2 = \text{RecursiveSolve}(l+1, z_2 + w_2)$ Compute  $y_1 = z_1 - U_{B_{l+1}}^{-1}L_{B_{l+1}}^{-1}F_{l+1}y_2$ 9: 10: 11: else 12:Solve the system  $S_0y_2 = z_2$  with  $\widetilde{S}_0^{-1}$  as a right preconditioner Compute  $y_1 = U_{B_0}^{-1} L_{B_0}^{-1} (b_1 - F_0 y_2)$ 13:14:end if 15:return  $y = (y_1^H, y_2^H)^H$ 16:17: end if 18: end procedure

Similarly to MSLR the HID ordering gives rise to  $B_l$  matrices that are block-284 diagonal in structure, and so all of these blocks can be factored in parallel. Further-285 more, the triangular solves associated with  $B_l$  can also be done in parallel for each 286 block. In addition, while Algorithm 2 generally provides an accurate approximation to 287  $C_l^{-1}$ , we must point out that due to the presence of the inner solve at level l = 0 (Line 288 13 of Algorithm 2), GMSLR is (potentially) more expensive per iteration than MSLR. 289 This expense can be lessened somewhat by the fact that the inner solves typically can 290 only require 1–2 digits of accuracy without radically affecting the convergence rate of 291 the outer solve. 292

5.3. Computational and memory complexity of the preconditioner. Let mem(ILU( $B_l$ )) denote the memory cost associated with the storage of the incomplete factorization of  $B_l$ . Then the total memory cost  $\mu_{GMSLR}^{(L)}$  of the GMSLR preconditioner using L levels is

$$\mu_{GMSLR}^{(L)} = \left(\sum_{l=0}^{L-1} \left[ \operatorname{mem}(\operatorname{ILU}(B_l)) + \max\left\{2s_lk_l + k_l^2, 3s_l^2\right\} \right] \right) + \operatorname{mem}(\operatorname{ILU}(C_{L-1})),$$

where the second term inside the summation accounts for the memory cost associated with the partial Schur decompositions of order  $1 \le k_l \le s_l$  at levels  $0 \le l \le L-1$ , and  $l_{100}$  and  $l_{10}$  denotes the number of interface variables at level l, i.e., the leading dimension of each  $C_l$ . For simplicity, we treat the upper triangular matrix  $H_{l,k_l}$  as a dense matrix. In the case where the incomplete factorization of matrices  $B_l$ ,  $l = 0, \ldots, L-1$ , and  $C_{L-1}$  are obtained by a thresholded version of ILU, with a maximum number of nonzero entries per row equal to  $\tau$ , the above memory cost is bounded by

$$\mu_{GMSLR}^{(L)} \le \left(\sum_{l=0}^{L-1} \left[ 2\tau d_l + \max\left\{ 2s_l k_l + k_l^2, 3s_l^2 \right\} \right] \right) + 2\tau s_{L-1},$$

where  $d_l$  denotes the leading dimension of  $B_l$ .

To obtain an estimate of the computational cost to apply the GMSLR precondi-307 tioner at level l, we need to consider the computational cost associated with all levels 308  $l + 1, \ldots, L - 1$ . In particular, let trisol(ILU( $B_l$ )) and trisol(ILU( $C_{L-1}$ )) denote the cost of the triangular solves with  $B_l$  and  $C_{L-1}$ , respectively, and let  $\gamma_{GMSLR}^{(L-1)}$  denote 309 310 the cost associated with level l = L - 1. At level l = L - 2, the cost to apply the 311 GMSLR preconditioner is equal to the sum of the cost to apply the preconditioner at 312 level l+1 = L-1 and the cost  $2 \times \text{trisol}(\text{ILU}(B_{L-2})) + O(s_{L-2}k_{L-2})$ . Continuing in 313 the same spirit, we finally get that the cost to apply the GMSLR preconditioner at 314 level  $l, \gamma_{GMSLR}^{(l)}$ , is equal to 315

<sup>316</sup> 
$$\gamma_{GMSLR}^{(l)} = \gamma_{GMSLR}^{(l+1)} + 2 \times \operatorname{trisol}(\operatorname{ILU}(B_l)) + O(s_l k_l), \quad l = 0, \dots, L-2,$$

317 where

<sup>318</sup> 
$$\gamma_{GMSLR}^{(L-1)} = \text{trisol}(\text{ILU}(C_{L-1})) + 2 \times \text{trisol}(\text{ILU}(B_{L-1})) + O(s_{L-1}k_{L-1}).$$

6. Eigenvalue analysis. This section studies the spectra of linear systems preconditioned by GMSLR. We only consider a 2-level decomposition since the recursive nature of both algorithms makes the analysis difficult. In what follows, let  $\tilde{B}_0$  denote an approximation to  $B_0$  and  $\tilde{S}_0$  the GMSLR approximation to the Schur complement

 $S_0 = C_0 - E_0 B_0^{-1} F_0$ , respectively. GMSLR starts with a 2 × 2 block partition of the 323 original matrix A, i.e., 324

$$A_0 = \begin{pmatrix} B_0 & F_0 \\ E_0 & C_0 \end{pmatrix},$$

where  $B_0$  is  $n_B \times n_B$  and  $C_0$  is  $s \times s$ . 326

As was already seen, the GMSLR preconditioner is based on the block-LU fac-327 torization of (6.1), so at level 0 we have 328

$$A_0 = \begin{pmatrix} B_0 & F_0 \\ E_0 & C_0 \end{pmatrix} = \begin{pmatrix} I & 0 \\ E_0 B_0^{-1} & I \end{pmatrix} \begin{pmatrix} B_0 & F_0 \\ 0 & S_0 \end{pmatrix} = \mathcal{L}_0 \mathcal{U}_0,$$

and the preconditioner  $\widetilde{\mathcal{U}}_0^{-1}$  is 330

$$\widetilde{\mathcal{U}}_0^{-1} = \begin{pmatrix} \widetilde{B}_0^{-1} & 0\\ 0 & I \end{pmatrix} \begin{pmatrix} I & -F_0\\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0\\ 0 & \widetilde{S}_0^{-1} \end{pmatrix}.$$

A simple calculation shows that 332

$$A_0 \widetilde{\mathcal{U}}_0^{-1} = \begin{pmatrix} B_0 \widetilde{B}_0^{-1} & (I - B_0 \widetilde{B}_0^{-1}) F_0 \widetilde{S}_0^{-1} \\ E_0 \widetilde{B}_0^{-1} & S_0 \widetilde{S}_0^{-1} \end{pmatrix}.$$

If we assume that  $\widetilde{B}_0 = B_0$ , then (6.2) simplifies to 334

335 (6.3) 
$$A_0 \widetilde{\mathcal{U}}_0^{-1} = \begin{pmatrix} I & 0 \\ E_0 B_0^{-1} & S_0 \widetilde{S}_0^{-1} \end{pmatrix},$$

336

which has eigenvalues  $\lambda(A_0 \widetilde{\mathcal{U}}_0^{-1}) = \{1, \lambda(S_0 \widetilde{S}_0^{-1})\}$ . Convergence will be rapid if the eigenvalues of  $S_0 \widetilde{S}_0^{-1}$  are also close to 1. To illustrate the influence the rank has on convergence, we show in Figure 6.1 the spectra 339 340 of  $S_0 \tilde{S}_0^{-1}$  for a small test problem. Here A is the discretized shifted Laplacian operator 341  $-\Delta u - cu = f$  with c = 0.0 (left figure) and c = 0.5 (right figure) and homogeneous 342 Dirichlet boundary conditions. For reference, when c = 0.5, this  $8000 \times 8000$  matrix 343 has 35 negative eigenvalues. This is a matrix selected for illustrative purposes, so we 344 use two levels with equal ranks  $k_0, k_1$  and compute the exact LU factorization of  $B_0$ . 345 As the ranks  $k_0, k_1$  increase, the real part of the eigenvalues of  $S_0 \tilde{S}_0^{-1}$  clusters more 346 tightly around 1. 347

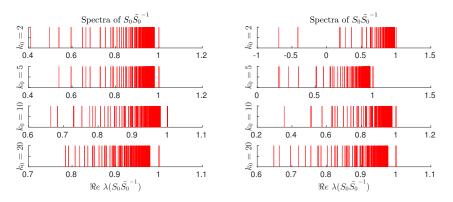


FIG. 6.1. The spectrum of  $S_0 \tilde{S}_0^{-1}$  for different values of  $k_0 \equiv k_1$  (L = 2). Left: c = 0.0. Right: 337 338 c = 0.5.

A10

7. Numerical experiments. All experiments were run on a single node of the 348 Mesabi Linux cluster at the Minnesota Supercomputing Institute. This node has a 349 memory of 64 GBs and consists of two sockets each having a twelve core 2.5 GHz Intel 350 Haswell processor. The GMSLR preconditioner was written in C++ and compiled 351 by Intel's C++ compiler using -03 optimization. Simple thread-level parallelism was 352 achieved with OpenMP with a maximum of 24 threads. The  $B_l$  blocks are factored by 353 the ILUT routine from ITSOL. The Intel Math Kernel Library (MKL) was used for 354 the BLAS and LAPACK routines. We use flexible GMRES [40] with a fixed restart 355 size of 40 as the outer solver, denoted by FGMRES(40). The inner solve in Step 14 356 of Algorithm 2 is also done with FGMRES. Unless otherwise noted, we follow the 357 methodology of [32, 41, 46] where the right-hand side vector b is given by Ae = b, 358 where e is the vector of all ones. 359

The HID ordering was obtained by the function PartGraphRecursive from the 360 METIS [30] package. The diagonal blocks of each  $B_l, C_l, l = 0, \ldots, L-1$ , were 361 reordered using the approximate minimum degree (AMD) ordering [15, 16] in order 362 to reduce the fill-in generated by their ILU factorizations. In our experiments the 363 reported preconditioner construction time comes from the factorization of the  $B_l$ 364 blocks and the computation of the low rank correction matrices. The reordering time 365 is regarded as preprocessing and is therefore not reported. Similarly, the iteration 366 time is the combined time spent on the inner and outer solves. 367

The parameters we are most interested in varying are the number L of levels in the HID and the maximum rank used in the low rank correction, i.e., the number of steps of Arnoldi's method (see section 4.2), denoted by rk. In particular we set  $k_l$ in (4.13) to be equal to rk for any l = 0, ..., L - 1, and thus all Arnoldi vectors are included in the low rank correction terms.

- <sup>373</sup> We use the following notation in the results that follow:
- fill =  $\frac{nnz(prec)}{nnz(A)}$ , where nnz denotes the number of nonzero entries of the input matrix;
- p-t: wall clock time to build the preconditioner (in seconds);
- its: number of *outer* iterations of preconditioned FGMRES(40) required for  $||r_k||_2 < 10^{-6}$ . We use "F" to indicate that FGMRES(40) did not converge after 500 iterations;
- i-t: wall clock time for the iteration phase of the solver;
  - rk: max rank used in building the low rank corrections.

The value of nnz(prec) is the sum of the nonzero entries associated with the incomplete factorizations (ILU) and low rank correction (LRC) terms. These quantities are computed as  $\sum_{l=0}^{L-1} [(nnz(U_{B_l}) + nnz(L_{B_l})] + (nnz(U_{C_{L-1}}) + nnz(L_{C_{L-1}})))$ for ILU and  $\sum_{l=0}^{L-1} [2s_l rk + rk^2]$  for LRC, respectively.

7.1. Problem 1. We begin our tests with the symmetric indefinite problem  

$$-\Delta u - cu = f \text{ in } \Omega,$$

388 (7.1)  $u = 0 \text{ on } \partial\Omega,$ 

381

where  $\Omega = (0, 1)^3$ . The discretization is via finite differences with the standard 7-point stencil in three dimensions. This test problem is useful for testing robustness with respect to definiteness. For reference, GMRES preconditioned by standard AMG fails to converge when applied to (7.1) with even a small positive shift on a  $32 \times 32$  regular mesh.

**7.1.1. Varying the number of levels.** First, we study the effect of adding more levels to the preconditioner. We solve (7.1) with c > 0 in order to make the problem indefinite. In the cases where c > 0, we shift the diescretized Laplacian operator by sI, where  $s = h^2c$  for mesh size h. For this first example, we set s = 0.5.

#### TABLE 7.1

The fill factor and iteration counts for solving (7.1) with s = 0.5 on a  $32^3$  grid with the FGMRES-GMSLR method. Here, the maximum rank for the LRC matrices was fixed at 50.

L	ILU fill	LRC fill	fill	p-t	i-t	its
2	34.61	.23	34.84	5.16	1.25	16
3	21.03	.68	21.71	.986	2.69	16
4	15.64	1.35	16.99	.382	1.03	12
5	8.69	2.46	11.15	.169	.97	19
6	5.56	3.96	9.52	.172	.95	17

The associated coefficient matrix has 163 negative eigenvalues. The maximum rank 406 was fixed at 50. By Table 7.1 we can see that, as L grows larger, the ILU fill factor 407 decreases monotonically while the low rank correction fill factor increases monoton-408 ically. The optimal number of levels occurs when these two quantities are roughly 409 equal. For this particular example, we pick  $L_{opt} = 6$  as it strikes the right balance of 410 fill, iteration count, and total computational time. Note that as L increases, so does 411 the number of interface variables at the root level,  $s_0$ . This can be verified immedi-412 ately by looking at Table 7.2 where we list  $s_0$  for all values of L from L = 2 to L = 6. 413 Figure 7.1 plots the number of inner iterations performed by GMSLR as a function 414 of the rank rk for different values of the drop tolerance (denoted by tol) in the ILU 415 factorizations. 416

TABLE 7.2 TABLE 7.2 Comparison between GMSLR with only  $\mathcal{U}_0^{-1}$  and GMSLR with  $\mathcal{L}_0^{-1}$  and  $\mathcal{U}_0^{-1}$  on (7.1) with s = 0.5 on a  $32^3$  grid. The maximum rank was fixed at 50.

		GMSI	LR - $\mathcal{U}_0^-$	$^{-1}$ only	GMS	LR - $\mathcal{U}_0^-$	$^{-1}\mathcal{L}_{0}^{-1}$
L	$s_0$	p-t	i-t	its	p-t	i-t	its
2	1,024	5.16	1.25	16	5.15	3.59	47
3	2,016	.986	2.69	16	1.01	5.24	37
4	2,977	.382	1.03	12	.391	2.88	34
5	4,955	.169	.97	19	.181	1.49	27
6	6,699	.172	.95	17	.176	1.43	24

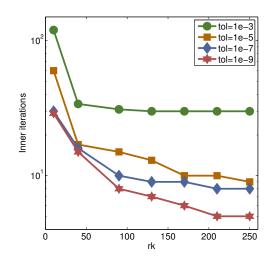


FIG. 7.1. Number of inner iterations in GMSLR as a function of rk for different values of the drop tolerance tol in the incomplete factorizations of  $B_l$  and  $C_{L-1}$ . We set L = 2.

394

Finally, recall that we could have used the inexact version of (3.4) instead of (3.2). For SPD problems there is not a significant difference in the results obtained by either preconditioner. However, as shown in Table 7.2, for an indefinite problem such as (7.1) with s = 0.5, (3.2) performs better. The likely explanation for this behavior is that (3.2) involves fewer solves with the  $B_l$  matrices which are highly indefinite and therefore admit poor ILU factorizations.

7.1.2. Varying the maximum rank in the low rank corrections. Next, we 423 keep the number of levels fixed but increase the maximum rank. We again solve (7.1)424 with s = 0.5 discretized on a  $32^3$  regular grid. The ILU fill factor is constant because 425 we are keeping the number of levels fixed at 6. The fill factor from the low rank 426 corrections increases at an almost constant rate. Increasing the maximum rank has 427 the unfortunate effect of increasing the fill factor and the preconditioner construction 428 time. As we see in Table 7.3, the effect of increasing the rank (at least for this model 429 problem) is difficult to predict. As a general rule, it seems as though a large maximum 430 rank is unavoidable for highly indefinite problems. 431

**7.1.3.** Increasingly indefinite problems. The model problem (7.1) becomes 438 significantly more difficult to solve as s increases. Here, we increase s from 0 to 439 1 while tuning the maximum rank and number of levels to compensate for solving 440 this increasingly difficult problem. We report the results that give the best balance 441 between iteration count and fill in Table 7.4. The fill factor increases dramatically for 442 two reasons: first, we must increase the rank of the low rank correction, and second, 443 we must keep the number of levels low, which, as was observed in section 7.1.1, leads 444 to increased fill-in for the same drop tolerance. If the rank is too low or the number of 445 levels is too high, FGMRES(40) simply will not converge. Recall that the construction 446 of the low rank correction is based on finding approximate eigenvalues of the matrix 447  $E_l U_{B_l}^{-1} L_{B_l}^{-1} F_l C_l^{-1}$  using Arnoldi's method. When  $B_0$  is indefinite, as is the case here, 448 the eigenvalues we seek get pushed deeper inside the spectrum; i.e., they become 449 interior eigenvalues. Since the Arnoldi process does a poorer job for these interior 450

TABLE 7.3 TABLE 7.3 Iteration counts for solving (7.1) with s = 0.5 on a  $32^3$  grid with the FGMRES-GMSLR method. The number of levels was fixed at 6.

rk	ILU fill	LRC fill	fill	p-t	i-t	its
20	5.56	1.58	7.14	.091	1.34	24
30	5.56	2.37	7.93	.118	1.14	19
40	5.56	3.17	8.73	.139	1.04	18
50	5.56	3.96	9.52	.174	.972	17
60	5.56	4.75	10.31	.208	1.29	22
70	5.56	5.24	10.8	.221	1.35	24
80	5.56	5.99	11.55	.291	.968	15

435

TABLE 7.4

Results of solving symmetric linear systems with increasing shift values s on a 32<sup>3</sup> regular mesh
 with GMSLR.

s	L	max rank	fill	p-t	i-t	its
0	8	20	5.89	.109	.068	3
.25	6	30	7.59	.117	.449	8
.5	6	50	9.52	.174	.973	17
.75	5	80	12.77	.291	.826	13
1.0	5	120	13.73	.406	1.87	29

eigenvalues than it does for extreme ones, we are forced to take more Arnoldi steps
in order to approximate them.

453 **7.2. Problem 2.** The second problem of interest is nonsymmetric:

$$-\Delta u - \alpha \cdot \nabla u - cu = f \quad \text{in } \Omega,$$

455 (7.2) 
$$u = 0 \text{ on } \partial\Omega$$

where  $\Omega = (0, 1)^3, \alpha \in \mathbb{R}^3$ . This problem is simply a shifted convection-diffusion equation, again discretized by the 7-point finite difference stencil. As before we shift the discretized convection-diffusion operator by sI where  $s = h^2c$ .

**7.2.1. Varying the number of levels.** In this next set of experiments we fix  $\alpha = [.1, .1, .1]$  and solve (7.2) in three dimensions with no shift and then with a shift of s = .25. As before, we start by increasing the number of levels. The results of the first problem with a maximum rank of 20 are in Table 7.5. These results are comparable to those obtained from the SPD problem (7.1) with s = 0; i.e., for this problem, the convergence rate is not adversely affected by the loss of symmetry.

<sup>473</sup> Next, we solve (7.2) with s = .25. The shift significantly increases the number <sup>474</sup> of eigenvalues with negative real parts, so we increase the maximum rank to 50. The <sup>475</sup> results can be found in Table 7.6. It is interesting to note that the fill from the low <sup>476</sup> rank correction is almost exactly the same as in Table 7.1. This is due to the fact <sup>477</sup> that both problems used a maximum rank of 50 to build the low rank corrections.

**7.3. Problem 3.** The third model problem is a Helmholtz equation of the form

479 (7.3) 
$$\left(-\Delta - \frac{\omega^2}{v(x)^2}\right)u(x,\omega) = s(x,\omega).$$

In this formulation,  $\Delta$  is the Laplacian operator,  $\omega$  the angular frequency, v(x)the velocity field, and  $s(x,\omega)$  is the external forcing function with corresponding

459	TABLE 7.5
460	The fill factor and iteration counts for solving (7.2) with no shift and $\alpha = [.1, .1, .1]$ on a $32^3$
461	grid with the FGMRES-GMSLR method. Here, the maximum rank for the LRC matrices was fixed
462	<i>at</i> 20.

\_ \_

L	ILU fill	LRC fill	fill	p-t	i-t	its
2	11.69	.092	11.78	.505	.159	7
3	10.13	.272	10.4	.234	.079	6
4	8.8	.539	9.34	.126	.044	5
5	6.47	.983	7.46	.09	.041	5
6	4.89	1.58	6.47	.086	.074	4
7	3.8	2.34	6.14	.092	.066	4
8	2.53	3.35	5.88	.116	.066	3

463

TABLE 7.6

The fill factor and iteration counts for solving (7.2) with s = .25 and  $\alpha = [.1, .1, .1]$  on a  $32^3$ grid with the FGMRES-GMSLR method. Here, the maximum rank for the LRC matrices was fixed at 50.

L	ILU fill	LRC fill	fill	p-t	i-t	its
2	24.11	.23	24.34	2.03	.88	16
3	15.44	.681	16.12	.58	.61	13
4	11.64	1.35	12.99	.237	.381	12
5	7.25	2.46	9.71	.149	.91	19
6	5.16	3.96	9.12	.167	.741	13
7	3.91	5.86	9.77	.214	1.00	14
8	2.56	8.39	10.95	.288	4.54	53

TABLE 7.7

Results from solving (7.3) on a sequence of 3D meshes with GMSLR. All problems have q = 8points per wavelength. The second set of results is with a small complex shift added to the  $B_{\ell}$ matrices.

490

				GMSLR - no shift				GMS	LR w/	complex	x shift
$\omega/(2\pi)$	$n = N^3$	L	$\mathbf{rk}$	fill	p-t	i-t	its	fill	p-t	i-t	its
2.5	$20^{3}$	5	16	3.79	.063	.318	14	3.56	.062	.205	17
3	$30^{3}$	6	16	5.18	.156	.308	13	4.72	.135	.547	16
5	$40^{3}$	7	16	6.19	.282	1.94	57	5.43	.251	.556	17
6	$50^{3}$	7	16	8.16	.768	3.52	54	6.64	0.54	1.3	21
8	$60^{3}$	8	16	7.73	.867	29.53	F	6.52	0.73	2.05	21
10	$80^{3}$	9	16	7.85	1.57	65.57	F	6.64	1.4	6.31	28

time-harmonic wave field solution  $u(x, \omega)$ . The computational domain is the unit 482 cube  $\Omega = (0,1)^3$  where we again use the 7-point finite difference discretization on a 483 regular mesh. The perfectly matched layer (PML) boundary condition is used on all 484 faces of  $\Omega$ . The resulting linear systems are complex non-Hermitian. If we assume 485 that the mean of v(x) is 1 in (7.3), then the wave number is  $\omega/(2\pi)$  and  $\lambda = 2\pi/\omega$  is 486 the wavelength. The number of grid points in each dimension is  $N = q\omega/(2\pi)$ , where 487 q is the number of points per wavelength. As a result, the discretized system is of size 488  $n = N^3 \times N^3.$ 489

We test the performance of the GMSLR preconditioner on six cubes, setting q = 8, 494 and report the results in Table 7.7. Since q is fixed, an increase in the wave number 495 means an increase in N, so the higher frequency problems lead to much larger linear 496 systems. In these experiments, we set the inner solve tolerance to  $10^{-2}$  or a maximum 497 of 10 iterations. Results reported under the legend "GMSLR - no shift" stand for the 498 regular GMSLR preconditioner. Results reported under the legend "GMSLR w/ 499 complex shift" stand for runs where the GMSLR preconditioner was built by first 500 shifting  $B_l$  by  $\sigma = \left(\sum_{j=1}^{d_l} (B_l)_{jj}/d_l\right) * .05 * i$ . Without a complex shift, these problems 501 can be much more difficult, especially as the matrix size grows. Indeed, for the last two 502 examples no convergence was achieved after 300 outer iterations. On the other hand, 503 the shift benefits all test problems as it allows for an increased number of levels (and 504 thus less fill-in introduced by ILU) while also keeping the number of outer iterations 505 relatively small (the number of outer iterations only increased from 17 to 28 as the 506 matrix size grew from  $20^3$  to  $80^3$ ). 507

7.4. General sparse matrices. To further illustrate the robustness of the GMSLR preconditioner, we tested it on several large matrices from the SuiteSparse Matrix
Collection [17]. These matrices come from a wide range of application areas, not just
PDEs. As a benchmark, we also tested ILUT for these nonsymmetric matrices. Information about the matrices is shown in Table 7.8. Table 7.9 shows the results of these
experiments. The ILUT parameters were chosen such that the fill of both methods
was comparable.

Results are shown in Table 7.9, where F indicates a failure to converge in 500 iterations. As can be seen, for these problems, GMSLR is superior to ILUT. It is worth adding that ILUT is a highly sequential preconditioner both in its construction and its application. In contrast, GMSLR is by design a domain decomposition-type preconditioner that offers potential for excellent parallelism.

Figure 7.2 plots the value of i-t and p-t as both L and the drop tolerance "tol" of the incomplete factorizations are varied for matrices "barrier2-1" and "offshore." In agreement with the results reported so far, an increase in the value of L reduces

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## 515

### TABLE 7.8

516 Set of test matrices from the SuiteSparse Matrix Collection where nnz is the number of nonzero

517 entries in the matrix.

Matrix	Order	nnz	SPD	Origin
cbuckle	13,681	676,515	yes	structural problem
epb2	25,228	175,027	no	thermal problem
wang4	26,068	177, 196	no	semiconductor device problem
barrier2 - 1	113,076	3,805,068	no	semiconductor device problem
Cage12	130,228	2,032,536	no	directed weighted graph
offshore	259,789	4,242,673	yes	electromagnetics problem
CoupCons	416,800	22,322,336	no	structural problem
AtmosModd	1,270,432	8,814,880	no	atmospheric model
AtmosModL	1,489,752	10,319,760	no	atmospheric model
Cage14	1,505,785	27,130,349	no	directed weighted graph
Transport	1,602,111	23,500,731	no	CFD problem

518

TABLE 7.9

519 Comparison between GMSLR and ILUT preconditioners for solving the above problems. ILUT

520 parameters were chosen so that the fill factor was close to that of GMSLR. Both sets of tests use 521 the same reordered matrix.

Matrix			GM	ISLR			ILUT				
Wattix	fill	L	rk	p-t	i-t	its	fill	p-t	i-t	its	
cbuckle	2.13	5	5	.22	.10	9	2.27	.38	.32	22	
epb2	3.63	5	15	.23	.13	4	3.43	.98	.76	19	
wang4	4.83	2	35	.14	.08	13	4.92	.45	.41	18	
barrier $2-1$	3.72	5	10	.60	1.91	6	3.69	44.19	14.32	F	
Cage12	0.95	5	25	.23	.28	4	1.00	.24	.31	5	
offshore	0.99	12	35	1.27	2.35	5	1.09	1.02	1.60	10	
CoupCons	1.82	10	16	1.68	.64	5	1.64	17.49	2.03	23	
AtmosModd	5.86	10	4	1.23	3.05	11	5.68	8.10	8.60	47	
AtmosModL	5.81	11	4	1.67	2.12	7	6.03	11.35	6.37	30	
Cage14	1.54	6	4	3.10	.89	4	1.57	5.09	0.70	4	
Transport	2.52	11	4	1.85	7.45	23	2.59	27.91	59.7	116	

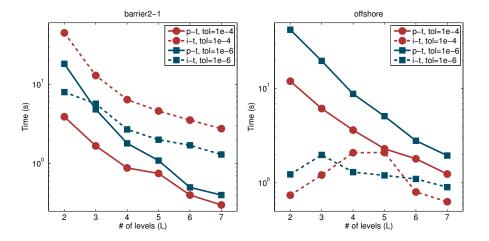


FIG. 7.2. Amount of time spent on building the GMSLR preconditioner and solving the linear
 system as the number of levels L and the drop tolerance tol in the incomplete factorizations vary.
 The rank rk was fixed to 10.

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the time to construct and apply the preconditioner. On the other hand, an increase in the value of L might also lead to a larger number of inner iterations necessary to achieve convergence and thus might lead to higher iteration times.

8. Conclusion. The GMSLR preconditioner combines several ideas. First is the 536 HID ordering method, which has a recursive multilevel structure. The (1,1) block of 537 each level of this structure is block diagonal, which means that solves with this block 538 are easily parallelizable. Motivated by the block LU factorization of the reordered 539 matrix, we use a block triangular preconditioner at the bottom level of the HID tree. 540 For the other levels, we use approximate inverse factorizations exploiting a recursive 541 relationship between the different levels. Finally, we approximate the inverse Schur 542 complement at each level of the HID tree via a low rank correction technique. 543

Because it is essentially an approximate inverse preconditioner, GMSLR is capable of solving a wide range of highly indefinite problems that would be difficult to solve by standard methods such as ILU. The numerical experiments we showed confirm this. Additional benefits of GMSLR include its inherent parallelism and its fast construction.

GMSLR is also promising for use in eigenvalue computations, especially in the context of rational filtering eigenvalue solvers where complex, indefinite linear systems need be solved [29, 47]. The factorization of these systems can be slow and costly for large 3D problems. We plan on investigating the use of Krylov subspace methods preconditioned by GMSLR to solve such systems. Among other objectives, we also plan to implement and publicly release a fully parallel, domain-decomposition based version of GMSLR.

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