HIFIR: Hybrid Incomplete Factorization with Iterative Refinement for Preconditioning Ill-conditioned and Singular Systems

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We introduce a software package called HIFIR for preconditioning sparse, unsymmetric, ill-conditioned, and potentially singular systems. HIFIR computes a hybrid incomplete factorization, which combines multilevel incomplete LU factorization with a truncated, rank-revealing QR factorization on the final Schur complement. This novel hybridization is based on the new theory of \(\epsilon\)-accurate approximate generalized inverse. It enables near-optimal preconditioners for consistent systems and enables flexible GMRES to solve inconsistent systems when coupled with iterative refinement. In this paper, we focus on some practical algorithmic and software issues of HIFIR. In particular, we introduce a new inverse-based rook pivoting into ILU, which improves the robustness and the overall efficiency for some ill-conditioned systems by significantly reducing the size of the final Schur complement for some systems. We also describe the software design of HIFIR in terms of its efficient data structures for supporting rook pivoting in a multilevel setting, its template-based generic programming interfaces for mixed-precision real and complex values in C++, and its user-friendly high-level interfaces in MATLAB and Python. We demonstrate the effectiveness of HIFIR for ill-conditioned or singular systems arising from several applications, including the Helmholtz equation, linear elasticity, stationary incompressible Navier–Stokes equations, and time-dependent advection-diffusion equation.

CCS Concepts:
- Mathematics of computing → Computations on matrices; Solvers
- Software and its engineering → Software libraries and repositories.

Additional Key Words and Phrases: preconditioning, hybrid incomplete factorization, multilevel ILU factorization, rank-revealing factorization, singular systems, approximate generalized inverse, iterative refinement

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1 INTRODUCTION

We consider the problem of preconditioning an iterative solver for a linear system,

\[ Ax = b, \]

where \( A \in \mathbb{C}^{n\times n} \) is sparse and potentially singular, \( x \in \mathbb{C}^n \), and \( b \in \mathbb{C}^n \), or as in many applications, \( A \in \mathbb{R}^{n\times n} \), \( x \in \mathbb{R}^n \), and \( b \in \mathbb{R}^n \). For generality, we will assume complex-valued systems in our discussions. In general, (1) is inconsistent in that \( \|b - AA^+b\| \gg \epsilon_{\text{mach}} \|b\| \), where \( A^+ \) denotes the Moore–Penrose pseudoinverse of \( A \) and \( \epsilon_{\text{mach}} \) denotes the...
machine epsilon of a given floating-point number system. In this case, we must seek a least-squares solution of (1), i.e.,
\[
x_{\text{LS}} = \arg \min_x \|b - Ax\|_2.
\]
or often preferably the pseudoinverse solution of (1), i.e.,
\[
x_{\text{PI}} = \arg \min_x \|x\|_2 \quad \text{subject to} \quad \min \|b - Ax\|_2,
\]
or equivalently, \(x_{\text{PI}} = A^+b\). When \(A\) is large-scale, it is preferable to solve (1) using a Krylov subspace (KSP) method, such as GMRES [71], which seeks a solution in the \(k\)th KSP
\[
\mathcal{K}_k(A, v) = \text{span} \{v, Av, \ldots, A^{k-1}v\}
\]
at the \(k\)th iteration, where \(v\) is typically equal to \(b\). It is well known that KSP methods can benefit from robust and effective preconditioners for ill-conditioned problems. This work introduces a software package called HIFIR, which delivers robust and computationally efficient preconditioners for singular systems. As a side product, HIFIR also improves the robustness in preconditioning ill-conditioned systems.

Compared to nonsingular systems, preconditioning (nearly) singular systems is a very challenging problem. Several software packages offer fairly robust and easy-to-use preconditioners for nonsingular systems, such as the multilevel ILU (MLILU) in ILUPACK [15], the supernodal ILU in SuperLU [57], and various parallel preconditioners in PETSc [5]. Conceptually, such software packages construct a preconditioner \(M \in \mathbb{C}^{n \times n}\) that approximates \(A\) in that \(M^{-1} \approx A^{-1}\).

Given \(M\), a right-preconditioned KSP method seeks a solution to
\[
AM^{-1}y = b
\]
in \(\mathcal{K}_k(AM^{-1}, v)\), where typically \(v = b\), and then \(x = M^{-1}y\). Ideally, the preconditioned KSP methods would converge significantly faster than the unpreconditioned ones. However, when \(A\) is (nearly) singular and the system (1) is inconsistent, there is a lack of robust algorithms and software. Some earlier techniques used a CGLS-type KSP method (e.g., [14, 30, 64]), which is mathematically equivalent to solving the normal equation using CG [14, 43] or MINRES [30, 63]. Those KSP methods tend to converge slowly due to the squaring of the condition number by the normal equation in the corresponding KSP [48]. More recently, there has been significant interest in preconditioning GMRES-type methods for singular systems or least-squares problems [40, 48, 61]. For example, the so-called AB-GMRES [40] solves the system \(ABy = b\) using GMRES with \(\mathcal{K}_k(AB, b)\), and then \(x = By\). Here, \(B\) plays a similar role as \(M^{-1}\), except that \(B\) may be singular (or rank deficient if \(A\) is rectangular). Hayami et al. [40] constructed \(B\) based on robust incomplete factorization (RIF) of Benzi and Tůma [11, 12], which was originally developed for CGLS-type methods. Although RIF could accelerate the convergence of AB-GMRES in [40], it was not robust in general [61]. In more recent works [35, 61], \(B\) in AB-GMRES is typically chosen to be \(A^H\) (or \(A^T\) for real matrices), which unfortunately squares the condition number (analogous to CGLS) and in turn can slow down the convergence. This work aims to deliver a right preconditioner that is more efficient and robust than RIF, and more importantly, enables near-optimal convergence rates. We achieve this goal by leveraging the new theory of \(\epsilon\)-accurate approximated generalized inverse (AGI) [48], as outlined in Section 2.

Our development of HIFIR was based on our earlier software package called HILUCSI [20], which was a prototype implementation of an MLILU for nonsingular saddle-point problems. Compared to single-level ILUs (such as ILU(k)) and

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\[1\] We consider only right preconditioning because left preconditioning alters the computation of residual vector \(r = b - Ax\) and in turn may lead to false stagnation or early terminations for ill-conditioned systems [33].

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ILUTP, etc. [70, Chapter 10]), MLILU is generally more robust for nonsingular indefinite systems [20, 33]. HILUCSI leveraged several techniques in a novel way to achieve superior efficiency and robustness for saddle-point problems than other MLILU libraries (such as ARMS [72], ILUPACK [15], and ILU++ [60]). In particular, HILUCSI achieved high efficiency by introducing a scalability-oriented dropping in a dual-thresholding strategy in the fan-in ILU² for linear-time complexity in its factorization and solve. It improved robustness by leveraging mixed symmetric and unsymmetric preprocessing techniques at different levels and combining static and dynamic permutations. HIFIR inherits some of these core algorithmic components of HILUCSI, as described in Section 3. However, as an MLIU technique, HILUCSI was not robust for singular systems, for example, when its final level is singular. HIFIR is designed to overcome this deficiency by leveraging a rank-revealing factorization in its final level, introducing iterative refinement to build a variable preconditioner, and introducing a new pivoting strategy in its ILU portion, as we will detail in Section 3.

The main contributions of this work are as follows. First and foremost, we introduce one of the first software libraries to improve the robustness for ill-conditioned and (nearly) singular systems to achieve near machine precision. Our software library, called HIFIR, or Hybrid Incomplete Factorization with Iterative Refinement, computes an AGI [48] by hybridizing incomplete LU and rank-revealing QR (RRQR) in a multilevel fashion. When used as a right-preconditioner for GMRES, this hybridization enables (near) optimal convergence for consistent or ill-conditioned systems. When fortified with iterative refinement in FGMRES [69], HIFIR enables the robust computation of the left null space and the pseudoinverse solution of inconsistent systems. We have implemented HIFIR using template-based objective-oriented programming in C++. For user-friendliness, the C++ HIFIR library is header-only, with easy-to-use high-level interfaces in MATLAB and Python. The software is open-source and has been made available at https://github.com/hifirworks/hifir.

Second, this work also introduces a novel inverse-based rook pivoting (IBRP) in the fan-in ILU. We describe efficient data structures for the efficient implementation of IBRP and show that this new pivoting strategy improves the robustness and efficiency for some challenging singular systems. Third, HIFIR offers some advanced features, such as the support of complex arithmetic, the ability to precondition both \( A \) and \( A^H \) using the same factorization, and the ability to multiply by an AGI of the preconditioning operator. These features enable the use of HIFIR as building blocks for advanced preconditioners, such as (parallel) block preconditioners. In addition, HIFIR supports mixed precision (e.g., double precision combined with single or potentially half precision) for the input matrix and the preconditioner, which is beneficial for heterogeneous hardware platforms and limited-memory settings.

The remainder of this paper is organized as follows. In Section 2, we give an overview of the theoretical foundation of HIFIR, including optimality conditions, treatment for singular systems, etc. In Section 3, we describe the algorithmic components of HIF and highlight some implementation details. Section 4 describes how to apply HIF as a preconditioner, including iterative refinement. In Section 5, we introduce the application programming interfaces of HIFIR in C++, MATLAB, and Python with example implementations. Section 6 demonstrates HIFIR for some large-scale applications with indefinite ill-conditioned and singular inconsistent systems. Finally, Section 7 concludes the paper with a discussion on future directions. For completeness, we present the details of our data structures in Appendix A and the complexity analysis of IBRP in Appendix B.
2 THEORETICAL FOUNDATIONS

In this section, we give an overview of the theoretical foundations of HIFIR. Most of the theory was based on that in [48], except that we generalize the results from real matrices to complex ones. We present some of the most relevant theoretical results for completeness, but we omit the proofs because they follow the same arguments as those in [48].

2.1 Mathematically optimal right-preconditioning operators for consistent systems

Let us first consider the issue of optimal preconditioning for a consistent system (1), where \( b \) is in the range of \( A \) (i.e., \( b \in \mathcal{R}(A) \)). In floating-point arithmetic, the convergence rate of a KSP method for such systems depends on the following generalized notion of condition numbers.

**Definition 1.** Given a potentially singular matrix \( A \in \mathbb{C}^{m \times n} \), the 2-norm condition number of \( A \) is the ratio between the largest and the smallest nonzero singular values of \( A \), i.e., \( \kappa(A) = \sigma_1(A)/\sigma_r(A) \), where \( r = \text{rank}(A) \).

To accelerate a KSP method for such a system, we solve a right-preconditioned system

\[
AGy = b,
\]

using a KSP method, and then \( x = Gy \). We refer to \( G \) as a right preconditioning operator (RPO). Ideally, we would like \( \kappa(AG) \ll \kappa(A) \). For nonsingular systems, \( G \) is equivalent to \( M^{-1} \) in (5); for singular systems, \( G \) generalizes \( M^{-1} \). The symbol \( G \) signifies that it is based on a generalized inverse.

**Definition 2.** [67, Definitions 2.2] Given a potentially rank-deficient \( A \in \mathbb{C}^{m \times n} \), \( A^\# \) is a generalized inverse of \( A \) if and only if \( AA^\# A = A \).

It is worth noting that the Moore–Penrose pseudoinverse \( A^+ \) is a special case of generalized inverses. Although it might be tempting to construct the RPO \( G \) to approximate \( A^+ \), the pseudoinverse is overly restrictive. The following two properties of generalized inverses make them particularly relevant to right-preconditioning singular systems.

**Proposition 1.** [48, Proposition 3.4] If \( A^\# \) is a generalized inverse of \( A \in \mathbb{C}^{m \times n} \), then \( AA^\# \) is diagonalizable, and its eigenvalues are all zeros and ones. In other words, there exists a nonsingular matrix \( X \in \mathbb{C}^{m \times m} \), such that \( AG = X \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} X^{-1} \), where \( I_r \) is the \( r \times r \) identity matrix with \( r = \text{rank}(A) \). Conversely, if there exists a nonsingular \( X \) such that \( AG = X \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} X^{-1} \) for \( r = \text{rank}(A) \), then \( G \) is a generalized inverse of \( A \).

**Proposition 2.** [48, Proposition A.1] Given \( A \in \mathbb{C}^{n \times n} \) of rank \( r = \text{rank}(A) \) and a generalized inverse \( A^\# \) with \( AA^\# = X \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} X^{-1} \), the condition number of \( AA^\# \) is bounded by \( \kappa(X) \), i.e., \( \kappa( AA^\# ) \leq \kappa(X) \).

From Proposition 1, it is easy to show that any generalized inverse \( A^\# \) (or a nonzero scalar multiple of \( A^\# \)) enables a mathematically optimal RPO for consistent systems in the following sense.

**Theorem 1.** [48, Theorem 3.6] Given \( A \in \mathbb{C}^{n \times n} \) and a generalized inverse \( A^\# \), then GMRES with RPO \( \alpha A^\# \) with \( \alpha \neq 0 \) converges to a least-squares solution \( x_{LS} \) of (1) after one iteration for all \( b \in \mathcal{R}(A) \) and \( x_0 \in \mathbb{C}^n \). Conversely, if GMRES with RPO \( G \) converges to a least-squares solution \( x_{LS} \) in one iteration for all \( b \in \mathcal{R}(A) \) and \( x_0 \in \mathbb{C}^n \), then \( G \) is a scalar multiple of a generalized inverse of \( A \).
A corollary of Theorem 1 is that if \( \mathcal{R}(A^\dagger) = \mathcal{R}(A^H) \), then the computed \( x_{LS} \) is the pseudoinverse solution of (1). Let \( \Pi_{\mathcal{R}(A^H)} \) denote a projection onto \( A^H \). Given any \( A^\dagger \), it is easy to show that \( \Pi_{\mathcal{R}(A^H)}A^\dagger \) is also a generalized inverse, and the computed \( x_{LS} \) with \( \Pi_{\mathcal{R}(A^H)}A^\dagger \) as the RPO is then the pseudoinverse solution. Theorem 1 assumes exact arithmetic. With rounding errors, the condition number of \( AA^\dagger \) must be bounded by a small constant, which holds in general if \( \kappa(X) \) is bounded due to Proposition 2.

Although the above theory may seem abstract, it suggests a new approach for constructing RPO based on generalized inverses. In particular, one option to construct \( A^\dagger \) is to hybridize multilevel ILU with a rank-revealing decomposition on its final Schur complement. As an illustration, consider the following example that combines LU factorization without pivoting with QR factorization with column pivoting (QRCP) [34].

**Example 1.** Given \( A \in \mathbb{C}^{n \times n} \), after \( n_1 \) steps of Gaussian elimination,

\[
A = \begin{bmatrix} L_1 & I_{n_1} \\ I_{n_2} & S \\ L_2 & I_{n_2} \end{bmatrix},
\]

where \( S \in \mathbb{C}^{n_2 \times n_2} \) is the Schur complement. Clearly, \( \text{rank}(A) = n_1 + \text{rank}(S) \). Let the QRCP of \( S \) be

\[
SP = Q \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix},
\]

where \( Q \in \mathbb{C}^{n \times n_2} \) is unitary and \( R_1 \in \mathbb{C}^{n_1 \times s} \) for \( s = \text{rank}(S) \) (i.e., the (numerical) rank of \( S \)). Let \( \hat{P} \) and \( \hat{Q} \) be composed of the first \( s \) columns of \( P \) and \( Q \), respectively. Then, \( S^\dagger = \hat{P}R_1^{-1}\hat{Q}^H \) is a generalized inverse of \( S \) with \( SS^H = \hat{Q}Q^H = QI_sQ^H \). Furthermore,

\[
G = \begin{bmatrix} U_1 & U_2 \\ I_{n_1} & I_{n_2} \end{bmatrix}^{-1} \begin{bmatrix} L_1 & I_{n_1} \\ L_2 & I_{n_2} \end{bmatrix}^{-1} = \begin{bmatrix} U_1 & U_2 \\ I_{n_1} & I_{n_2} \end{bmatrix}^{-1} \begin{bmatrix} P & 0 \\ 0 & Q^H \end{bmatrix} \begin{bmatrix} L_1 & \vdots \\ L_2 & I_{n_2} \end{bmatrix}^{-1}
\]

is a generalized inverse of \( A \), with \( X = \begin{bmatrix} L_1 & \vdots \\ L_2 & I_{n_2} \end{bmatrix}^{-1} \begin{bmatrix} I_{n_1} \\ Q \end{bmatrix} \) for \( X \) as in Proposition 1.

We refer to the preceding construction of \( G \) as a **hybrid factorization**. It enables a more efficient approach to construct an optimal RPO, for example, compared to applying QRCP to \( A \) if \( n_2 \ll n \). For the strategy to be successful, we must address some practical issues. First, we need to allow droppings in the factorization to reduce computational cost and memory requirement, especially for larger-scale systems. Second, we need to control \( \kappa \left( \begin{bmatrix} L_1 \\ L_2 \\ I \end{bmatrix} \right) \) to limit \( \kappa(AG) \), for example, by leveraging pivoting and equilibration [26]. Third, it is desirable to make \( S \) as small as possible before we apply QRCP. Hereafter, we will address the first two issues from a theoretical perspective and then address the third issue in Section 3.

### 2.2 Near-optimal right-preconditioning operators via approximate generalized inverses

Although a mathematically optimal RPO enables the most rapid convergence of KSP methods, the computational cost per iteration may be prohibitively high, so is the memory requirement. In practice, it may be more desirable to construct "near-optimal" RPOs by approximating a generalized inverse. The following definition and theorem establish the guideline for constructing such approximations.

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Definition 3. [48, Definition 3.8] Given \( \mathbf{A} \in \mathbb{C}^{n \times n} \), \( G \) is an \( \epsilon \)-accurate approximate generalized inverse (AGI) if there exists \( \mathbf{X} \in \mathbb{C}^{n \times n} \) such that
\[
\left\| \mathbf{X}^{-1} \mathbf{AGX} - \begin{bmatrix} \mathbf{I}_r & 0 \\ 0 & 0 \end{bmatrix} \right\| = \epsilon \leq 1,
\]
where \( \mathbf{I}_r \) is an \( r \times r \) identity matrix with \( r = \text{rank}(\mathbf{A}) \). A class of AGIs is \( \epsilon \)-accurate if \( \epsilon \) tends to 0 as its control parameters are tightened. \( G \) is a stable AGI if \( \kappa(\mathbf{X}) \leq C \) for some \( C \approx 1/\text{mach} \).

Theorem 2. [48, Theorem 3.9] GMRES with an \( \epsilon \)-accurate AGI \( G \) of \( \mathbf{A} \) converges to a least-squares solution \( \mathbf{x}_{LS} \) of (1) in exact arithmetic for all consistent systems (i.e., \( \mathbf{b} \in \mathcal{R}(\mathbf{A}) \)) with any initial guess \( \mathbf{x}_0 \in \mathbb{C}^n \).

A corollary of Theorem 2 is that given an \( \epsilon \)-accurate AGI \( G \), \( \Pi_{\mathcal{R}(\mathbf{A}^H)} G \) is also an \( \epsilon \)-accurate AGI, and the computed \( \mathbf{x}_{LS} \) with \( \Pi_{\mathcal{R}(\mathbf{A}^H)} G \) as the RPO is the pseudoinverse solution. Mathematically, it is equivalent to compute \( \mathbf{x}_{LS} \) with \( G \) as the RPO and then project \( \mathbf{x}_{LS} \) onto \( \mathcal{R}(\mathbf{A}^H) \) to obtain the pseudoinverse solution.

Remark 1. In the literature, commonly used measures of accuracy and stability of a preconditioner \( \mathbf{M} \) for a nonsingular matrix \( \mathbf{A} \) were \( \| \mathbf{A} - \mathbf{M} \|_F \) and \( \| \mathbf{I} - \mathbf{A} \mathbf{M}^{-1} \|_F \), respectively; see, e.g., [8]. Our new definitions of accuracy and stability in Definition 3 are more general in that they apply to singular systems. In addition, they are more rigorous in that they are based on Theorem 2 and Proposition 2, respectively, instead of based on empirical evidence [8].

Theorem 2 and Example 1 suggest that we can construct AGIs by replacing the LU factorization in hybrid factorization with some ILU variants. We will refer to the combination of ILU with a rank-revealing factorization on the Schur complement as a hybrid incomplete factorization (HIF). From the perspective of AGI, a good candidate ILU should satisfy three critical criteria. First, the ILU needs to have prudent dropping strategies to make the approximation as accurate as possible. Second, we must be able to control \( \kappa(\mathbf{AG}) \) effectively for stability. Third, the computational cost and storage requirement should ideally scale linearly (or near-linearly) with respect to the input size. In the ILU literature [16, 22, 70], there had been significant attention to the first criterion. However, the second criterion excludes simple ILU techniques without pivoting, such as ILU(k) [70]. The third criterion excludes ILU with relatively simple pivoting strategies, such as ILUTP [22, 70] and its supernodal variants [57], which suffer from superlinear complexity [20, 33].

Although the second and third criteria may appear self-contradicting for traditional ILU techniques, they can be met by a well-designed MLILU technique. Before delving into the details of MLILU algorithms, let us briefly review MLILU and more importantly, show that MLILU can be used to construct accurate and stable AGIs. First, consider a two-level ILU (or more precisely, ILDU) of \( \mathbf{A} \in \mathbb{C}^{n \times n} \),
\[
P^T \mathbf{W} \mathbf{A} \mathbf{V} \mathbf{Q} = \begin{bmatrix} \mathbf{B} & \mathbf{F} \\ \mathbf{E} & \mathbf{C} \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{B}} & \tilde{\mathbf{F}} \\ \tilde{\mathbf{E}} & \tilde{\mathbf{C}} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_B & \mathbf{D}_B \\ \mathbf{L}_E & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{B}_U & \mathbf{U}_F \\ \mathbf{S} & \mathbf{I} \end{bmatrix},
\]
where \( \mathbf{B} \approx \tilde{\mathbf{B}} = \mathbf{L}_B \mathbf{D}_B \mathbf{U}_B \) is an ILDU of the leading block, \( \mathbf{E} \approx \tilde{\mathbf{E}} = \mathbf{L}_E \mathbf{D}_B \mathbf{U}_B \), \( \mathbf{F} \approx \tilde{\mathbf{F}} = \mathbf{L}_B \mathbf{D}_B \mathbf{U}_F \), and
\[
\mathbf{S} = \mathbf{C} - \tilde{\mathbf{E}} \mathbf{B}^{-1} \tilde{\mathbf{F}} = \mathbf{C} - \mathbf{L}_E \mathbf{D}_B \mathbf{U}_F
\]
is the Schur complement; \( \mathbf{P} \) and \( \mathbf{Q} \) are row and column permutation matrices, respectively; \( \mathbf{W} \) and \( \mathbf{V} \) correspond to row and column scaling diagonal matrices, respectively. The Schur complement \( \mathbf{S} \) can be factorized recursively using the same ILU technique, leading to an \( m \)-level ILU preconditioners, namely,
\[
\mathbf{M} = \begin{bmatrix} \mathbf{W}_1^{-1} \mathbf{P}_1 \mathbf{L}_1 & \cdots & \mathbf{W}_m^{-1} \mathbf{P}_m \mathbf{L}_m \end{bmatrix} \begin{bmatrix} \mathbf{D} \\ \mathbf{S}_m \mathbf{U}_m \mathbf{Q}_m ^{-1} \mathbf{V}^{-1}_m & \cdots & \mathbf{U}_1 \mathbf{Q}_1 ^{-1} \mathbf{V}^{-1}_1 \end{bmatrix}.
\]
where $L_i = \begin{bmatrix} I_{n-n_i} & L_B^{(i)} \\ L_B^{(i)} & L_E^{(i)} & I \end{bmatrix} \in \mathbb{C}^{n \times n}$ for $L_B^{(i)} \in \mathbb{C}^{n_i \times n_i}$ in (11) at the $i$th level (similarly for $U_i$ and all other permutation and scaling matrices), $D$ is composed of the “union” of $D_B$ in (11) for all levels, and $S_m$ is the final Schur complement. As in Example 1, we apply QRCP to $S_m$ to obtain $S_mP = Q \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix}$, where $Q \in \mathbb{C}^{m \times m}$ is unitary and $R_1 \in \mathbb{C}^{n_s \times n_s}$ with $n_s = \text{rank}(S_m)$, $r_1 \geq r_2 \geq \cdots \geq r_{n_s} > 0$ along its diagonal, and $\kappa(R_1) \ll 1/\varepsilon_{\text{mach}}$. We define an RPO as

$$G = U^{-1} \begin{bmatrix} D^{-1} & S^g_m \\ 0 \end{bmatrix} L^{-1} = U^{-1} \begin{bmatrix} D^{-1} & 0 \\ R_1^{-1} & 0 \end{bmatrix} Q^H L^{-1},$$

where $L$, $U$, and $D$ are as in (13). We note the following fact.

**Proposition 3.** [48, Lemma 4.3] If no dropping is applied in MLILU, then $G$ in (14) is a generalized inverse of $A$ with $X = L \begin{bmatrix} I_{n-n_m} \\ Q \end{bmatrix}$ for $X$ as in Proposition 1.

Since $G$ without dropping is an optimal RPO for consistent systems due to Theorem 1, we claim that an $\varepsilon$-accurate and stable $G$ constitutes a near-optimal RPO for consistent systems. The near optimality requires sufficient small droppings and numerical stability, or more precisely, $X^{-1}AGX$ should be close to $I_r$ for $r = \text{rank}(A)$ and $\kappa(L)$ must be controlled by the algorithm. To this end, we utilize an MLILU technique called *HILUCSI*, which stands for *Hierarchical Incomplete LU-Crout with Scalability-oriented and Inverse-based droppings* [20]. HILUCSI leverages several techniques, including fan-in ILU [55], equilibration [26], static and dynamic pivoting across different levels [16, 20], etc., to meet the accuracy and stability requirements. As the name suggests, HILUCSI focuses on scalability in terms of problem sizes, and it has linear time complexity in each level for both the factorization and solve stages [20]. We defer the detailed description of these algorithmic components to Section 3.

**Remark 2.** Besides HILUCSI, there were several MLILU software packages, such as ARMS [72], ILU++ [59], ILUPACK [15], etc. Proposition 3 can also be applied to improve those packages to solve singular systems by applying QRCP to the final Schur complement. To harness this benefit, however, one must also extend them (especially ARMS and ILU++) to ensure the stability of the $L$ factor.

Finally, we note that it is sometimes needed to reuse HIF to construct preconditioners for both $A$ and $A^H$. To achieve, we note the following property:

**Proposition 4.** [48, Proposition 3.5] If $A^g$ is a generalized inverse of $A \in \mathbb{C}^{m \times n}$, then $A^gH \equiv (A^g)^H$ is a generalized inverse of $A^H$.

Conceptually, we can extend (11) to construct a preconditioner $\tilde{M}^H$ for $A^H$ as

$$Q^TVA^HW = \tilde{M}^H = \begin{bmatrix} \tilde{B}^H & \tilde{E}^H \\ \tilde{E}^H & C^H \end{bmatrix} = \begin{bmatrix} U_B^H & L_B^H \\ U_E^H & L_E^H \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} D_B & S^H \\ 0 & I \end{bmatrix}^H.$$

(15)
2.3 Variable preconditioning via iterative refinement for null-space computation

The preceding discussions focused on consistent systems. For inconsistent systems, i.e., \( \mathbf{b} \in \mathbb{C}^n \backslash \mathcal{R}(A) \), an AGI (or even a generalized inverse\(^3\)) cannot guarantee the convergence of GMRES due to the following fact.

**Theorem 3.** [48, Theorem 2.4] GMRES with RPO \( G \) does not break down until finding a least-squares solution \( x_{\text{LS}} \) of (1) for all \( \mathbf{b} \in \mathbb{C}^n \) and \( x_0 \in \mathbb{C}^n \) if and only if \( \mathcal{R}(G) = \mathcal{R}(A^H) \). Furthermore, \( x_{\text{LS}} \) is the pseudoinverse solution if \( \mathcal{R}(G) = \mathcal{R}(A^H) \).

**Remark 3.** The main challenge posed by Theorem 3 is that it is difficult, if not impossible, to ensure the range symmetry of \( \mathcal{R}(G) \) for an approximate generalized inverse \( G \). The requirement of range symmetry is the primary reason why \( A^H \) is often used as \( B \) in AB-GMRES [35, 61]. It is also a key factor for the prevalence of CGLS-type KSP methods [14, 30, 64] for solving singular and least-squares problems. Although such methods can be accelerated by applying some preconditioners, such as incomplete QR [47, 68] or RIF [11, 12], it is difficult for these preconditioners to overcome the slowdown caused by the squaring of the condition number.

Fortunately, this issue can be resolved by using flexible GMRES with variable preconditioners, as formalized by the following definition and theorem.

**Definition 4.** [48, Definition 2.1] Given a matrix \( A \in \mathbb{C}^{n \times n} \), an initial vector \( \mathbf{v} \in \mathbb{C}^n \), and variable preconditioners \( \mathcal{G}_{k-1} = [\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_{k-1}] \), the \( k \)-th flexible Krylov subspace (FKSP) associated with \( A, \mathbf{v}, \) and \( \mathcal{G}_{k-1} \) is

\[
\mathcal{K}_k(A, \mathbf{v}, \mathcal{G}_{k-1}) = \text{span}( \mathbf{v}, A\mathcal{G}_1(\mathbf{v}_1), \ldots, A\mathcal{G}_{k-1}(\mathbf{v}_{k-1}) ),
\]

where \( \mathbf{v}_{k-1} \in \mathcal{K}_{k-1}(A, \mathbf{v}, \mathcal{G}_{k-2}) \setminus \{0\} \) and \( \mathbf{v}_{k-1} \perp \mathcal{K}_{k-2}(A, \mathbf{v}, \mathcal{G}_{k-3}) \) for \( k \geq 2 \). The flexible Krylov matrix, denoted by \( K_k \), is composed of the basis vectors in (16).

The orthogonality of \( \mathbf{v}_{k-1} \) with \( \mathcal{K}_{k-2}(A, \mathbf{v}, \mathcal{G}_{k-3}) \) can be enforced using a generalization of Arnoldi iterations as in [69].

**Theorem 4.** [48, Theorem 2.5] If FGMRES with variable preconditioners \( \mathcal{G} = [\mathcal{G}_1, \mathcal{G}_2, \ldots] \) does not break down until step \( k + 1 \), where \( k = \text{rank}(A) \) for a specific \( \mathbf{b} \in \mathcal{R}(A) \) and \( k = \text{rank}(A) + 1 \) for \( \mathbf{b} \in \mathbb{C}^n \backslash \mathcal{R}(A) \), respectively. If \( \mathcal{R}(A) = \sum_{i=1}^{k} \mathcal{R}(A_i) \), then it finds a least-squares solution of (1) for an initial guess \( x_0 \in \mathbb{C}^n \).

One effective approach to construct variable preconditioners is to introduce iterative refinement (IR) in HIF, leading to HIFIR. Specifically, given an \( \varepsilon \)-accurate AGI \( G \) and an initial vector \( \mathbf{v}_0 \in \mathbb{C}^n \) (typically, \( \mathbf{v}_0 = 0 \)), we refine the solution of \( A\mathbf{v} = \mathbf{q} \) iteratively by obtaining \( \mathbf{v}_j \) for \( j = 1, 2, \ldots \) as

\[
\mathbf{v}_j = (I - GA)\mathbf{v}_{j-1} + G\mathbf{q}.
\]

Eq. (17) defines the \( j \)-th RPO \( \mathcal{G}_i \) in \( \mathcal{G} \), and different \( \mathcal{G}_i \) may use different numbers of IR iterations. Note that (17) in general does not converge by a standalone iterative solver in that \( \rho(I - GA) \geq 1 \) when \( G \) is a generalized inverse, and Eq. (17) cannot introduce additional nonlinearity into the variable preconditioner \( G \) and in turn undermine the robustness of FGMRES due to Theorem 4. Hence, we shift our attention to its use as a variable preconditioner in the context of computing null-space vectors. In particular, we apply the technique to compute the left null space of \( A \) (i.e., \( \mathcal{N}(A^H) \)), which allows us to convert an inconsistent system into a consistent one. Furthermore, by applying the same

\[^3\]When \( G = A^H \), then right-preconditioned GMRES converges to a weighted-least-squares (WLS) solution for inconsistent systems, instead of least-squares solution [48, Theorem 3.7]. We cannot convert the WLS solution into a pseudoinverse solution by projecting it onto \( \mathcal{R}(A^H) \).
3 RECURSIVE CONSTRUCTION OF HYBRID INCOMPLETE FACTORIZATION

In this section, we describe the overall algorithm for constructing HIF. Similar to that of HILUCSI [20] and other MLILU algorithms, HIF is a recursive algorithm. As shown in Figure 1, at each level, HIF takes an input matrix \( A \). HIF first performs symmetric or unsymmetric preprocessing depending on whether \( A \) is (nearly) pattern symmetric, i.e., np(A) \( \approx \) np(A^T); see Section 3.4. The process leads to \( \hat{P}^T WAV\hat{Q} = \hat{P}^T \hat{A}\hat{Q} \), where \( \hat{P}, W, V, \) and \( \hat{Q} \) are obtained from preprocessing. If \( A \) is nearly pattern symmetric, the preprocessing step may involve static deferring, which splits \( \hat{P}^T \hat{A}\hat{Q} \) into a 2-by-2 block matrix, i.e., \( \hat{P}^T \hat{A}\hat{Q} = \begin{bmatrix} B & \hat{F} \\ E & \hat{C} \end{bmatrix} \). Depending on whether the leading block \( B \) is Hermitian, we then perform incomplete \( LDL^H \) or \( LDU \) factorizations, respectively, where \( L \) and \( U \) are unit lower and upper triangular matrices, respectively (i.e., their diagonal entries are ones). We compute these factorizations using fan-in updates (aka the Crout version of ILU), which update the \( k \)-th column of \( L \) using columns 1 through \( k - 1 \) and update the \( k \)-th row of \( U \) using rows 1 through \( k - 1 \) at the \( k \)-th step, respectively. For stability, we combine fan-in updates with dynamic deferring and scalability-oriented droppings; see Section 3.1. In addition, HIF enables rook pivoting when the previous level had too many deferrals as indicated by the Boolean tag ibrp in Figure 1; see Section 3.2. The dynamic deferring may permute some rows and columns in \( \hat{B} \) after \( \hat{E} \) and \( \hat{F} \) to obtain a new 2-by-2 block structure \( \begin{bmatrix} B & \hat{F} \\ \hat{E} & \hat{C} \end{bmatrix} \), where \( \hat{E} \) and \( \hat{F} \) are the leading rows and blocks in \( E \) and \( F \), respectively. We then compute the Schur complement \( S \) corresponding to \( C \) and factorize \( S \) either directly using RRQR or recursively using HIF, depending on whether \( S \) is sufficiently small or nearly dense; see Section 3.3. Some of the components above are the same as those in HILUCSI [20], the predecessor of HIF. The key differences between HIF and HILUCSI are that 1) HIF introduces a variant of the rook pivoting [66] to improve robustness, and 2) HIF uses a rank-revealing QR factorization [18] on \( S_m \). In the following, we first focus on these two aspects and then briefly outline the other components. We will describe how to apply HIF as a preconditioner in Section 4.

3.1 Incomplete \( LDU \) with dynamic deferring and scalability-oriented and inverse-based droppings

The core of HIF at each level is incomplete \( LDU \) factorization, or its variant of incomplete \( LDL^H \) factorization. For robustness, we leverage the fan-in ILU, scalability-oriented dropping, inverse-based dropping, and dynamic deferring, as shown in Algorithm 1. Hereafter, we outline the dual thresholding and dynamic deferring steps in fan-in ILU. An optional step in Algorithm 1 is the inverse-based rook pivoting activated by the Boolean flag ibrp. We will dedicate Section 3.2 to this new pivoting strategy.

In Algorithm 1, the input matrix \( \hat{A} = WAV \) is obtained from applying preprocessing techniques on either the input matrix \( A \) or the Schur complement from the previous level. Note that in the actual implementation, we do not form \( \hat{A} \) explicitly; instead, we rescale the entries in \( A \) by \( W \) and \( V \) in a ”just-in-time” fashion. The procedure \texttt{ilu_factorize} also takes \( \hat{P} \) and \( \hat{Q} \) as input, which were obtained from preprocessing along with \( W \) and \( V \) (see Figure 1 and Section 3.4). The main loop in Algorithm 1 factorizes \( \hat{B} \), the leading block of \( \hat{A} \), using fan-in ILU similar to those in [54, 55], which delays the computation of the Schur complement as late as possible. Unlike [54, 55], however, \texttt{ilu_factorize} dynamically...
permutes (aka defers) rows and columns in \( \tilde{B} \) to the end of \( \tilde{E} \) and \( \tilde{F} \). The procedure computes

\[
P^T W A V Q \approx \begin{bmatrix} \tilde{B} & \tilde{F} \\ \tilde{E} & ? \end{bmatrix} = \begin{bmatrix} L_B & 0 \\ L_E & I \end{bmatrix} \begin{bmatrix} D_B & 0 \\ 0 & ? \end{bmatrix} \begin{bmatrix} U_B & U_F \\ 0 & I \end{bmatrix}
\]

(18)

where the first and second question marks ("?") in (18) correspond to \( C \) and \( S \), which we will describe their computations in Section 3.3. Algorithm 1 returns \( L_B, D_B, U_B, L_E, U_F, P, \) and \( Q \), from which \( \tilde{E} \) and \( \tilde{F} \) (along with \( C \)) can be computed.

A noteworthy feature of \texttt{ilu\_factorize} is its scalability-oriented dropping, which differs from the dropping strategies in [54, 55] and [15]. Consider the step \( k \) of ILU at a particular level. Using the MATLAB’s colon notation, let \( \ell_{k+1:n,k} \) and \( u_{k,k+1:n} \) denote the \( k \)th column and row of \( \begin{bmatrix} L_B \\ L_E \end{bmatrix} \) and \( \begin{bmatrix} U_B & U_F \end{bmatrix} \), respectively. Our dropping strategy limits \( \text{nnz} (\ell_{k+1:n,k}) \) and \( \text{nnz} (u_{k,k+1:n}) \) to be proportional to numbers of nonzeros in the corresponding column and row of
Algorithm 1 ilu_factorize\( (A, p, q, n_1, \text{params}, \text{level}, \text{ibrp}, \text{nr}, \text{nc}) \)

**inputs:**
- \( A \): input scaled matrix of size \( n \times n \) (i.e., \( \hat{A} = WAV \), passed in as \( A \), \( W \), and \( V \) separately)
- \( p, q \): row and column permutation vectors of \( A \) after preprocessing, respectively
- \( n_1 \): the dimension of the current leading block (i.e., \( B = A_{p_1:n_1, q_1:n_1} \))
- \( \text{params} : \{\alpha_l, \alpha_U, \kappa, \kappa_f, \tau_L, \tau_U\} \) (adapted for present level), max\_steps (for rook pivoting)
- level: current level
- ibrp: Boolean tag for enabling inverse-based rook pivoting
- nr, nc: number of nonzeros per row and column entry of the original user input matrix, respectively

**outputs:**
- \( L_B, d_B, U_B \): approximate LDU factors of the leading block
- \( L_E, U_F \): off-diagonal blocks of (11)
- \( p, q \): updated row and column permutation vectors, respectively
- \( n_1 \): updated leading block dimension

1: \( L \leftarrow [1]; U \leftarrow [1]; d \leftarrow [1] \)
2: for \( k = 1 \) to \( n_1 \) do
3: \hspace{1em} if ibrp then
4: \hspace{2em} \( p, L, d, U, q \leftarrow \text{ib_rook_pivot} (A, k, p, L, d, U, q, k, n_1, \text{max\_steps}) \) \[\text{[perform inverse-based root pivoting, typically only if level} > 1]\]
5: \hspace{1em} else
6: \hspace{2em} \( d_k \leftarrow d_{p_k,q_k} - \ell_{k,1:k-1}D_{1:k-1,1:k-1}u_{1:k-1,k} \) \[\text{[fan-in update of diagonal entry]}\]
7: \hspace{1em} end if
8: \hspace{2em} \( \tilde{\kappa}_L \leftarrow \left\| L_{1:k,1:k}^{-1} \right\|_\infty; \tilde{\kappa}_U \leftarrow \left\| U_{1:k,1:k}^{-1} \right\|_1 \) \[\text{[estimate inverse norms of current } L \text{ and } U \text{ factors]}\]
9: while \( \kappa_f \left| d_k \right| < 1 \) or \( \max \left\{ \kappa_L, \kappa_U \right\} > \kappa \) do
10: \hspace{2em} permute entries \( \ell_{k,1:k-1}, d_k \) and \( u_{1:k-1,k} \) to the end; update \( p \) and \( q \) accordingly
11: \hspace{2em} break if \( k \equiv n_1 \)
12: \hspace{2em} \( \tilde{\kappa}_L \leftarrow \left\| L_{1:k,1:k}^{-1} \right\|_\infty; \tilde{\kappa}_U \leftarrow \left\| U_{1:k,1:k}^{-1} \right\|_1 \) \[\text{[update inverse norms]}\]
13: \hspace{2em} \( d_k \leftarrow d_{p_k,q_k} - \ell_{k,1:k-1}D_{1:k-1,1:k-1}u_{1:k-1,k} \) \[\text{[recompute diagonal entry due to pivoting]}\]
14: \hspace{2em} \( n_1 \leftarrow n_1 - 1 \) \[\text{[decrease leading block for factorization]}\]
15: end while
16: \( \ell_{k+1:n,k} \leftarrow \frac{1}{d_k} \left( a_{p_{k+1:n},q_k} - l_{k+1:n,1:k-1}D_{1:k-1,1:k-1}u_{1:k-1,k} \right) \) \[\text{[fan-in update } k \text{th column in } L]\]
17: \( u_{k+1:n} \leftarrow \frac{1}{d_k} \left( a_{p_{k+1:n},q_k} - \ell_{k,1:k-1}D_{1:k-1,1:k-1}u_{1:k-1,k+1:n} \right) \) \[\text{[fan-in update } k \text{th row in } U]\]
18: select largest \( \left\{ a_{l_j,n_k} \right\} \) and \( \left\{ u_{l_j,k+1:n} \right\} \) entries in \( \ell_{k+1:n,k} \) and \( u_{k+1:n,k} \) respectively \[\text{[scalability-oriented dropping]}\]
19: drop entries \( \left\{ \ell_{l_j} \in \ell_{k+1:n,k} \left| \kappa_D \tilde{\kappa}_L \left| \ell_{l_j} \right| \leq \tau_L \right\} \) and \( \left\{ u_{l_j} \in u_{k+1:n,k} \left| \kappa_D \tilde{\kappa}_U \left| u_{l_j} \right| \leq \tau_U \right\} \) \[\text{[inverse-based dropping]}\]
20: end for
21: \( L_B \leftarrow L_{1:n_1,1:n_1}; d_B \leftarrow d_{1:n_1,1:n_1}; U_B \leftarrow U_{1:n_1,1:n_1}; L_E \leftarrow L_{n_1+1:n_1,1:n_1}; U_E \leftarrow U_{n_1+1:n_1,1:n_1}; U_F \leftarrow U_{1:n_1,1:n_1+1:n_1} \)
22: return \( L_B, d_B, U_B, L_E, U_E, p, q, n_1 \)

the original (i.e., the top level instead of the present level) input matrix, respectively; see line 18. This dropping strategy plays an important role for HILUCSI and HIF to achieve (near) linear complexity in both space and time. Besides this symbolic dropping, HILUCSI and HIF also adopted an inverse-based dropping [9], which drops every entry \( \ell_{l_j} \) such that \( \kappa_f \left| \ell_{l_j} \right| \leq \tau_L \), where \( \kappa_f \) and \( \tau_L \) are user-specified thresholds for the upper bound of \( \left\| D_{1:k,1:k}^{-1} \right\|_\infty \) and the drop tolerance, respectively (see Section 5.2). The dropping for \( U \) is similar; see line 19.

Another core component in ilu_factorize is the inverse-based dynamic deferring. In particular, during the fan-in ILU, we dynamically defer \( \ell_{k,1:k-1} \) and \( u_{1:k-1,k} \) (line 10) if we encounter small \( |d_k| \) or large \( \left\| L_{1:k,1:k}^{-1} \right\|_\infty \) and \( \left\| U_{1:k,1:k}^{-1} \right\|_1 \)
defer the $k$th row and $k$th column

$L_{k-1}$ and $U_{k-1}$ are shorthand for $L_{1:k-1,1:k-1}$ and $U_{1:k-1,1:k-1}$, respectively. When encountering ill-conditioned factors ($|d_k| < 1/k^2$ or $\max \|L_{1:k,1:k}\|_\infty, \|U_{1:k,1:k}\|_1 > k$) due to $f_{k,1:k-1}$ or $u_{1:k-1,k}$ (green regions in left panel), we dynamically defer both $f_{k,1:k-1}$ and $u_{1:k-1,k}$ to next level (right panel).

(line 9). Figure 2 illustrates the process of dynamic deferring. This deferring is similar to that in [15, 16]; in Section 3.2, we will extend it to support rook pivoting. Note that the inverse-based dropping in line 19 can be replaced by a different dropping strategy, such as that in [59], but we utilized the inverse-based dropping since we are already estimating the inverse norms for deferring.

We note some implementation details. First, in line 18, we use quickselect [44], which has expected linear time complexity. Second, since we need to access both rows and columns of $\hat{A}$ while computing the fan-in updates (lines 16 and 17), we need to store $\hat{A}$ (or more precisely, $A$) in both row and column majors. We will describe the data structures in Section 3.5 and Appendix A. Third, the output $L_E$ and $U_F$ will only be used to compute the Schur complement in Section 3.3. Afterwards, $L_E$ and $U_F$ are discarded, since they can be reconstructed from $\tilde{E} = \hat{A}_{p_{n_1+1:n_1}, q_{1:n_1}}$ and $\tilde{F} = \hat{A}_{p_{1:n_1}, q_{1:n_1}}$, respectively as in (11).

3.2 Inverse-based rook pivoting for coarse levels

Dynamic deferring symmetrically permutes rows and columns. Such a permutation strategy works well for reasonably well-conditioned matrices. However, we observe that symmetric permutations alone sometimes lead to relatively large Schur complements for highly ill-conditioned unsymmetric systems. To overcome this issue, we introduce an inverse-based rook pivoting (IBRP) for the fan-in ILU, by adapting the rook pivoting [66] for complete LU factorization.

In the standard rook pivoting [66], a pivot is found by searching in the row and column in alternating order until its magnitude is no smaller than those of all other entries in the row and column within the Schur complement. This strategy has a comparable cost as partial pivoting for dense matrices but enables superior stability. However, in the context of fan-in ILU, only the $k$th row and column of the Schur complement $S$ are updated at the $k$th step; the remaining part of the Schur complement is not available. Hence, we must modify the pivoting procedure to interleave the search with dynamic permutation and “just-in-time” fan-in updates. Figure 3 illustrates one step of the IBRP. Note that this permutation is more general than the dynamic deferring in Figure 2, in that it can exchange $f_{k,1:k-1}$ with a row in the middle of $L_{k+1:n_1,1:k-1}$, and similarly for the rows in $U$. Furthermore, the row and column interchanges are not
Fig. 3. Illustration of inverse-based rook pivoting in HIF. At the upper-left panel, we update $d_k$ and nonzeros in $\ell_{k+1,n,k}$, find a pivot, and then interchange $\ell_{k,1:k-1}$ with the pivot row (indicated by curved arrow). The lower-left panel shows the process for $U$.

symmetric in general. Note that IBRP requires a more sophisticated data structure to support the row and column interchanges, which we will address in Section 3.5.

Besides the difference dictated by the fan-in update, there are two other significant differences between IBRP and the standard rook pivoting. First, we do not simply use the magnitude to determine the pivot, since it may conflict with dynamic deferring. Instead, we add an inverse-based constraint when searching the pivot, so that the pivot row in $L$ and pivot column in $U$ would not arbitrarily enlarge the condition numbers of the $L$ and $U$, respectively. Second, we do not locate the optimal rook pivot whose magnitude is the largest among its row and column; instead, we impose a maximum number of steps of IBRP, controlled by the parameter max_steps. For completeness, Algorithm 2 details the inverse-based rook pivoting. Note that we do not scale $\ell$ and $u$ by $1/d_k$ in lines 2 and 9 in Algorithm 2, compared to $t_{k,n,k}$ and $u_{k,k,n}$ in lines 16 and 17 in Algorithm 1. This omission of scaling is for efficiency purposes, because the choice of pivot does not depend on the scaling of the entries.

We note an important practical issue. The IBRP can result in significantly denser $L$ and $U$ factors because the pivoting may undo the effects of the fill-reduction reordering in the preprocessing step. Hence, we enable IBRP only on the coarser levels (typically for level $> 1$) when dynamic deferring is found to be ineffective. At the coarser levels, we
Algorithm 2 ib_rook_pivot($\hat{A}, k, p, L, d, U, q, \kappa, n_1, \text{max\_steps}$)

**inputs:**

- $\hat{A}$: input scaled matrix (i.e., $\hat{A} = WAV$, passed in as $A$, $W$, and $V$ separately)
- $k$: step count in ILU factorization
- $p, q$: row and column permutation vectors of $A$, respectively
- $L, U$: $L$ and $U$ factors at step $k$, i.e., $L_k \cup L_F$ and $U_B \cup U_F$, respectively
- $d$: diagonal entries at step $k$
- $\kappa$: inverse-norm threshold
- $n_1$: leading block dimension
- max\_steps: maximum number of rook pivoting steps

**outputs:**

- $p, q$: updated row and column permutation vectors, respectively
- $L, U$: updated $L$ and $U$ factors, respectively
- $d$: diagonal entries with updated $d_k$

1. **for** $i = 1$ to max\_steps **do**
2. \[ \ell_{k,n} \leftarrow \hat{a}_{k:n}q_k = L_{k:n,1:k-1}\hat{D}_{1:k-1,1:k-1}u_{1:k-1,k}[\text{fan-in update of } d_k \text{ and } \ell_{k+1,n,k} \text{ without scaling by diagonal}] \]
3. \[ r \leftarrow \arg \max \left\{ \ell_k \mid k + 1 \leq r \leq n_1 \text{ and } \left\| L_{1:k-1,1:k-1} \ell_r \right\|_1 \leq \kappa \right\} \text{ [find pivot in } \ell_{k+1,n} \right\} \]
4. **if** $r \neq \emptyset$ **and** $|\hat{\ell}_k| < |\hat{\ell}_r|$ **then**
5. \[ \ell_{k+1,k-1} \leftarrow \ell_{r,1:k-1}; \ell_{r,k} \leftarrow \ell_k \text{ [perform row interchange]} \]
6. **else if** $i > 1$ **then**
7. \[ d_k \leftarrow \hat{u}_1; \text{ break} \text{ [extract } d_k \text{ from } \ell_{k:n} \right\} \]
8. **end if**
9. \[ \hat{u}_{k:n} \leftarrow \hat{a}_{p_k}q_{k:n} = L_{k:n,1:k-1}\hat{D}_{1:k-1,1:k-1}U_{1:k-1,k:n}[\text{fan-in update of } d_k \text{ and } u_{k,k+1:n} \text{ without scaling by diagonal}] \]
10. \[ c \leftarrow \arg \max \left\{ |\hat{u}_c| \mid k + 1 \leq c \leq n_1 \text{ and } \left\| U_{1:k-1,1:k-1} \hat{u}_{k,c} \right\|_1 \leq \kappa \right\} \text{ [find pivot in } \hat{u}_{k+1:n} \right\} \]
11. **if** $c \neq \emptyset$ **and** $|\hat{u}_k| < |\hat{u}_c|$ **then**
12. \[ u_{1:k-1,k} \leftarrow u_{1:k-1,c}; q_k \leftarrow q_c; \hat{u}_k \leftarrow \hat{u}_r \text{ [perform column interchange]} \]
13. **else**
14. \[ d_k \leftarrow \hat{u}_k; \text{ break} \text{ [extract } d_k \text{ from } \hat{u}_{k:n} \right\} \]
15. **end if**
16. **end for**
17. **return** $p, L, d, U, q$

also enlarge the scalability-oriented fill factors $a_L$ and $a_U$ to preserve more fills introduced by IBRP. Our experiments show that applying IBRP on coarser levels can significantly reduce the size of the final Schur complement for some challenging problems, as demonstrated by the example in Table 1.

### 3.3 Computing and factorizing Schur complements

After finishing **iliu_factorize**, we need to compute the Schur complement $S$ based on (12). This step involves a sparse matrix-matrix (SpMM) multiplication, for which we adopt the algorithm as described in [6]. The space and time complexity of SpMM depends on the nonzeros in $L_E$ and $U_F$. To achieve near-linear complexity, we apply scalability-oriented dropping before SpMM to the rows and columns of $L_E$ and $U_F$, respectively. Recall that in **iliu_factorize** we already applied scalability-oriented dropping to the columns and rows of $L_E$ and $U_F$, respectively. Hence, the nonzeros both rows and columns in $L_E$ and in $U_F$ are well controlled, allowing us to effectively bound the complexity of $S$. In
Table 1. Effectiveness of IBRP for reducing the final Schur complement size for the testing matrix shyy161 from the SuiteSparse Matrix Collection [23]. \( \dim(N) \) indicates the dimension of the null space, and \( S_m \) denotes the final Schur complement in HIF. We factorized the testing matrix using HIF with and without IBRP, and we report the factorization time (factor time) and nnz ratio (i.e., \( \text{nnz}(M) / \text{nnz}(A) \), aka fill ratio in [57]). We solved the consistent system with right-hand side \( b = A1 \) (where \( 1 = [1, 1, \ldots, 1]^T \)) using GMRES(30) with relative residual tolerance \( 10^{-6} \). The computing environment for running the test can be found in Section 6. Timing results for GMRES were negligible thus omitted.

| \( n \) | \( \text{nnz} \) | \( \dim(N(A)) \) | w/ IBRP | \( S_m \) in HIF | \( \dim(N(S_m)) \) | fac. time | \#levels | nnz ratio | GMRES iter. |
|---|---|---|---|---|---|---|---|---|---|
| 76,480 | 329,762 | \( \geq 50 \) | yes | 1,407 | 50 | 2.51 | 5 | 12.0 | 15 |
| | | | no | 9,394 | 48 | 226 | 2 | 304 | 2 |

Algorithm 3 \( \text{rrqr\_final\_schur}(S, \kappa_{\text{rrqr}}) \)

inputs:
- \( S \): final Schur complement of size \( n_S \times n_s \)
- \( \kappa_{\text{rrqr}} \): condition number threshold for determining numerical rank (default value is \( \epsilon_{\text{mach}}^{-2/3} \))

outputs:
- \( Q, R \): \( Q \) and \( R \) factors of \( S \)
- \( p \): permutation vector in QRCP
- \( r \): numerical rank of \( S \)

1: factorize \( S = \text{QRPT} \) \{compute QRCP via xGEQP3\}
2: for \( r = 1 \) to \( n_S \) do
3: update estimated \( \|R_{1, r, 1, r}\|_2 \) and \( \|R_{1, r, 1, r}^{-1}\|_2 \) \{incremental condition number estimation via xLAIC1\}
4: if \( \|R_{1, r, 1, r}\|_2 \|R_{1, r, 1, r}^{-1}\|_2 < \kappa_{\text{rrqr}} \) then
5: \( r \leftarrow r + 1 \)
6: break
7: end if
8: end for
9: return \( Q, R, p, r \)

contrast, if we applied dropping after SpMM, the complexity of SpMM may be higher. Note that after computing \( S \), we drop both \( L_E \) and \( U_F \) as they can be reconstructed from the other terms as in (11), and then factorize \( S \) recursively.

In HIF, the final Schur complement is factorized by rank-revealing QR (or truncated QRCP) in order to guarantee the stability of the preconditioner. Algorithm 3 outlines the procedure. We note a couple of details in the algorithm. First, line 1 computes QRCP \( S_P = QR \) for \( S \in \mathbb{R}^{n_S \times n_S} \), where \( P \) is a permutation matrix, and \( r_{11} \geq r_{22} \geq \ldots \geq r_{n_S n_S} \geq 0 \). The QRCP has a time complexity of \( O \left( n_S^3 \right) \). Second, lines 2–8 determine the numerical rank of \( S \) by comparing the estimated condition number against a threshold \( \kappa_{\text{rrqr}} \), which defaults to \( \kappa_{\text{rrqr}} = \epsilon_{\text{mach}}^{-2/3} \). We estimate the 2-norm condition number using the incremental estimator in [13], which has a linear complexity per step. Hence, the overall computational cost is dominated by QRCP. For efficiency, we implement the QRCP and condition-number estimator using LAPACK kernel functions xGEQP3 and xLAIC1, respectively.

Due to the cubic time complexity of QRCP, we would like to make \( n_S \) as small as possible, and ideally have \( n_S = O \left( \sqrt{n} \right) \), where \( n \) is the number of unknowns in the original system. This high complexity was the motivation to use IBRP within multilevel ILU. In addition, we would also like to prevent having too many low-quality ILU levels. As a tradeoff, we trigger QRCP based on the following criteria. In \textbf{ilu\_factorize}, let \( n_0 \) be the initial leading block dimension.
after preprocessing, i.e., the input $n_1$ in Algorithm 1, and let $d$ be the total number of dynamic deferrals. If more than 75% entries are dynamically deferred during fan-in update, i.e., $d/n_0 \geq 0.75$, then we discard incomplete factorization in that level and use RRQR on its input. In addition, if more than 60% entries are dynamically deferred, i.e., $d/n_0 \geq 0.6$, then we apply RRQR on the remainder Schur complement.

3.4 Preprocessing with static deferring

In Figure 1, an important step was the preprocessing at each step, which computes a block structure $\begin{bmatrix} B & F \\ E & C \end{bmatrix}$. The preprocessing in HIF performs equilibration, static deferring, and fill-reduction reordering, in that order. Equilibration improves stability by computing $P^T W A V Q = \tilde{A}$, where $W$ and $V$ correspond to row and column scaling matrices, and $P$ and $Q$ correspond to row and column permutation matrices. We utilize MC64 [26], which computes unsymmetric equilibration, for which $Q = I$. For (nearly) pattern symmetric levels, we symmetrize the output of MC64 by setting $W = V = \sqrt{WV}$ and $Q = P$ as in [53]. Note that for structurally singular systems, MC64 sometimes yields unstable scaling factors that may be arbitrarily large or small [48]. The symmetrization process overcomes the issue; for unsymmetric equilibration, we also symmetrize the scaling factors by setting $w_i = q_i = \sqrt{w_i q_i}$ if $\max\{w_i, q_i\} / \min\{w_i, q_i\} > \beta$, where $\beta$ is 1000 by default. After symmetric equilibration, we permute a row and its corresponding column to the lower-right corner if its diagonal entry is nearly zero. We refer to this process as static deferring, which naturally yields a block structure $\begin{bmatrix} B & F \\ E & C \end{bmatrix}$. Afterwards, we apply fill-reduction reordering on $B$ and then permute $E$ and $F$ correspondingly, which leads to the final block structure $\begin{bmatrix} B & F \\ E & C \end{bmatrix}$. We use RCM [31] and AMD [2] for symmetric and unsymmetric reordering, respectively, because RCM is more efficient and has been shown to work better for symmetric ILU [10, 38].

3.5 Efficient data structures and complexity analysis

To implement HIF efficiently, we must perform all its core operations in linear time with respect to the number of nonzeros. In particular, the fan-in updates of $L_k^{+1, n, k}$ and $U_k^{+1, n, k}$ at $k$th ilu_factorize (cf. lines 16 and 17 in Algorithm 1 and lines 2 and 9 in Algorithm 2) requires efficient sequential access of $L$ and $U$ in both rows and columns. More importantly, the deferring and pivoting operations require interchanging rows and columns in $L$ and $U$ dynamically. Although the data structure in [55] supports fan-in updates efficiently, it does not support deferring or rook pivoting. Under these considerations, we developed flexible, three-tiered data structures, which extended the data structure in [55] to support deferring and pivoting, as we describe in Appendix A. This three-tiered data structure augments the standard compressed sparse column or row (aka CSC and CSR) formats either partially or fully. We use the partially augmented version when rook pivoting is disabled, especially at the top levels, since it has a smaller memory footprint; the fully augmented version is used when rook pivoting is enabled, which in general occurs only at coarser levels.

Assuming the number of nonzeros per row and column in the input mesh is bounded by a constant, which is typically the case for linear systems arising from partial differential equations, the augmented data structures enable all the core components in HIF to be performed in linear time at each level. We outline the analysis as follows. First, the fan-in update can be performed in linear time proportional to the number of nonzeros, thanks to the use of augmented data structure [55]. Second, the incremental update of $L_{k-1, k, 1:n}$ and $U_{k-1, k, 1:n}$ also costs linear time with respect to the number of nonzeros in $L$ and $U$, respectively (see e.g., [34]). Third, the partially augmented data structures allow the
permutations in deferring can be performed in linear time complexity, as shown in [20]. Fourth, the fully augmented data structures allow each row interchange in rook pivoting to be performed in time proportional to the number of nonzeros, assuming the number of nonzeros in each row is a constant. This step is the most complicated, and we defer its analysis to Appendix B. Fifth, the time complexity of SpMM in Section 3.3 is proportional to the number of nonzeros in the product. Since the scalability-oriented dropping ensures that each row and column of $L_E$ and $U_F$ is bounded by a constant $C$, so the number of nonzeros per row and per column in the product $L_E D_B U_F$ is bounded by $C^2$. Finally, assuming the number of rows in the final Schur complement is bounded by $O(n^{1/3})$, we conclude that HIF guarantees linear time complexity per level (excluding its preprocessing steps) under the assumptions as mentioned above.

Note that HIF does not guarantee that the number of levels is bounded by a constant. Furthermore, the time complexity of AMD reordering is quadratic in the worst-case case [41]. Hence, the total time complexity of HIF may not be linear. Nevertheless, the number of levels is typically a small constant, and the computational cost of AMD is typically negligible. Hence, we do observe linear asymptotic growth for the overall HIF across all levels empirically.

### 4 MULTILEVEL TRIANGULAR SOLVES AND MATRIX-VECTOR MULTIPLICATIONS

To use the HIF as a preconditioner, we typically need a procedure similar to triangular solves. We shall refer to it as a multilevel triangular solver. As an illustration, let $y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$ be a block vector corresponding to $B$ and $C$ in the two-level ILU $M$ in (11). In this case, $W^{-1}P \tilde{M} \tilde{Q}^T V^{-1}$ is a preconditioner of $A$. The multilevel solver computes

$$M^\delta y = \begin{bmatrix} \tilde{B}^{-1} y_1 \\ 0 \end{bmatrix} + \begin{bmatrix} -\tilde{B}^{-1} F \\ I \end{bmatrix} S^\delta \begin{bmatrix} y_2 - E \tilde{B}^{-1} y_1 \end{bmatrix}. \tag{19}$$

We further compute $S^\delta y_1$ recursively, which leads to the multilevel solver. Algorithm 4 details this recursive procedure. Note that Algorithm 4 also supports the use of $M^H$ to construct a preconditioner for $A^H$ based on (15).

When solving inconsistent systems, such as the computation of the null-space vector, using $G = \tilde{M}^\delta$ as the preconditioning operator may be insufficient. In this setting, it is desirable to enable iterative refinement with HIF to construct a variable preconditioner for FGMRES, as described in [48]. Specifically, given equation $A v = q$, HIFIR iteratively computes

$$v_j = (I - M^\delta A) v_{j-1} + M^\delta q = v_{j-1} - M^\delta r_{j-1} \tag{20}$$

for $j = 1, 2, \ldots$, where $r_{j-1} = q - A v_{j-1}$ is the residual vector with $v_0 = 0$, and $M^\delta r_{j-1}$ is computed by Algorithm 4. Note that when computing null-space vectors, the condition number of $R_1$ in the RRQR of $S_m$ can be as large as $1/\epsilon_{\text{mach}}$, so it would have a different numerical rank of $S_m$ compared to that when solving consistent systems as described in Section 3.3. For this reason, Algorithm 4 has a parameter $r$ to allow the user passing in different numerical ranks of $S_m$.

When choosing the number of iterations in the iterative refinement, HIFIR terminates the iteration after a maximum number of iterations. We increase this upper bound on the iterations at every restart for FGMRES. We refer readers to [48] for the analysis of this adaptive procedure.

Besides multilevel triangular solves, HIF also supports the computation of the multiplication $\tilde{M}$ with a vector. As an illustration, given $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ in a two-level factorization, the multiplication can be written as

$$\tilde{M} x = \begin{bmatrix} \tilde{B} \\ E \end{bmatrix} x_1 + \begin{bmatrix} I \\ E \tilde{B}^{-1} \end{bmatrix} F x_2 + \begin{bmatrix} 0 \\ S x_2 \end{bmatrix}. \tag{21}$$
Algorithm 4  hif_solve\((M, y, r, \text{trans}, \text{level} = 1)\)

inputs:
\- \(M\): a structure containing HIF preconditioner
\- \(y\): right-hand side vector
\- \(r\): numerical rank used in the final RRQR factorization
\- \(\text{trans}\): Boolean flag indicating whether to solve \(M^H y\)
\- \(\text{level}\): level counter in the HIF preconditioner (default to 1 at top level)

output:
\- \(x\): solution vector \(M^y\) or \(M^H y\)

1: extract \(n_1, n, L_B, D_B, U_B, E, F, P, Q, W, \) and \(V\) for current level from \(M\)
2: if \(\text{trans}\) then
3: \(L_B, U_B \leftarrow U_B^H, L_B^H; D_B \leftarrow \bar{D}_B\) \[construct\ conjugate\ transpose\]
4: \(E, F \leftarrow P^H, E^H\)
5: \(W \leftarrow V; P \leftarrow Q\)
6: end if
7: \(y \leftarrow P^T Wy\) \[scale\ and\ permute\ right-hand\ side\]
8: \(x_{1:n_1} \leftarrow U_B^{-1} D_B^{-1} L_B^{-1} y_{1:n_1}\)
9: \(x_{n_1+1:n} \leftarrow y_{n_1+1:n} = Ex_{1:n_1}\)
10: if final level then
11: extract \(\hat{Q}, \hat{R}, \) and \(\hat{P}\) of QRCP of \(S_m\) (or of \(S_m^H\) if \(\text{trans}\)) from \(M\)
12: \(x_{n_1+1:n} \leftarrow \hat{P}_{1:r} \hat{R}_{r:r} \hat{Q}_{1:r}^H x_{n_1+1:n}\) \[solve\ on\ final\ Schur\ complement\ with\ numerical\ rank\ \(r\)]
13: else
14: \(x_{n_1+1:n} \leftarrow \text{hif_solve} (M, x_{n_1+1:n}; r, \text{trans}, \text{level} + 1)\)
15: end if
16: \(x_{1:n_1} \leftarrow y_{1:n_1} = Fx_{n_1+1:n}\)
17: \(x_{1:n_1} \leftarrow U_B^{-1} D_B^{-1} L_B^{-1} x_{1:n_1}\)
18: return \(VQx\) \[scale\ and\ permute\ \(x\)\]

The multiplication of \(x_2\) by the Schur complement, i.e. \(Sx_2\), is then computed recursively, leading to the multilevel matrix-vector multiplication. The control flow of this recursive algorithm is similar to that of Algorithm 4, and it is helpful when we need \(\hat{M}\) as an approximation of \(A\) (instead of using \(\hat{M}^H\) as an approximation to \(A^H\)). In addition, it is also useful for some advanced preconditioners for singular systems, which we will report in the future.

5 SOFTWARE DESIGN AND USER INTERFACES

In this section, we describe our software design and the user interfaces of HIFIR, including its C++ programming interface as well as the high-level interfaces for Python and MATLAB. We refer the readers to the official documentation https://hifirworks.github.io/hifir/ for more detailed documentation of HIFIR.

5.1 Design considerations

When designing HIFIR, we have focused on three key factors: efficiency, flexibility, and ease-of-integration into other codes. Under these considerations, we chose to implement the core components of HIFIR in C++-11 using C++ templates in a header-only fashion while providing high-level interfaces in Python and MATLAB. C++ is a powerful programming language for scientific computing and is highly efficient. For efficient kernel computations, we link HIFIR with LAPACK and we ease the linking by leveraging compiler directives and macros. In terms of flexibility, HIFIR supports different data types, such as float, double, and std::complex<double>, through C++ templates. In addition, mixed data types are
supported, for example, to compute the factorization in double precision while exporting it in single precision during
the solve step. In addition, the use of C++ also makes it easier to integrate with other linear-algebra packages (such as
Eigen [36], Blaze [46], SuperLU [56], PETSc [5], etc.) and scientific-computing packages (such as Trilinos [42]). The use
of C++ in HIFIR eases its integration with such libraries. The header-only design of HIFIR is similar to that of Eigen
[36]. This design significantly simplifies the installation and build process in that the user only needs to include the
header file hifir.hpp and link with LAPACK libraries. For ease of prototyping, we also provide high-level interfaces in
Python and MATLAB through hifir4py and hifir4m, respectively; see Section 5.4.

5.2 Control parameters
The algorithm described in Section 3 involved several control parameters, as we summarize some key parameters
in Figure 4 as a C++ structure. The first six parameters correspond to $\alpha_L$, $\alpha_U$, $\kappa$, $\kappa_D$, $\tau_L$, and $\tau_U$ for the top level in
Algorithm 1; note that HIF automatically adapt these parameters for coarser levels. Their default values were obtained
based on the experiments in [20]. The seventh and eighth parameters in Figure 4 corresponds to $\beta$ described in Section 3.4
and $\kappa_{rrqr}$ in Algorithm 3, respectively. We omit some additional parameters for simplicity.

The default values typically work well for PDE-based systems. They are appropriate for both double- and single-
precision computations, since the thresholds are far greater than their corresponding machine epsilons. We present
some guidelines in tuning the first six parameters, based on theoretical analysis and extensive experimentation:

- $\alpha_L$, $\alpha_U$: These control the scalability-oriented dropping, and they are critical in achieving linear-time
  complexity of HIFIR at each level. The recommended values are between 2 and 20. While the default values
  $\alpha_L = \alpha_U = 10$ are robust, the user may reduce them to $\alpha_L = \alpha_U = 3$ for PDE-based systems (including
  saddle-point problems) for better efficiency;
- $\kappa$, $\kappa_D$: These control the inverse norms of the triangular factors ($L$ and $U$) and diagonal factor ($D$),
  respectively. Their recommended range is between 3 and 5. The default values $\kappa = \kappa_D = 3$ are robust, but the
  user may increase them to $\kappa = \kappa_D = 5$ for PDE-based systems for better efficiency;
- $\tau_L$, $\tau_U$: These control numerical droppings and they are secondary compared to $\alpha_L$ and $\alpha_U$. The default
  values $\tau_L = \tau_U = 10^{-4}$ are robust; one may increase them to $\tau_L = \tau_U = 10^{-2}$ for PDE-based systems for better
  efficiency. One could even set them to zero without losing (near) linear time complexity, as long as $\alpha_L$ and $\alpha_U$
  are within the recommended ranges. Note that large $\kappa$ and $\kappa_D$ may implicitly reduce the drop tolerances.
5.3 Programming interfaces in C++

The core components of HIFIR are implemented using generic object-oriented programming with C++-11. All data structures and algorithms in HIFIR are implemented as C++ template classes and functions.

5.3.1 Basic data types. HIFIR has two basic data types: sparse matrices and vectors. The sparse matrices in HIF include CSC, CSR, and their partially or fully augmented counterparts as described in Appendix A. We will use CSR as the demonstration in the following. The class of CSR matrix in HIF is hif::CSR<ValueType, IndexType>, of which the two template arguments correspond to the value data type (e.g., float, double, std::complex<double>, etc.) and the index data type (e.g., int, long, etc.), respectively. For instance, a commonly used type is hif::CSR<double, int>. A CSR instance can either wrap or own the data; the former mode allows the user to create a “view” into a CSR matrix owned by another software library, so it is more memory efficient and is preferred. For example, to wrap external data for read-only access by HIF, one can use the helper function

```cpp
template <ValueType, IndexType> const hif::CSR<ValueType, IndexType> hif::wrap_const_csr(IndexType nrows, IndexType ncols, const IndexType *row_ptr, const IndexType *col_ind, const ValueType *vals);
```

where row_ptr, col_ind, and vals are read-only. HIF also provides an interface to construct a CSR matrix from scratch; we omit the details for simplicity. Note that the augmented CSC and CSR data structures are used internally by HIF, so we omit their interface definitions.

When using HIF as a preconditioner, the right-hand side and solution vectors need to be passed in as arrays. HIF uses a generic interface compatible with STL sequence containers such as std::vector. For memory efficiency, HIF also provides a container hif::Array<ValueType> for wrapping user-allocated arrays. The user can create mutable and immutable instances by using one of the helper functions:

```cpp
template <ValueType> hif::Array<ValueType> hif::wrap_array(std::size_t n, ValueType *vals);

template <ValueType> const hif::Array<ValueType> hif::wrap_const_array(std::size_t n, const ValueType *vals);
```

If C++-20 is used, then std::span<ValueType> can be used in place of hif::Array<ValueType>. Note that hif::Array can also own the data; in this case, one can use a construct of hif::Array similar to that of std::vector.

5.3.2 Interfaces for HIF preconditioners. The algorithms for HIF are encapsulated in a class hif::HIF<ValueType=double, IndexType=int>, of which the two template arguments are similar to those of hif::CSR and specify the data types used by the internal augmented CSC and CSR formats as well as the output format. The class has two main interfaces: factorization and multilevel solve. In the following, we will use dHIF as an alias for hif::HIF<double, int> as a demonstration.

We first describe the member functions for computing the factorization, which is provided by the template function

```cpp
template <class MatType> void dHIF::factorize(const MatType &A, const hif::Params &params=hif::DEFAULT_PARAMS);
```

where MatType is typically hif::CSR<ValueType, IndexType> or hif::CSC<ValueType, IndexType>. However, the interface allows the use of different ValueType and IndexType for hif::HIF and MatType. For example, the input may be in double precision, and the preconditioner can be built in single precision. However, if the input matrix is complex, then
ValueType of hif::HIF must also be complex and vice versa. The second argument passes in the control parameters as described in Section 5.2, where the default is a static variable in hif.

The interface for the multilevel solve is provided by the template function

\[
\text{template < class RhsType, class SolType > void dHIF::solve ( const RhsType &b, SolType &x, bool trans=false, int rnk=0);}
\]

where \( b \) and \( x \) are the right-hand side and the solution vector, respectively. The interfaces for RhsType and SolType should be compatible with const hif::Array<ValueType> and hif::Array<ValueType>, respectively, where their ValueType may differ from each other and also differ from that of hif::HIF. The optional Boolean argument \( \text{trans} \) indicates whether to apply the preconditioner itself or the (conjugate) transpose. The argument \( \text{rnk} \) specifies the rank for the RRQR for the final Schur complement; its default value 0 indicates to use the rank determined by hif::HIF from \( \kappa_{\text{rrqr}} \). The user can set \( \text{rnk} \) to \(-1\) to use a larger rank determined from \( \kappa_{\text{rrqr}} = 1/\epsilon_{\text{mach}} \) for the computation of the null spaces.

Besides the above main interfaces, hif::HIF also offers hif::HIF::hifir for multilevel solve with iterative refinement and hif::HIF::mmultiply for multilevel matrix-vector multiplication. Their interfaces are as follows:

\[
\text{template < class MatType, class RhsType, class SolType > void dHIF::hifir ( const MatType &A, const RhsType &b, SolType &x, int nirs, bool trans=false, int rnk=-1);}
\]

\[
\text{template < class RhsType, class SolType > void dHIF::mmultiply ( const RhsType &b, SolType &x, bool trans=false, int rnk=-1);}
\]

These two functions are more useful for solving singular systems, and hence their default values for \( \text{rnk} \) is \(-1\) instead of 0. The argument \( \text{nirs} \) specifies the number of iterations of iterative refinement.

### 5.4 High-level interfaces for MATLAB and Python

It is often more productive for prototyping and academic research to use a high-level programming language such as MATLAB, GNU Octave, and Python. For this reason, we have developed hifir4m and hifir4py to allow the users to access HIFIR from these languages.

For the MATLAB interface, hifir4m, which also supports GNU Octave, provides three key functions in its high-level programming interface. The first function constructs a handle to a HIF object for a matrix \( A \) from either \( A \) itself or an optional "sparsifier" \( S \), with the interface

\[
\text{function hif = hifCreate (A [, S, varargin])}
\]

where \( A \) and \( S \) can be MATLAB’s built-in sparse format matrices or MATLAB struct containing the three CSR fields, and varargin specifies name-value pairs, such as \( (\ldots, \text{’alpha}_L’, 5, \text{’alpha}_U’, 5, \text{’mixed’, true}) \). The matrix \( A \) and \( S \) can be single or double precision and can be real or complex. The second function applies the preconditioner, with the interface

\[
\text{function y = hifApply (hif, x [, op, rnk, nirs])}
\]

where the optional argument \( \text{op} \) can be one of 'S', 'SH', 'M', and 'MH' for \( M^T x, M^{TH} x, M x, \) and \( M^{HT} x \), respectively. \( \text{rnk} \) specifies the rank for truncated RRQR, and \( \text{nirs} \) specifies the number of iterative refinements for \( M^T x \) and \( M^{TH} x \). To destroy the HIF object, the user can call

\[
\text{delete (hif)}
\]

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manually, or leave it to MATLAB to delete it automatically. In addition, hifir4m offers two high-level drivers, gmresHif and pipitHifir, for solving nonsingular and singular systems, respectively. Their interfaces are similar to MATLAB’s build-in gmres.

For the Python interface, hifir4py offers two sets of interfaces: an intermediate-level interface consistent with the C++ version implemented using Cython [7], and a high-level interface consistent with the MATLAB version with support for SciPy sparse matrices [77].

6 ILLUSTRATIONS OF HIFIR FOR VARIOUS APPLICATIONS

For HIFIR and its predecessor HILUCSI, we have reported extensive comparisons with some prior state-of-the-art preconditioners [20, 21, 48, 49]: In [20], we compared HILUCSI with supernodal ILUTP in SuperLU [56, 57] and multilevel ILU in ILUPACK [15] for indefinite systems; in [21], we compared HILUCSI with some customized preconditioners (including pressure convection diffusion (PCD) [51, 74], least-squares commutator (LSC) [28], and modified augmented Lagrangian preconditioner [9, 62]) in Newton-GMRES method for solving the stationary incompressible Navier–Stokes equations; in [49], we compared HILUCSI with ILU(0) [70] and BoomerAMG in hypre [45] as building blocks for several block preconditioners for solving time-dependent advection-diffusion equations with high-order finite element and finite difference discretizations and fully implicit multistage Runge–Kutta schemes; in [48], we compared HIFIR with RIF-preconditioned LSMR [12, 30] and implicitly restarted Lanczos bidiagonlization [4] for computing null-space vectors and for solving inconsistent singular systems. In this section, we illustrate HIFIR for some of these applications, using some of the aforementioned state-of-the-art techniques as points of reference. We conducted our tests on a single node of a cluster running CentOS 7.4 with dual 2.5 GHz 12-core Intel Xeon E5-2680v3 processors and 64 GB of RAM. We compiled HIFIR by GCC with optimization options -O3 and -ffast-math. For all the tests, we used right-preconditioned GMRES with restart [70, Section 9.3.2], and the dimension of KSP space is limited to 30, i.e., GMRES(30).

6.1 Helmholtz equation

As the first illustration, we solved the Helmholtz equation over $\Omega = [0, 1]^3$

$$-\Delta u - k^2 u = f$$

(22)

with Dirichlet boundary conditions $u = u_D$ on $\partial \Omega$, where $k > 0$ is the wave number and $f$ is a source term. Such systems are notoriously difficult to solve for large wave numbers [29]. We discretized the equation using the Galerkin finite element methods (FEM) with quadratic tetrahedral (aka $P_2$) elements, which we implemented using FEniCS v2019.1.0 [1, 58]. We constructed the right-hand side and the boundary conditions using the method of manufactured solutions with the exact solution $u(x, y, z) = \cos(\pi x) \sin(\pi y) \sin(\pi z)$. Given a consistent numerical discretization method for (22), we arrive at the following system of equations

$$\left(K - k^2 M\right) u_h = f_h,$$

(23)

where $K$ and $M$ are the stiffness and mass matrices, respectively, and $u_h$ and $f_h$ are vectors containing nodal values of $u$ and $f$, respectively. Note that $K$ and $M$ are (symmetric) positive definite, but the coefficient matrix $K - k^2 M$ can be positive definite, indefinite, or even singular. We chose three different wave numbers, $k = 1, 5,$ and $10$. The first two resulted in positive-definite systems, and the third resulted in indefinite systems.
Table 2. Results for systems arising from the Helmholtz equation discretized by $P_2$ FEM, solved using GMRES(30) with HIF compared to with supernodal ILUTP in SuperLU and ILUTP in WSMP as the right preconditioner. The condition numbers were estimated using condest function in MATLAB. Times are in seconds. Leaders are in boldface.

| mesh  | $n$   | nnz         | $k$ | cond. | HIF | supernodal ILUTP | WSMP/ILUTP |
|-------|-------|-------------|-----|-------|-----|------------------|------------|
|       |       |             |     |       | fac. | tot. | time | iter. | fac. | tot. | time | iter. | fac. | tot. | time | iter. | fac. | tot. | time | iter. |
| coarse| 132,651| 3,195,529   | 1   | $8.8e4$| 3.15 | 3.46 | 8    | 20.2 | 21.1 | 11   | 2.25 | 2.91 | 23   |      |      |      |      |      |
|       | 5     | 6.4e5       | 2   | $2.4e5$| 9.82 | 9.62 | 8    | 115  | 117  | 12   | 7.85 | 10.8 | 30   |      |      |      |      |      |
|       | 10    | 6.5e5       | 2   | $2.4e5$| 8.9  | 10.7 | 16   | 116  | 120  | 24   | 7.9  | 25.1 | 192  |      |      |      |      |      |
| medium| 357,911| 9,070,749   | 1   | $7.4e5$| 30.1 | 34.1 | 11   | 918  | 944  | 16   | 35.4 | 47.9 | 37   |      |      |      |      |      |
|       | 5     | 5.4e6       | 2   | $7.4e5$| 29.8 | 33.8 | 11   | 903  | 941  | 15   | 35.5 | 46.1 | 32   |      |      |      |      |      |
|       | 10    | 5.5e6       | 2   | $7.4e5$| 29.8 | 35.5 | 16   | 903  | 954  | 20   | 35.1 | 77.4 | 141  |      |      |      |      |      |

To assess the effectiveness of HIF, we assembled three systems using meshes with 93,750, 257,250, and 795,906 quadratic elements, respectively. We solved the systems using $rtol = 10^{-6}$ GMRES(30) and $\tau = 10^{-2}$, $\kappa = 5$, and $\alpha = 3$ for double-precision HIF. For each of these systems, HIF ended up producing a four-level factorization with $mnz$ ratios (i.e., the number of nonzeros in the preconditioner versus that in the input matrix) of about 2.7. As points of reference, we also solved the systems using GMRES(30) with the supernodal ILUTP in SuperLU v5.2.2 [56, 57] and ILUTP in WSMP v20.12 [37, 39] as the right preconditioners with $droptol = 10^{-2}$. As can be seen from Table 2, HIF was the fastest for seven out of nine cases, and WSMP was the fastest for two small cases. SuperLU was substantially slower than both HIF and WSMP. Nevertheless, SuperLU was relatively insensitive to the wave numbers in terms of factorization and total times, as was HIF. In contrast, WSMP had a significant increase in the solve times for $k = 10$, indicating that ILUTP in WSMP is less optimized for indefinite systems than for positive-definite systems. In addition, the computational cost of WSMP increased at a faster rate than HIF as the problem size increased. As a result, HIF was about a factor of 2.2 faster than WSMP for $k = 10$ on the finest mesh. The better performance of HIF was mostly due to its scalability-oriented dropping. It is worth noting that WSMP supports parallel ILUTP and all of our comparisons were conducted in serial. Parallel ILUTP in WSMP may potentially outperform HIF on a multicore computer, but parallel ILUTP is less robust than serial ILUTP in WSMP and caused GMRES to stagnate for larger systems in our tests.

6.2 Linear elasticity with pure traction boundary conditions

In this illustration, we considered the linear-elasticity model of a solid body $\Omega \subset \mathbb{R}^3$,

$$-\nabla \cdot \sigma = f,$$  \hspace{1cm} (24)

where $\sigma$ and $f$ are Cauchy stress tensor and body force per unit volume, respectively. For isotropic material, $\sigma = \lambda (\nabla \cdot u) I + \mu (\nabla u + (\nabla u)^T)$, where $u$ is the displacement, and $\lambda$ and $\mu$ are Lamé’s parameters. We applied pure traction (aka Neumann) boundary conditions to (24), i.e.,

$$\sigma \cdot n = t \quad \text{on } \partial \Omega,$$  \hspace{1cm} (25)

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where \( n \) and \( t \) are unit outward surface normal and surface traction, respectively. Discretizing (24) and (25) using a Galerkin FEM leads to a singular system

\[
K u_h = f_h,
\]

(26)

where the stiffness matrix \( K \in \mathbb{R}^{n \times n} \) is symmetric positive semidefinite (SPSD), and \( u_h \) and \( f_h \) contain nodal values of \( u \) and \( f \), respectively. The continuum equation is invariant to translation and rotation, so the null space of (26) is six dimensional. As in [52], we constructed the solid domain \( \Omega \) by first rotating a box \([-1/4, 1/4] \times [-1/2, 1/2] \times [-1/8, 1/8]\) around \( x \)-, \( y \)-, and \( z \)-axes by \( \pi/2 \), \( \pi/4 \), \( \pi/5 \) in that order and then by translating it by \([0.1, 0.2, 0.3]^T\). We discretized the domain using three linear tetrahedral meshes with 24,576, 196,608, and 2,058,000 \( P_1 \) elements, respectively. We computed the body force \( f \) and surface traction \( h \) using the manufactured solution \( u(x, y, z) = \frac{1}{4}(\sin(\frac{\pi}{4} x), z^3, -y) \).

Due to discretization errors, the resulting linear system (26) may be inconsistent, which poses significant challenges for computing a stable solution for \( u_h \). Note that the nullspace of \( K \) corresponds the rigid-body motion, of which an orthonormal basis may be computed analytically if the mesh and the finite-element basis functions are known; see e.g., [52]. However, an algebraic solver should be able to compute the nullspace from the matrix directly, for example, when the solver does not have access to the mesh or the basis functions.

To solve the inconsistent system, we use the solver PIPIT (or PseudoInverse solver via Preconditioned Iterations) [48], which is based on HIFIR and is composed of three steps:

1. Compute orthonormal basis \( V \in \mathbb{R}^{n \times 6} \) of \( N(K^T) = N(K) \) for \( K \) in (26) using HIFIR-preconditioned FGMRES.
2. Find a least-squares solution \( u_{LS} \) of the consistent system \( Ku_{LS} = (I - VV^T)f_h \) using HIF-preconditioned GMRES.
3. Obtain the pseudoinverse solution \( u_{PI} \) via orthogonal projection, i.e., \( u_{PI} = (I - VV^T)u_{LS} \).

All three steps reuse the same incomplete factorization. We refer readers to [48] for more detail. If the nullspace is known \textit{a priori}, such as in [52], then Step 1 can be omitted. When computing the null-space vectors, we used FGMRES(30) with Householder QR for the Arnoldi process and terminated when the Hessenberg matrix became ill-conditioned. We used the default parameters (see Section 5.2) for HIFIR except that rtol was set to \( 10^{-10} \) in step 2. For these meshes, HIF ended up having three, four, and five levels with nnz ratios 8.84, 10.4, and 10.7, respectively. Table 3 summarizes the timing results of PIPIT for these singular systems. As a point of reference, we used LSMR [30] preconditioned with RIF [12]. Since LSMR did not converge in our test without a preconditioner and a preconditioned LSMR can only compute a least-squares solution, we compare the computational cost of PIPIT for computing a least-squares solution (i.e., the factorization cost of HIF and step 2 of PIPIT) with RIF+LSMR. It can be seen that PIPIT was more than an order of magnitude more efficient than RIF+LSMR for the small and medium meshes. For the large mesh, RIF+LSMR failed to converge to the desired precision after 10,000 iterations. In addition, Table 3 also shows the runtimes for step 1 of PIPIT, which were comparable to solving for \( u_{LS} \) since the same HIF preconditioner was reused. In addition, we report the accuracy of the first (\( v_1 \)) and sixth (\( v_6 \)) null-space vectors as examples, both of which converted to (near) machine precision. Note that for RIF+LSMR to compute \( u_{PI} \) instead of \( u_{LS} \), it would also need to compute the null-space vectors, presumably using preconditioned LSMR [30], which could not converge at least for the largest system.

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Table 3. Results for singular systems arising from linear elasticity with pure traction boundary conditions using \( P_1 \) finite elements. We compare the costs of step 2 of PIPIT with RIF+LSMR, where leaders are in boldface and ‘−’ indicated non-convergence after 10,000 iterations. The last three columns show the cost and accuracy of null-space computations in step 1 of PIPIT. Times are in seconds.

| mesh   | \( n \)    | nnz       | PIPIT for \( u_{LS} \) | RIF+LSMR for \( u_{LS} \) | null-space computation |
|--------|------------|-----------|-------------------------|-----------------------------|------------------------|
|        | fac. time | tot. time | iter. | fac. time | tot. time | iter. | time | \( \| K_{U_1} \| / \| K \| \) | \( \| K_{U_2} \| / \| K \| \) |
| coarse | 15,147    | 610,929   | 3.5 | 3.82 | 15 | 12.5 | 30.5 | 2,588 | 3.01 | 7e-16 | 3e-14 |
| medium | 109,395   | 4,652,505 | 39.4 | 44  | 35 | 308  | 741  | 8,673 | 126  | 3e-15 | 4e-16 |
| fine   | 1,081,188 | 47,392,074 | 511 | 700 | 152 | −    | −    | −    | 3.1e3 | 4e-15 | 6e-16 |

6.3 Stationary incompressible Navier–Stokes equations

As a third illustration, we solve the incompressible Navier–Stokes (INS) equations for modeling fluids. We consider the INS equations with normalized density on a domain \( \Omega \subset \mathbb{R}^3 \), which read

\[
\begin{align*}
\dot{u}_t - \nu \Delta u + u \cdot \nabla u + \nabla p &= g, \\
\nabla \cdot u &= 0,
\end{align*}
\]

where \( u \) and \( p \) are velocities and pressure, respectively, \( \nu \) is the kinetic viscosity, and the subscript \( t \) denotes the temporal derivative. After dropping off the temporal-derivative term, we arrive at the stationary INS, for which the momentum equation (27) becomes

\[
- \nu \Delta u + u \cdot \nabla u + \nabla p = g.
\]

When integrating (27) in time, (29) is equivalent to having the time step equal to infinity. We discretize the INS in space using the \( P_2-P_1 \) Taylor–Hood (TH) elements [76], which leads to a system of nonlinear systems of equations. We then solve it using Newton-GMRES, an inexact Newton method [24] that uses the preconditioned GMRES in the inner iterations of Newton’s method. At iteration \( k \), Newton’s method solves a linear problem

\[
J_k \begin{bmatrix} \delta u_k \\ \delta p_k \end{bmatrix} = J_k \begin{bmatrix} f_k \\ y_k \end{bmatrix},
\]

where \( K, E, C_k, \) and \( W_k \) correspond to \( \nu \Delta u, \nabla \cdot \delta u, u_k \cdot \nabla u, \) and \( \delta u \cdot \nabla u_k \), respectively, and \( \delta u_k \) and \( \delta p_k \) denote increments in velocity and pressure, respectively. Since \( J_k \) is fairly dense in Newton’s method, we constructed a “sparsifier” \( B_k \) by omitting \( W_k \) when building the preconditioner. For robustness, we start with Picard iterations, which uses \( B_k \) in place of \( J_k \) at each Newton’s step, and then switch to Newton’s iterations once the solution is sufficiently accurate. For the initial guess \( \begin{bmatrix} u_0, p_0 \end{bmatrix}^T \), we obtained it by solving the corresponding Stokes equation, i.e., \(- \nu \Delta u + \nabla p = g\). For more details, see [21].

As a demonstration, we solved the 3D flow-over-cylinder benchmark problem [73], where a cylinder of diameter \( D = 0.1 \) is placed in a channel of length 2.5 with square cross-sections of height \( H = 0.41 \). The inflow boundary condition is imposed on the left side of a box, which reads \( u_{in} = (U(y, z), 0, 0) \), where \( U(y, z) = 16 \times 0.45 yz(H - y)(H - z)/H^4 \). A “do-nothing” velocity is imposed for the outflow (right face) along with a zero pressure. The rest boundaries are no-slip walls. The kinetic viscosity was \( \nu = 1 \times 10^{-3} \), so the Reynolds number is \( Re = 4 \times 0.45 D/(9 \nu) = 20 \). We generated three sets of unstructured tetrahedral meshes using Gmsh [32], with 71,031, 268,814, and 930,248 elements, respectively. Figure 5 shows a coarse sample mesh along with the computed speed. We assembled the matrices \( J_k \) and \( B_k \) using our in-house FEM code. Table 4 shows the performance of HIF+GMRES(30) for a representative Newton step, with \( rtol = 10^{-6} \) in GMRES and \( \tau = 10^{-2} \), \( \kappa = 5 \), and \( \alpha = 3 \) for HIF. As a point of reference, we solved the same systems...
Fig. 5. Cut-off view of the speed for the 3D flow-over-cylinder problem with a coarse sample mesh.

Table 4. Results for stationary INS with TH elements in one representative Newton’s step solved by GMRES(3) preconditioned by HIF on the sparsifier $B_k$ in comparison with ILUPACK. ‘×’ indicates out of memory. Times are in seconds. Leaders are in boldface.

| mesh      | $n$    | nnz($J_k$) | nnz($B_k$) | HIF-GMRES(30) | ILUPACK-GMRES(30) |
|-----------|--------|------------|------------|----------------|-------------------|
|           |        |            |            | nnz rat. | fac. time | tot. time | iter. | nnz rat. | fac. time | tot. time | iter. |
| coarse    | 262,912| 21,870,739 | 9,902,533  | 3.47     | 20.3     | 22.6     | 17    | 8.34     | 130       | 133       | 11    |
| medium    | 1,086,263| 98,205,997 | 43,686,979 | 3.4     | 106      | 124      | 33    | 13.4     | 1,92e3    | 1,94e3    | 14    |
| fine      | 3,738,327| 343,357,455| 152,438,721| 3.47    | 442      | 586      | 68    | ×        | ×         | ×        | ×     |

using ILUPACK [15] with droptol = $10^{-2}$ and other default parameters. As we can see, HIF-preconditioned GMRES performed consistently well, even for the finest mesh. Its overall performance was faster than ILUPACK by a factor about six and 16 for the coarse and intermediate-level meshes, although ILUPACK used fewer GMRES iterations. More importantly, ILUPACK ran out of the 64 GB main memory for the largest problem. In [21], we also compared HIF with the direct solve MUMPS [3], which also ran out of memory for the largest case as ILUPACK, and with ILU(1) and ILU(2), for which GMRES failed to converge.

6.4 Advection-diffusion equation with fully implicit Runge–Kutta schemes

As our final illustration, we consider the time-dependent advection-diffusion (AD) equation for $u$: $\Omega \times [0, T] \rightarrow \mathbb{R}$,

$$u_t - \mu \Delta u + v \cdot \nabla u = f,$$

(31)

where $\mu \geq 0$ is the diffusion coefficient, $v$ is a divergence-free velocity field, and $f$ is some source term. As a demonstration, we chose $\Omega = [0, 1]^3$ and computed $f$ and the Dirichlet boundary conditions from the manufactured solution $u(x, y, z, t) = \sin(1.5 \pi t) \sin(\pi x) \sin(\pi y) \sin(\pi z)$. We used the fourth and sixth-order finite difference method (FDM) to discretize (31), leading to the semi-discretization form

$$u_t(t) = Ju(t) + f(t),$$

(32)

where $J \in \mathbb{R}^{n \times n}$ denotes the Jacobian matrix corresponding to the operator $(\mu \Delta - v \cdot \nabla)$. Eq. (32) is a system of stiff ordinary differential equations (ODEs) and can be integrated using high-order fully implicit Runge–Kutta (FIRK) schemes, such as $s$-stage Gauss–Legendre schemes, which are $2s$-order accurate and are unconditionally stable. A Runge–Kutta scheme can be expressed by the Butcher tableau $\begin{bmatrix} c \vert A \end{bmatrix} b^T$, where $A \in \mathbb{R}^{s \times s}$, $c \in \mathbb{R}^s$, and $b \in \mathbb{R}^s$ [17].

Given a time step $\delta t$, Eq. (32) leads to an $sn \times sn$ linear system

$$AK = B \quad \text{with} \quad A = I_{sn} - \delta t A \otimes J.$$

(33)
where $I_m$ denotes the $m$-dimension identity matrix, $\otimes$ denotes the Kronecker-product operator, $A \in \mathbb{R}^{m \times m}$, $B \in \mathbb{R}^{m}$, and $K \in \mathbb{R}^{m}$. We refer readers to [49] for more details.

To assess HIF for complex-valued matrices, we use an optimal preconditioner, called block CSD or BCSD, developed in [49]. BCSD is based on the complex Schur decomposition (CSD) of the Butcher matrix $A$ (i.e., $A = QUQ^H$, where $Q \in \mathbb{C}^{n \times n}$ is unitary and $U \in \mathbb{C}^{n \times n}$ is upper triangular), and it reads

$$M = (Q \otimes I_n)(U \otimes I_n)$$

with $U = I_{sn} - \delta U \otimes J$. \hspace{1cm} (34)

$M$ is optimal in that $AM^{-1} = I_{sn}$, where $M^{-1} = (Q \otimes I_n)U^{-1}(Q^H \otimes I_n)$; see [49] for more details. Note that $U$ in (34) is block upper triangular, so computing $U^{-1}X$ for a vector $X$ only requires (approximately) factorizing the diagonal blocks of $U$, i.e., $M_i = I_n - \delta \lambda_i J \in \mathbb{C}^{n \times n}$ for $i = 1, 2, \ldots, s$, where $\lambda_i \in \mathbb{C}$ are the diagonal entries of $U$, which are the eigenvalues of $A$. For Gauss–Legendre schemes, there are $\lfloor \frac{s}{2} \rfloor$ distinct conjugate pairs of complex eigenvalues of $A$, and given $M_i \in \mathbb{C}^{n \times n}$, $y = M_i^{-1}x \Rightarrow \bar{y} = M_i^{-1}\bar{x}$. Hence, we only need to factorize $\lfloor \frac{s}{2} \rfloor$ distinct complex-valued diagonal blocks for BCSD. We constructed the blocks in the Jacobian matrices $J$ in (32) using our in-house high-order FDM code on equidistant structured grids with grid sizes $h = 1/32, 1/64, 1/128$ and a velocity field $v = [1, 1, 1]^T$. We factorized $M_i$ using double-precision complex HIF with parameters $\tau = 10^{-3}$, $\kappa = 5$, and $\alpha = 5$. With these parameters, HIF ended up producing three to four levels. Table 5 shows the performance of HIF-based BCSD preconditioner for the two- and four-stage Gauss–Legendre schemes for the first time step with $\delta t = 1/8$. As a point of reference, Table 5 also reports the results using MATLAB’s built-in (precompiled) ilu function without fills (aka ILU(0)) with preprocessing steps (including equilibration [26] and fill-reduction reordering [19]). We chose ILU(0) as a baseline since it is commonly used in the literature for the diagonal blocks [50, 65]. It can be seen HIF was significantly faster than ILU(0) overall, although ILU(0) was more efficient in terms of factorization cost. In addition, BCSD with ILU(0) failed to converge for the largest case. In [49], we also compared HIF with BoomerAMG in hypre v2.21.0 [45] for some real-valued block preconditioners, and HIF was about a factor of eight faster than BoomerAMG for larger problems. We do not compare BoomerAMG for BCSD, since hypre does not yet support complex arithmetic.

7 CONCLUSION AND FUTURE WORK

In this work, we introduced a software package, HIFIR, for preconditioning GMRES and FGMRES for solving unsymmetric sparse linear systems. Unlike previous software packages, HIFIR is designed to solve singular and near-singular (aka...
ill-conditioned) systems, including finding least-squares solutions for consistent singular systems, null-space vectors of singular matrices, and pseudoinverse solutions for inconsistent systems. This unique feature is backed by a new theory of $\varepsilon$-accurate AGI, and a new algorithm that combines multilevel incomplete LU factorization with an RRQR on the final Schur complement. Compared to its predecessor HILUCSI, HIFIR also introduces an algorithmic innovation, namely IBRR, which improves the robustness and significantly reduces the size of the final Schur complement for some systems. HIFIR was implemented in C++, with user-friendly high-level interfaces for MATLAB and Python in hifir4m and hifir4py, respectively. We have released them as open-source software. We described the software design of HIFIR in terms of its efficient data structures and its template-based generic programming interfaces for mixed-precision real and complex values. We also demonstrated the effectiveness of HIFIR for ill-conditioned or singular systems arising from several applications, including the Helmholtz equation, linear elasticity, incompressible Navier–Stokes equations, and advection-diffusion equation. As presented in this work, HIFIR was serial. However, it can be used as the computational kernel in a domain-decomposition preconditioner [75] by factorizing the diagonal blocks within each processor. In addition, we are presently developing a multi-threaded implementation with the option of applying the multilevel solver and multilevel matrix-vector multiplication on GPUs, which we plan to release in the future.

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A FLEXIBLE ARRAY-BASED SPARSE MATRIX DATA STRUCTURE

We describe a flexible, three-tiered, array-based (instead of pointer-based) sparse matrix data structure to support fan-in updates, deferring, and rook pivoting, respectively. We focus on the column-oriented version for $L$, the data structure for $U$ uses a corresponding row-oriented version.

A.1 Partially augmented CSC for fan-in updates

We first briefly describe the baseline data structure as in [55], which extends the standard CSC format. Recall that the CSC format has the following three arrays:

- **val**: a floating-point array of size equal to the total number of nonzeros, with nonzeros stored column by column;
- **row_ind**: an integer array of size equal to that of row_ind, storing the row indices in each column;
- **col_start**: an integer array of size $n+1$, storing the starting index of each column in row_ind, where col_start$(k)$ stores the starting position for the $k$th column in row_ind.

To support fan-in update in Algorithm 1, we maintain two additional arrays Lstart and Llist in [55], where Lstart is a size-$n$ integer array storing the first entry in each column of $L$ whose row index is no smaller than $k$ at the $k$th step, and Llist is a size-$n$ array-based linked list storing the index of each column that has a nonzero entry in $\ell^T_k$. The combination of Lstart and Llist allows efficient access of the $k$th row in $L$. We refer to this baseline data structure as partially augmenter CSC (PACSC). The data structure for $U$ uses the counterpart PACSR, which partially augments CSR.

A.2 Partially augmented CSC with gaps

PACSC is memory efficient, but it does not support permutations, such as static or dynamic deferring. To support static and dynamic deferring, we extend the data structure to allow a “gap” of size $d$ between $L_B$ and $L_E$ if there have been $d$ deferrals. We maintain the gap as follows. At the $k$th step, suppose there have been $d - 1$ deferrals in the preceding steps. Before performing computation on the $k$th row, we first move $\ell^T_{k+d-1}$ to $\ell^T_k$ in $L$ to eliminate the gap. If row $k$ needs to be deferred, we directly move the row from $\ell^T_{k+d-1}$ to row $\ell^T_{n+d}$ in $L$, which increases the gap to $d$. Figure 6 illustrates these operations. To avoid dynamic expansion of the arrays, we pre-allocate the CSC storage to allow up to $2n$ rows, and also enlarge Llist and Ulist to size $2n$. At the end of ilu_factorize, we eliminate the gap by moving $L_{n+1} + d: n+d$ to $L_{n+1}$. We refer to the above data structure as PACSC-G; the data structure for $U$ uses the corresponding PACSR-G. It is worth noting that in Algorithm 1, row $i$ in $L$ for $i \geq k$ refers to row $i + d$ in PACSC-G, and similarly, column $j$ in $U$ for $j \geq k$ refers to column $j + d$ in PACSR-G. Note that ILUPACK [15] also extended CSC to support deferring, but we could not find its implementation details in its documentation for comparison.

A.3 Fully augmented CSC for rook pivoting

To support row interchanges of $L$ in rook pivoting, we need to access its $i$th row for $k \leq i \leq n_1$. The PACSC (with or without gap) is insufficient for this purpose. To support rook pivoting, we need to access any row in $L_{k,n,1:k}$ and any column in $U_{1:k,k:n}$. To support this, we replace the Lstart and Llist arrays in PACSC with the following additional arrays, analogous to those in the CSR (Compressed Sparse Row) format:

- **val_pos**: an integer array of size equal to the total number of nonzeros, storing the indices of the nonzeros in the val array in the underlying CSC format;
- **inv_val_pos**: an integer array storing the inverse mapping of val_pos.
- **col_ind**: an integer array of size equal to that of val_pos, storing the column indices within val_pos in each row;
\begin{itemize}
  
  \item row_start: an integer array of size \( n \), storing the starting index of each row in \( \text{col\_ind} \);
  
  \item row_next: an integer array of the same size as \( \text{col\_ind} \), storing the index in \( \text{col\_ind} \) for the next nonzero in the same row;
  
  \item row_end: an integer array of size \( n \), storing the last index of each row in \( \text{col\_ind} \).
\end{itemize}

We refer to this data structure as the fully augmented CSC (or FACSC). Here, val_pos and inv_val_pos play the same role as val in CSR; we introduced them to avoid duplicating the numerical values. col_ind and row_start play the same roles as their respective counterparts in CSR. The arrays row_next and row_end essentially maintain Llist for all rows in \( L_{k,n;1:k} \) instead of for just the \( k \)th row. When interchanging rows \( i \) and \( r \) in \( L \) during pivoting, besides updating val and row_ind in CSC, we need to swap row_start \((i)\) and row_end \((i)\) with row_start \((r)\) and row_end \((r)\), respectively, while keeping the other arrays intact. The data structure for \( U \) uses FACSR, which fully augments CSR.

\section*{B TIME COMPLEXITY OF INVERSE-BASED ROOK PIVOTING}

We analyze the time complexity for partial row interchanges in \( L \); the analysis for column interchanges in \( U \) is similar. In Algorithm 2, there are three key steps: 1) computing the \( k \)th column vector \( \ell \) (line 2), 2) finding a potential pivot \( r \) (line 3), and 3) interchanging the \( k \)th and \( r \)th rows in \( L \) (line 5). The total number of floating-point operations in computing \( \ell \) is bounded by \( O \left( \text{nnz} \left( \bar{a}_{p_k} \right) + \sum_{i \in \text{nnz}(u_k)} \text{nnz} \left( L_{k+1:n,n,i} \right) \right) \). Under the assumption that the averaged number of nonzeros per row and column in the input is a constant (say, bounded by \( C \)), the scalability-oriented dropping ensures that this cost is also bounded by a constant (proportional to \( C^2 \)). The inverse-based constraint in line 3 also introduces extra cost in estimating the inverse norm. A brute-force implementation leads to \( O \left( \sum_{i \in \text{nnz}(\ell)} \text{nnz} \left( \ell_i \right) \right) \) cost in the worst case, which can be improved to \( O \left( \text{nnz} \left( \bar{\ell} \right) \log \left( \text{nnz} \left( \bar{\ell} \right) + \text{nnz} \left( \ell_i \right) \right) \right) \) if we sort \( \ell \) first and then estimate the inverse norm only once. Finally, with the FACSC data structure, interchanging the \( k \)th row and the \( r \)th row in \( L \) can be done in \( O(1) \) (or more precisely, \( O(C^2) \)) operations. Therefore, the time complexity is bounded by constant per row interchange in rook pivoting. Since we limit the maximum number of row and column interchanges in rook pivoting by a constant, the total operations in rook pivoting is no greater than that of the fan-in update in ILU, and hence rook pivoting does not increase the overall time complexity.