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

GEOFFREY DILLON†, YUANZHE XI†, AND YOUSEF SAAD†

Abstract. Nonsymmetric and highly indefinite linear systems can be quite difficult to solve via iterative methods. This paper combines ideas from the Multilevel Schur Low-Rank preconditioner developed by Y. Xi, R. Li, and Y. Saad [*SIAM J. Matrix Anal.*, 37 (2016), pp. 235–259] with classic block preconditioning strategies in order to handle this case. The method to be described generates a tree structure $\mathcal{T}$ that represents a hierarchical decomposition of the original matrix. This decomposition gives rise to a block structured matrix at each level of $\mathcal{T}$. An approximate inverse based on the block LU factorization of the system is computed at each level via a low-rank property inherent in the difference between the inverses of the Schur complement and 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 with respect to indefiniteness for a few discretized Partial Differential Equations (PDEs) and publicly available test problems.

Key words. block preconditioner, Schur complements, multilevel, low-rank approximation, Krylov subspace methods, domain decomposition, Nested Dissection ordering.

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

1. Introduction.

In this paper we focus on the solution of large nonsymmetric sparse linear systems

$$Ax = b \tag{1.1}$$

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 2-sided preconditioners. Ideally, M is an approximation to A such that it is significantly easier to solve the linear systems with it than with the original A.

A commonly used preconditioner is the Incomplete LU (ILU) factorization of A, where $A \approx LU = M$. ILU preconditioners can be very effective for certain types of linear systems. However, if the original matrix A is poorly conditioned or highly indefinite then ILU methods can fail due to very small pivots or unstable factors [10, 36]. Here, note that by 'indefinite matrix' we refer to matrices that have eigenvalues on both sides of the imaginary axis. ILU methods are also known to have poor performance on high-performance computers, e.g., those with GPUs [29] or Intel Xeon Phi processors.

Algebraic multigrid (AMG) is another popular technique for solving problems arising from discretized PDEs. Multigrid methods are provably optimal for a wide range of SPD matrices and also perform well in parallel. However, without specialization, multigrid will fail on even mildly indefinite problems. Considerable efforts must be made to make multigrid work on these types of linear systems and even then the method must be tailored to the specific PDE being solved (e.g. multigrid for Maxwell's equations).

Sparse approximate inverses emerged in the 1990s as alternatives to ILU factorizations [7, 11, 19]. These methods were mostly abandoned due to their high cost both in terms of arithmetic and memory usage. A subsequent class of preconditioners were based on *rank-structured matrices* [8]. Two such types of matrices are $\mathcal{H}^2$-matrices [20, 21] and hierarchically semiseparable (HSS) matrices [42, 43, 44]. Both of these forms are the result of a partition of the original matrix where some of the off-diagonal blocks are approximated by low rank matrices. These ideas have been used to develop both sparse direct solvers and preconditioners [45].

Recently, a new class of approximate inverse preconditioners was developed. The first of these was the Multilevel Low-Rank (MLR) preconditioner descibed in [28]. Within the domain decomposition framework came the Schur complement low-rank (SLR) preconditioner [30], the Fast contour integral (FCI) preconditioner [41] followed by the Multilevel Schur complement Low-Rank (MSLR) preconditioner [39]. The MSLR preconditioner uses a multilevel Hierarchical interface decomposition (HID) ordering [22] along

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with an efficient Schur complement approximation. This approach is shown to be much less sensitive to indefiniteness than the classical ILU and domain decomposition based methods. However, MSLR is designed for symmetric problems.

In this paper, we present a preconditioner that incorporates a modified hierarchical low rank approximation of the inverse Schur complement from the MSLR preconditioner into a block preconditioner based on the block LU factorization of A. The resulting method will be called a Generalized Multilevel Schur complement Low-Rank (GMSLR) preconditioner. Two characteristics of the proposed methods are worth highlighting. First *GMSLR is designed to be applicable to a wide range of problems.* The preconditioner is nonsymmetric and it changes at each iteration, since it incorporates inner solves. As a result we use flexible GMRES [34] as the accelerator. The method also performs well with symmetric matrices. As observed in [5, Section 10.1.2], the loss of symmetry incurred by application of a nonsymmetric preconditioner is not a major concern provided that good approximations to certain blocks of A are available. The numerical experiments will confirm this observation. Second, a property that is inherited from MSLR is that the *GMSLR preconditioner computes a recursive, multilevel approximation to the inverse of the Schur complement.* GMSLR is a block preconditioner with inner sub-solves required at every outer iteration. These inner solves can themselves be preconditioned in order to reduce computational costs. One of these required inner solves is with the Schur complement, i.e., we must solve $Sy = g$. For most problems, this inverse Schur complement approximation turns out to be an effective preconditioner for these inner solves.

We have developed a code consisting of a set of C/C++ routines that implement the GMSLR preconditioner. This code was used in the numerical results section to solve SPD, symmetric indefinite, nonsymmetric, and complex non-Hermitian linear systems. The code reorders the matrix, builds the preconditioner, and then solves the linear system. Intel MKL routines are used along with thread-level parallelism via OpenMP. A truly parallel code using MPI is in progress.

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 two level analysis of the preconditioned eigenvalues is presented in Section 6. Then, in Section 7, we present some numerical results from test problems and problems from the SuiteSparse matrix collection [15]. Concluding remarks and some ideas for future work are found in Section 8.

2. HID ordering. Reordering the original system matrix A is essential for the performance of direct as well as iterative methods [6, 27, 33, 37]. GMSLR uses one such reordering technique known as the *Hierarchical Interface Decomposition (HID)* [22]. This ordering is applicable to a wide class of sparse matrices, not just those that originate from PDEs. An HID ordering can be obtained in a number of ways. A particular method for obtaining such an ordering is the well known nested dissection method [18]. Nested dissection recursively partitions the adjacency graph of A into bipartite subgraphs. The vertices whose removal leads to two disjoint subgraphs are called *vertex separators*. Each level of bisection produces a new separator and new subgraphs. This level information can be represented by an HID tree $\mathcal{T}$. The matrix itself is reordered according to level, starting with level 0 and ending with level L.

Since we assume that A is large, sparse, and nonsymmetric, then an HID ordering has the multilevel, recursive structure

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

In this notation, A_0 denotes the original matrix A after HID ordering whereas A_L is the submatrix associated with the L^{th} level connector. The B_l block itself has a block diagonal structure due to the block independent set ordering [37], making solves with B_l ideally suited for parallel computation. Figure 2.1 shows an example of the HID ordering for a 3D convection-diffusion operator discretized with the standard 7-point finite difference stencil.

3. Block Preconditioning. Domain decomposition reordering gives rise to linear systems of the form

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix}, \tag{3.1}$$

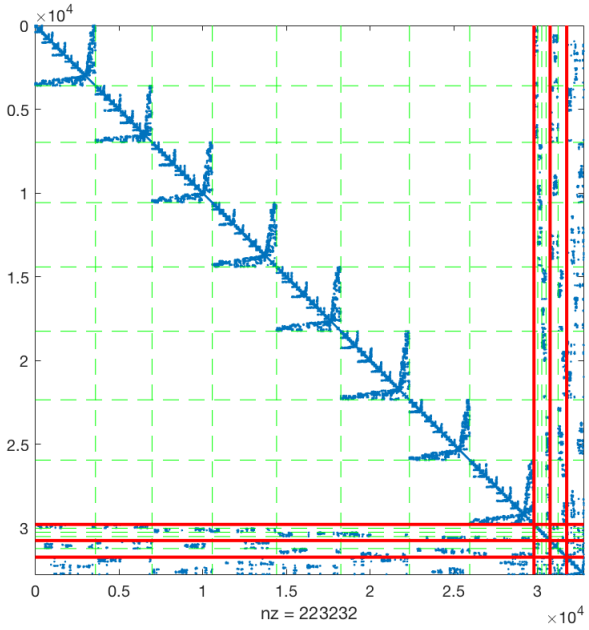


Fig. 2.1: *A 4-level HID ordered 3D convection-diffusion matrix with zero Dirichlet boundary conditions. The original matrix is discretized on a* $32 \times 32 \times 32$ *regular grid with the standard 7-point stencil. The red lines separate the different levels.*

see [2, 9]. 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 [4, 5, 25, 31, 32]. For examples of preconditioning other coupled systems of PDEs, see [12, 23, 24].

At the initial level GMSLR uses a block triangular preconditioner of the form

$$\mathcal{P} = \begin{pmatrix} \widetilde{B}_0 & F_0 \\ 0 & \widetilde{S}_0 \end{pmatrix} \tag{3.2}$$

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

In the ideal case where $\widetilde{B}_0 = B_0$ and $\widetilde{S}_0 = S_0$, 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 [25, 32]. Therefore the total cost of the procedure based on the ideal form of (3.2) is 2 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 $\mathcal{P}_{\text{ideal}}^{-1}$:

$$\mathcal{P}_{\text{ideal}}^{-1} = \begin{pmatrix} B_0 & F_0 \\ & S_0 \end{pmatrix}^{-1} = \begin{pmatrix} B_0^{-1} & \\ & I \end{pmatrix} \begin{pmatrix} I & -F_0 \\ & I \end{pmatrix} \begin{pmatrix} I & \\ & S_0^{-1} \end{pmatrix}. \tag{3.3}$$

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

$$\mathcal{P}^{-1} = \begin{pmatrix} B_0^{-1} & \\ & I \end{pmatrix} \begin{pmatrix} I & -F_0 \\ & I \end{pmatrix} \begin{pmatrix} I & \\ & S_0^{-1} \end{pmatrix} \begin{pmatrix} I & \\ -E_0 B_0^{-1} & I \end{pmatrix}, \tag{3.4}$$

then in the ideal case we have an exact inverse of A_0 and a Krlyov 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, $\widetilde{B}_0$ and $\widetilde{S}_0$ 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 [30], we solve linear systems with the B blocks by using incomplete LU (ILU) factorizations. Approximations to the Schur complement are typically tailored specifically to the problem being studied (e.g. the pressure convection diffusion [17] and least-squares commutator [16] 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 [30, 39].

4. Schur complement approximation. GMSLR is an extension of the MSLR preconditioner of [39] based on approximating the block $\mathcal{LDU}$ factorization of (2.1):

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

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

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

Let the *complex* Schur decomposition of G_l be

$$G_l = E_l B_l^{-1} F_l C_l^{-1} = W_l R_l W_l^H \tag{4.3}$$

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

$$S_l = \left(I - W_l R_l W_l^H\right) C_l = W_l \left(I - R_l\right) W_l^H C_l. \tag{4.4}$$

Then, the Sherman-Morrison-Woodbury formula yields the inverse of S_l:

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

which reduces to

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

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. The resulting inverse Schur complement approximation is given in the following proposition.

PROPOSITION 4.1. *Let $G_l = E_l B_l^{-1} F_l C_l^{-1}, l = 0 \ldots L-1$ and $G_l = W_l R_l W_l^H$ be its Schur decomposition at level l. Let W_{l,k_l} be the matrix of the first k_l Schur vectors ($k_l < s$) of W_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 l^{th} level inverse Schur complement $\widetilde{S}_{l,k_l}^{-1}$ is given by*

$$\widetilde{S}_{l,k_l}^{-1} = C_l^{-1}(I + W_{l,k_l} H_{l,k_l} W_{l,k_l}^H). \tag{4.7}$$

where

$$H_{l,k_l} = [(I - R_{l,k_l})^{-1} - I]. \tag{4.8}$$

This inverse Schur complement approximation (4.7) will be used at every level $l = 0, \ldots, L-1$.

Finally, due to the potential size of the C_l blocks, we can only afford to factor C_{L-1} (i.e., at the top level) 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 [39] for approximating the action of C_l^{-1} on a vector. The details of this approximation will be shown in Section 5.

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.,

$$B_l = L_{B_l} U_{B_l},\ C_l = L_{C_l} U_{C_l}. \tag{4.9}$$

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 large, 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 of low-rank, again define the matrix G_l by

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

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 equation (4.6) the eigenvalues $\theta_1, \theta_2, \cdots, \theta_{s-1}, \theta_s$ of X_l are given explicitly by

$$\theta_i = \frac{\gamma_i}{1 - \gamma_i},\ i = 1, \ldots s \tag{4.11}$$

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

As long as the eigenvalues γ_i of G_l are not clustered at 1, the eigenvalues θ_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 [39, 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:

$$\begin{aligned} G_l U_m &= U_m H_m + h_{m+1,m} u_{m+1} e_m^T \\ U_m^T G_l U_m &= H_m \end{aligned}$$

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

$$Q^H H_m Q = T. \tag{4.12}$$

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, 38]. We approximate the low-rank matrices in (4.7) by

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

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 are non-singular.

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, b_0 respectively.

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

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

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.

Step 2: At level 1, we have

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

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

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

Next we move up a level again to define an approximate inverse for C_1, referring again to (2.1).

Step 3: At level 2 we have:

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

Our earlier analysis suggests that we approximate S_2^{-1} by C_2^{-1} plus a low-rank correction term, i.e.,

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

At this level, we decide that C_2 is sufficiently small and compute its 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 forward-backward 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 eigenvalues and eigenvectors of the matrix G_l, we need to be able to compute matrix vector products with the matrix $E_lB_l^{-1}F_lC_l^{-1}$ at each level l. We already have the factors of B_l, so any matrix-vector product with B_l^{-1} can be computed with one forward and one backward substitution. The same does not hold true for C_l, since we only compute its factorization at level $L-1$. However, we already have an approximate factorization of A_{l+1}^{-1} and since $C_l^{-1} = A_{l+1}^{-1}$ 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 defined product of C_l^{-1} with a vector b are given in Algorithm

2.

Algorithm 1 Generalized Multilevel Schur Low-Rank (Construction phase)

procedure GMSLR
  Apply an L-level reordering to A (A_0 = reordered matrix).
  for level l from $L-1$ to 0 **do**
    if $l = L-1$ **then**
      Compute ILU factorization of C_{L-1}, $C_{L-1} \approx L_{C_{L-1}} U_{C_{L-1}}$
    end if
    Compute ILU factorization of B_l, $B_l \approx L_{B_l} U_{B_l}$.
    Perform k_l steps of the Arnoldi process ▷ *Call Algorithm 2 to apply* C_l^{-1}

$$[V_l, K_l] = \text{Arnoldi}(E_l U_{B_l}^{-1} L_{B_l}^{-1} F_l C_l^{-1}, k_l)$$

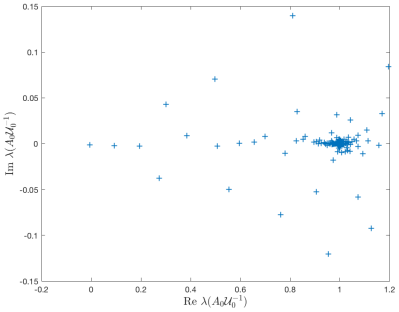
    Compute the complex Schur decomposition $K_l = WTW^T$.
    Compute $W_{l,k_l} = V_l W$ and set $R_{l,k_l} = T_{1:k_l,1:k_l}$.
    Compute $H_l = (I - R_{l,k_l})^{-1} - I = R_{l,k_l}(I - R_{k_l})^{-1}$.
  end for
end procedure

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

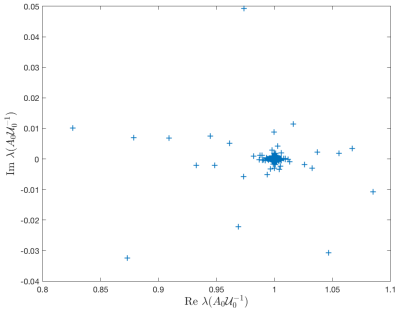
1: **procedure** `RecursiveSolve`(l, b)
2: **if** $l = L-1$ **then**
3: return $y = U_{C_{L-1}}^{-1} L_{C_{L-1}}^{-1} b$
4: **else**
5: Split $b = (b_1^T, b_2^T)^T$ conformingly with the blocking of C_l
6: Compute $z_1 = U_{B_{l+1}}^{-1} L_{B_{l+1}}^{-1} b_1$
7: Compute $z_2 = b_2 - E_{l+1} z_1$
8: **if** $1 \leq l < L-1$ **then**
9: Compute $w_2 = W_{l+1,k_{l+1}} H_{l+1} W_{l+1,k_{l+1}}^T z_2$
10: Compute $y_2 =$ `RecursiveSolve`$(l+1, z_2 + w_2)$
11: Compute $y_1 = z_1 - U_{B_{l+1}}^{-1} L_{B_{l+1}}^{-1} F_{l+1} y_2$
12: **else**
13: Solve the system $S_0 y_2 = z_2$ with $\widetilde{S}_0^{-1}$ as a right preconditioner
14: Compute $y_1 = U_{B_0}^{-1} L_{B_0}^{-1} (b_1 - F_0 y_2)$
15: **end if**
16: return $y = (y_1^T, y_2^T)^T$
17: **end if**
18: **end procedure**

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

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 $\widetilde{B}_0$ denote an approximation to B_0 and $\widetilde{S}_0$ 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



(a) Eigenvalues of shifted Laplacian preconditioned by GMSLR with a rank 2 correction.



(b) Eigenvalues of shifted Laplacian preconditioned by GMSLR with a rank 20 correction.

Fig. 6.1: *Spectra of (6.3). These figures were obtained by using a 2 level reordering (to complement the above analysis) and the exact LU decomposition of the B_l blocks.*

the original matrix A, i.e.,

$$A_0 = \begin{pmatrix} B_0 & F_0 \\ E_0 & C_0 \end{pmatrix} \tag{6.1}$$

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

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

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

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

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

A simple calculation shows that

$$A_0 \widetilde{\mathcal{U}}_0^{-1} = \begin{pmatrix} B_0 \widetilde{B}_0^{-1} & (I - B_0 \widetilde{B}_0^{-1}) F_0 \widetilde{S}_0^{-1} \\ E_0 \widetilde{B}_0^{-1} & S_0 \widetilde{S}_0^{-1} \end{pmatrix}. \tag{6.2}$$

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

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

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 the spectra of (6.3) for a small test problem in Figure 6.1. Here A is the discretized shifted Laplacian operator $-\Delta u - cu = f$ with $c = 0.5$ and homogeneous Dirichlet boundary conditions. For reference, this 8000×8000 matrix has 35 negative eigenvalues. Since this matrix is small, we use the LU factorization of B_0 in order for the preconditioned system to resemble (6.3) as much as possible. Figure 6.1(a) shows that with only a rank 2 correction, the spectrum of $A_0 \widetilde{\mathcal{U}}_0^{-1}$ is not particularly well clustered. Figure 6.1(b) shows that with a rank 20 correction, the spectrum of $A_0 \widetilde{\mathcal{U}}_0^{-1}$ is tightly clustered around 1. For this particular problem, GMSLR with a rank 20 low rank correction converges in 6 outer iterations while the rank 2 corrected version converges in 23.

7. Numerical experiments. Our goal is the efficient solution of large 2D and 3D problems. The experiments were all run on a single node of the `Mesabi` Linux cluster at the Minnesota Supercomputing Institute. This node has 64 GB memory and consists of two sockets each having a twelve core 2.5 GHz Intel Haswell processor. This preconditioner was written in C++ and compiled by Intel's C++ compiler using `-O3` optimization. Simple thread-level parallelism was achieved with OpenMP with a maximum of 24 threads. The B_l blocks are factored by the ILUT routine from ITSOL. The Intel Math Kernel Library (MKL) was used for many BLAS and LAPACK routines. We use flexible GMRES [34] with a fixed restart size of 40 as the outer solver, denoted by GMRES(40). The inner solve in step 14 of Algorithm 2 is also done with FGMRES. Unless otherwise noted, we follow the methodology of [28, 35, 39] where the right hand side vector b is given by $Ae = b$ where e is the vector of all ones.

The HID ordering was obtained by the function `PartGraphRecursive` from the METIS [26] package. The diagonal blocks of each B_l, C_l were reordered using the approximate minimum degree (AMD) ordering [13, 14] in order to reduce fill-in generated by their ILU factorizations. In our experiments the reported preconditioner construction time comes from the factorization of the B_l blocks and the computation of the low-rank correction matrices. The reordering time is regarded as preprocessing and is therefore not reported. Similarly, the iteration time is the combined time spent on the inner and outer solves.

The parameters we are most interested in varying are: the number 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.

We use the following notation in the results that follow:

- fill = $\frac{nnz(prec)}{nnz(A)}$;
- p-t: wall clock time to build the preconditioner (in seconds);
- its: number of *outer* iterations of preconditioned GMRES(40) required for $\|r_k\|_2 < 10^{-6}$. We use "`F`" to indicate that GMRES(40) did not converge after 500 iterations;
- i-t: wall clock time for the iteration phase of the solver. This time is not reported when GMRES(40) does not converge, as indicated by "–";
- rk: max rank used in building the low-rank corrections.

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

$$\begin{aligned} -\Delta u - cu &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{7.1}$$

where $\Omega = (0,1)^3$. The discretization is via finite differences with the standard 7-point stencil in 3D. 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 32×32 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 $s = h^2 c$ for mesh size h. For this first example, we set $s = 0.5$. The associated coefficient matrix has 163 negative eigenvalues. The maximum rank was fixed at 50. As Figure 7.1 shows, the ILU fill-factor curve is monotonically decreasing while the low-rank correction fill-factor increases monotonically. The optimal number of levels occurs when these two quantities are roughly equal. For this particular example, we pick $nlev_{opt} = 6$ as it strikes the right balance of fill, iteration count, and total computational time as shown in Table 7.1.

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 keep the number of levels fixed, but increase the maximum rank. We again solve (7.1) with $s = 0.5$ discretized on a 32^3 regular grid. The ILU fill factor is constant because we are keeping the number of levels fixed at 6. The fill factor from the low rank corrections increases at an almost constant rate. Increasing the maximum rank has the unfortunate effect of increasing the fill-factor and the preconditioner construction time. As we see in Table

lev	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

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.*

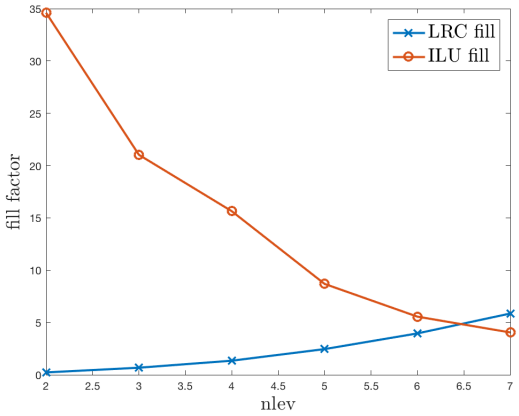


Fig. 7.1: *Illustration of the fill factors from ILU and low-rank corrections versus different levels in Table 7.1.*

7.3, the effect of increasing the rank (at least for this model problem) is difficult to predict. As a general rule, it seems as though a large maximum rank is unavoidable for highly indefinite problems.

7.1.3. Increasingly indefinite problems. The model problem (7.1) becomes significantly more difficult to solve as s increases. Here, we increase s from 0 to 1 while tuning the maximum rank and number of levels to compensate for solving this increasingly difficult problem. We report the results that give the best balance between iteration count and fill in Table 7.4. The fill factor increases dramatically for two reasons: first, we must increase the rank of the low rank correction and second, we must keep the number of levels low, which means the ILU factors will be denser. If the rank is too low or the number of levels is too high, GMRES(40) simply will not converge.

We are forced to dramatically increase the rank for these highly indefinite problems due to how we construct the low rank correction. Recall that the construction of the low rank correction is based on finding approximate eigenvalues of the matrix $E_l U_{B_l}^{-1} L_{B_l}^{-1} F_l C_l^{-1}$ using Arnoldi's method. When B_0 is indefinite, as is the case here, the eigenvalues we seek get pushed deeper inside the spectrum, i.e. they become interior eigenvalues. Since the Arnoldi process recovers extreme eigenvalues quickly, we are forced to take more steps of Arnoldi in order to approximate these eigenvalues.

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

$$\begin{aligned} -\Delta u - \alpha \cdot \nabla u - cu &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{7.2}$$

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 $s = h^2 c$.

	GMSLR - $\mathcal{U}_0^{-1}$ only			GMSLR - $\mathcal{U}_0^{-1}\mathcal{L}_0^{-1}$		
nlev	p-t	i-t	its	p-t	i-t	its
2	5.16	1.25	16	5.15	3.59	47
3	.986	2.69	16	1.01	5.24	37
4	.382	1.03	12	.391	2.88	34
5	.169	.97	19	.181	1.49	27
6	.172	.95	17	.176	1.43	24

Table 7.2: *Comparison between GMSLR with only using* $\mathcal{U}_0^{-1}$ *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.*

rank	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

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.*

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 3D 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.

Next, we solve (7.2) with $s = .25$. The shift significantly increases the number of eigenvalues with negative real parts, so we increase the maximum rank to 50. The results can be found in Table 7.6. It is interesting to note that the fill from the low rank correction is almost exactly the same as in Table 7.1. This is due to the fact 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

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

In this formulation, Δ is the Laplacian operator, ω the angular frequency, $v(x)$ the velocity field, and $s(x,\omega)$ is the external forcing function with corresponding time-harmonic wave field solution $u(x,\omega)$. The computational domain is the unit cube $\Omega = (0,1)^3$ where we again use the seven-point finite difference discretization on a regular mesh. The Perfectly Matched Layer (PML) boundary condition is used on all faces of Ω. The resulting linear systems are complex non-Hermitian. If we assume that the mean of $v(x)$ is 1 in (7.3), then the wave number is $\omega/(2\pi)$ and $\lambda = 2\pi/\omega$ the wavelength. The number of grid points in each dimension is $N = q\omega/(2\pi)$ where q is the number of points per wavelength. As a result, the discretized system is $n = N^3 \times N^3$.

We test the performance of the GMSLR preconditioner on 6 cubes with $q = 8$ and report the results in Table 7.7. Since q is fixed, an increase in wave number means an increase in N, so the higher frequency problems lead to much larger linear systems. These problems are much more sensitive to the number of levels used. Overall, we use a smaller number of levels (as compared to the real-valued test problems), which leads to larger fill factors. In these experiments, we set the inner solve tolerance to 10^{-1}. The number of outer iterations required only increases from 6 to 13 while the matrices grow from 20^3 to 80^3. The fill factors do increase as the problem gets larger, but not by too much. The last problem has a larger

s	nlev	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

Table 7.4: *Results of solving symmetric linear systems with increasing shift values s on a 32^3 regular mesh with GMSLR.*

lev	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

Table 7.5: *The fill factor and iteration counts for solving (7.2) with no shift 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 20.*

fill factor due to the fact that the maximum rank used is significantly higher than the other examples while the number of levels remains the same.

7.4. Other problems. To further illustrate the robustness of the GMSLR preconditioner, we tested it on several large, nonsymmetric matrices from the SuiteSparse Matrix Collection [15]. 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.

8. Conclusion. The GMSLR preconditioner combines several ideas. First is the HID ordering method, which has a recursive multilevel structure. The $(1, 1)$ block of each level of this structure is block diagonal, which means that solves with this block are easily parallelizable. Motivated by the block LU factorization of the reordered matrix, we use a block triangular preconditioner at the bottom level of the HID tree. For the other levels, we use approximate inverse factorizations thanks to the relationships between the different levels. Finally, we approximate the inverse Schur complement of each level of the HID tree via a low-rank property.

Because it is essentially an approximate inverse preconditioner, GMSLR is capable of solving a wide range of highly indefinite problems that would be difficult for 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. In several eigenvalue methods, such as shift and invert and rational filtering [40], one has to solve highly indefinite systems. 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 our other objectives, we are also planning to implement and publicly release a fully parallel, domain-decomposition based, version of GMSLR.

lev	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 7.6: *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.*

$\omega/(2\pi)$	q	$n = N^3$	nlev	rk	fill	p-t	i-t	its
2.5	8	20^3	4	16	5.43	.05	.035	6
3	8	30^3	5	16	6.65	.128	.147	8
5	8	40^3	6	16	7.56	.318	.775	8
6	8	50^3	6	16	10.45	1.01	1.72	9
8	8	60^3	6	20	15.09	3.35	3.33	9
10	8	80^3	6	40	22.44	19.34	14.54	13

Table 7.7: *Results from solving (7.3) on a sequence of 3D meshes with GMSLR. Here q denotes the number of points per wavelength.*

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Matrix	Order	nnz	SPD	Origin
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

Table 7.8: *Set of nonsymmetric test matrices from the SuiteSparse Matrix Collection.*

Matrix	GMSLR						ILUT			
	fill	nlev	rank	p-t	i-t	its	fill	p-t	i-t	its
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	8.1	8.6	47
AtmosModL	5.81	11	4	1.67	2.12	7	6.03	11.35	6.37	30
Cage14	1.54	6	4	3.1	.89	4	1.57	5.09	0.7	4
Transport	2.52	11	4	1.85	7.45	23	2.96	–	–	F

Table 7.9: *Comparison between GMSLR and ILUT preconditioners for solving the above problems. ILUT parameters were chosen so that the fill factor was close to that of GMSLR. Both sets of tests use the same reordered matrix.*

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