

HILUCSI: Simple, Robust, and Fast Multilevel ILU with Mixed Symmetric and Unsymmetric Processing

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Abstract

Incomplete factorization is a widely used preconditioning technique for Krylov subspace methods for solving large-scale sparse linear systems. Its multilevel variants, such as those in ILUPACK and ARMS, have been shown to be more robust for many symmetric or unsymmetric linear systems than the traditional, single-level incomplete LU (or ILU) techniques. However, multilevel ILU still lacked robustness and efficiency for some large-scale, nearly or partially symmetric, ill-conditioned, or indefinite systems, which often arise from systems of partial differential equations (PDEs). In this work, we address this issue by introducing *HILUCSI*, or Hierarchical Incomplete LU-Crout with Scalability-oriented and Inverse-based dropping. *HILUCSI* differs from the state-of-the-art multilevel ILU in three aspects. First, to strike a balance between robustness and efficiency, *HILUCSI* leverages some proven techniques for symmetric and unsymmetric matrices at the top and lower levels, respectively, for nearly or partially symmetric systems. Second, to simplify the treatment of indefinite systems, *HILUCSI* statically defers tiny diagonal entries to the next level during preprocessing instead of relying on dynamic partial or Bunch-Kauffman pivoting. Third, to improve the effectiveness for large-scale problems from PDEs, *HILUCSI* introduces a scalability-oriented dropping in conjunction with a modified inverse-based dropping. We demonstrate the robustness and efficiency of *HILUCSI* for benchmark problems from a wide range of applications against ILUPACK, the supernodal ILUTP in SuperLU, and multithreaded direct solvers in PARDISO and MUMPS.

1 Introduction

Krylov subspace (KSP) methods, such as GMRES [85, 87] and BiCGSTAB [100], are widely used for solving large-scale sparse unsymmetric or indefinite linear systems, especially those arising from numerical discretizations of partial differential equations (PDEs). For relatively ill-conditioned matrices, the KSP methods can significantly benefit from a robust and efficient preconditioner. Incomplete factorization techniques, such as incomplete LDL^T or Cholesky factorization for M-matrices [75] and symmetric and positive definite (SPD) systems [49, 59, 69, 93] and incomplete LU (or ILU) factorization for symmetric indefinite [63, 91] and unsymmetric [67, 71, 82] systems, are among the most robust preconditioners. Earlier ILU methods, such as ILUT [82], ILUP [81], ILUTP [29, 85], ILUC [63, 64, 71], etc., lacked robustness for many indefinite systems; see e.g. [29, 42, 46, 67, 110] for some challenging benchmark problems that caused failures. With the more recent development of multilevel ILU techniques, such as ARMS [86, 88], ILUPACK [20, 22], MDRILU [109], ILU++ [73, 74], etc., the robustness of ILU has improved significantly for many applications. However, robustness and efficiency are sometimes problematic for highly ill-conditioned or saddle-point systems, which often arise from discretizations of PDEs, such as Stokes, Navier-Stokes, and Helmholtz equations, in application areas such as computational fluid dynamics (CFD), climate modeling, materials science, structural mechanics, multiphysics coupling, etc.; see e.g. [86] and Section 5 in this work for some examples. The objective of this work is to improve the robustness and efficiency of multilevel ILU for such systems. To this end, we introduce a new preconditioner, called *HILUCSI* (pronounced as Hi-Luxi), which stands for Hierarchical Incomplete LU-Crout with Scalability-oriented and Inverse-based dropping.

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The development of HILUCSI was motivated by two observations. First, many linear systems from systems of PDEs are often *nearly* or *partially symmetric*, with some block structures. Without loss of generality, we assume the matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ has the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{B} & \mathbf{F} \\ \mathbf{E} & \mathbf{C} \end{bmatrix}, \quad (1.1)$$

where $\mathbf{B} \in \mathbb{R}^{n_1 \times n_1}$. By *near symmetry*, we mean that \mathbf{A} has a nearly symmetric nonzero pattern, and $\|\mathbf{A} - \mathbf{A}^T\| \ll \|\mathbf{A}\|$. This (near) pattern symmetry is intrinsic to some numerical methods, such as finite differences [62], finite elements [30, 41], or finite volumes [61], because the local support of the basis functions (a.k.a. trial functions in finite elements) and that of the test functions in the variational formulations are typically the same or have significant overlaps. The numerical asymmetry in these cases tends to be small when it is due to small non-self-adjoint terms (such as advection in a diffusion-dominant advection-diffusion problem [41, p. 243]) or due to truncation errors (such as in a Petrov-Galerkin method for a self-adjoint PDE [41, p. 88]). By *partial symmetry*, we mean that \mathbf{B} is nearly symmetric, although \mathbf{E} and \mathbf{F}^T may differ significantly. The strong asymmetry between \mathbf{E} and \mathbf{F} may be due to strongly imposed constraints in a variational formulation [40], high-order treatment of Neumann boundary conditions in finite elements [16] or finite differences [62], imposition of jump conditions in immersed/embedded boundary methods [58, 78], or a system of PDEs with mixed self-adjoint and non-self-adjoint subsystems (such as in a monolithically coupled fluid-structure interaction system [57]).

The second observation was that it is *sometimes* advantageous to treat a fully symmetric system as unsymmetric, especially for some indefinite systems. This claim seems to contradict the conventional wisdom that “it is rarely sensible to throw away symmetry in preconditioning” [106]. Indeed, some state-of-the-art packages for symmetric indefinite systems always try to preserve symmetry and use some variant of the Bunch-Kauffman pivoting [26, 47]; see e.g. [48, 63, 91, 92]. Such pivoting strategies require a mixture of 1×1 and 2×2 blocks, which not only complicate the implementation but also are sometimes less effective than unsymmetric ILU in avoiding small pivots. At the same time, the conventional wisdom is also sound in that leveraging symmetry can reduce the computational cost by nearly half for some problems, but may improve robustness, which we observe for some linear systems matrices from systems of PDEs. A novel feature of HILUCSI is to apply symmetric preprocessing at the top levels for nearly or partially symmetric matrices but unsymmetric factorization at lower levels for all indefinite systems, including symmetric indefinite systems. In addition, HILUCSI introduces a static deferring strategy for (nearly) symmetric saddle-point problems, which eliminates the need for 2×2 pivots for stability.

Due to the numerous applications of nearly or partially symmetric and indefinite systems, there have been significant interests in solving such systems in linear algebra, numerical PDE, and engineering communities. Many recent problems in the SuiteSparse Matrix Collections [33] and Matrix Market [17] belong to these classes, including some of the cases highlighted in [29, 67, 74, 86, 110]. To address these challenging problems, the PDE and multigrid communities have developed some customized preconditioners and solvers for specific equations; see [1, 2] for examples of special multigrid solvers and see [14] for a survey on special techniques for saddle-point problems. In terms of general-purpose solvers, a common practice is to treat such systems as general unsymmetric systems, such as in ARMS [88], ILU++ [73], supernodal ILUTP in SuperLU [67], etc. We note two exceptions. First, one may build a symmetric preconditioner for an unsymmetric \mathbf{A} , such as using $(\mathbf{A} + \mathbf{A}^T)/2$ in an algebraic preconditioner [32, 107] or using the self-adjoint terms in a physics-based preconditioner [3]. However, the symmetric part may not approximate \mathbf{A} accurately for some applications, and factorization of $(\mathbf{A} + \mathbf{A}^T)/2$ may break down for partially symmetric systems, for example, if $\mathbf{E} = -\mathbf{F}^T$ and $\mathbf{C} = \mathbf{0}$ in (1.1) as in the unsymmetric positive-definite variant of symmetric saddle-point problems [14]. Second, for a partially symmetric matrix where \mathbf{B} is symmetric but $\mathbf{E} \neq \mathbf{F}^T$ in (1.1), one may factorize \mathbf{B} using a symmetric ILU and then apply unsymmetric ILU on the Schur complement [14]. However, this approach breaks down if \mathbf{B} is singular, which can happen even if \mathbf{A} is well-conditioned [14]. HILUCSI differs from these earlier approaches in that it does not explicitly construct a symmetric approximation of \mathbf{A} , and it does not suffer from potential instabilities associated with factorizing a singular $\mathbf{A} + \mathbf{A}^T$ or \mathbf{B} .

Another novel feature of HILUCSI is its *scalability-oriented dropping* together with *modified inverse-based dropping* in the Crout version of multilevel ILU [22, 64]. Our scalability-oriented dropping shares some similarity to the space-based droppings (such as those in ILUT [82], ICMF [69], PARDISO 6 [92])

as well as area-based dropping in SuperLU [67]. Those space or area-based droppings traditionally focused on controlling space complexity. In contrast, the primary goal of our scalability-oriented dropping is to achieve (near) linear-time complexity in the number of nonzeros in the input matrix. Although linear time complexity implies linear space complexity as a side product, the converse is not true in general. Also, using a pseudo-spectral analysis, we derive a *modified inverse-based dropping* strategy, which is more robust than that of Bollhöfer in [18, 21] and is more efficient than that of Bollhöfer and Saad in [22]. Using a similar analysis, we propose a modification to the inverse-based deferring of Bollhöfer and Saad [22] to control not only the norms of \mathbf{L}^{-1} and \mathbf{U}^{-1} but also that of \mathbf{D}^{-1} . We show that our new dropping strategies along with mixed symmetric and unsymmetric processing enabled superior robustness and efficiency for HILUCSI compared to ILUPACK [20] and SuperLU [67]. In addition, we show that the serial performance of HILUCSI with optimized parameters is competitive with the state-of-the-art multithreaded direct solvers in MUMPS [6] and PARDISO [92] on 24 cores for large systems with more than one million unknowns.

The remainder of the paper is organized as follows. In Section 2, we review some background on incomplete LU factorization and its multilevel variants. In Section 3, we describe the algorithm components of HILUCSI for robustness. In Section 4, we address the efficiency issues with a focus on scalability with respect to problem sizes. In Section 5, we present numerical results with HILUCSI as a right preconditioner for restarted GMRES and compare its performance with some state-of-the-art packages. Finally, Section 6 concludes the paper with a discussion on future work.

2 Background and mathematical foundation

In this section, we review some incomplete LU preconditioners, especially multilevel ILU. Because there is a vast literature on preconditioning and ILU, we focus on only some of the most relevant techniques and mathematical analysis. For comprehensive reviews, we refer readers to some surveys [13, 27, 89, 106] and textbooks [85, 101].

2.1 Incomplete LDU factorizations

ILU, or more precisely *incomplete LDU* (or *ILDU*) *factorization with pivoting*, performs an approximate factorization

$$\mathbf{P}^T \mathbf{A} \mathbf{Q} \approx \mathbf{L} \mathbf{D} \mathbf{U}, \quad (2.1)$$

where \mathbf{L} and \mathbf{U} are unit lower and upper triangular matrices, respectively, and \mathbf{P} and \mathbf{Q} are row and column permutation matrices, which may be obtained from some static reordering, static or dynamic pivoting, or a combination of them. Let $\mathbf{M} = \mathbf{L} \mathbf{D} \mathbf{U}$, and $\mathbf{P} \mathbf{M} \mathbf{Q}^T$ is a *preconditioner* of \mathbf{A} , or equivalently \mathbf{M} is a preconditioner of $\mathbf{P}^T \mathbf{A} \mathbf{Q}$. We consider only right preconditioning in this work. In this context, when solving a linear system $\mathbf{A} \mathbf{x} = \mathbf{b}$ using an iterative method, especially a Krylov subspace method, one solves the right-preconditioned linear system

$$\mathbf{A} \left(\mathbf{P} \mathbf{M} \mathbf{Q}^T \right)^{-1} \mathbf{y} = \mathbf{b}, \quad (2.2)$$

which ideally would converge much faster than solving the original linear system, and then $\mathbf{x} = \left(\mathbf{P} \mathbf{M} \mathbf{Q}^T \right)^{-1} \mathbf{y} = \mathbf{Q} \mathbf{U}^{-1} \mathbf{D}^{-1} \mathbf{L}^{-1} \mathbf{P}^T \mathbf{y}$.

2.1.1 Single-level ILU

We refer to the ILU with the basic form in (2.1) as a *single-level ILU*. Such a technique has been used to solve linear systems from PDEs since 1950s; see e.g. [104]. In 1977, Meijerink and van der Vorst [75] showed that incomplete Cholesky (IC) factorization is stable for a symmetric M-matrix, i.e., a matrix with nonpositive off-diagonal entries and nonnegative entries in its inverse. Since then, IC has been extended to and become popular for SPD systems [49, 59, 69, 93]. However, ILU for unsymmetric or indefinite systems had turned out to be much more challenging, and it has been an active research topic over the past few decades; see e.g. [7, 19, 22, 29, 28, 72, 67, 82, 86].

In its simplest form, ILU does not involve any pivoting, and \mathbf{L} and \mathbf{U} preserve the sparsity patterns of the lower and upper triangular parts of $\mathbf{P}^T \mathbf{A} \mathbf{Q}$, respectively. This approach is often referred to as *ILU0*

or $ILU(0)$. To improve its robustness, one may allow *fills*, a.k.a. *fill-ins*, which are new nonzeros in the \mathbf{L} and \mathbf{U} factors. The fills may be introduced based on their levels in the elimination tree or based on the magnitude of numerical values. The former leads to the so-called $ILU(k)$, which zeros out all the fills of level $k + 1$ or higher in the elimination tree. The combination of the two is known as *ILU with dual thresholding* ($ILUT$) [82]. The level-based fills may be replaced with some other dropping to control the numbers of fills in each row or column. The ILU implementations in PETSc [9] and hypre [96] use some variants of ILUT with dual thresholding.

ILUT may encounter zero or tiny pivots, which can lead to a breakdown of the factorization. One may replace tiny pivots with a small value, but such a trick is not robust [29]. The robustness may be improved by using pivoting, leading to the so-called $ILUP$ [81] and $ILUTP$ [85]. The ILU implementations in MATLAB [97], SPARSKIT [83], and SuperLU [67], for example, are based on ILUTP. However, ILUTP cannot prevent small pivots [86], so it is still not robust in practice; see [67, 74, 86] and Section 5 in this work for some failed cases with ILUTP.

2.1.2 Multilevel ILU

A more sophisticated form of ILU takes advantage of the global block structure of \mathbf{A} similar to that in (1.1) to compute a block factorization of \mathbf{B} . Specifically, let \mathbf{P} and \mathbf{Q} denote the row and column permutation matrices. A block-structured preconditioner $\hat{\mathbf{M}}$ for the permuted matrix $\mathbf{P}^T \mathbf{A} \mathbf{Q}$ can be constructed via the approximation

$$\mathbf{P}^T \mathbf{A} \mathbf{Q} = \begin{bmatrix} \hat{\mathbf{B}} & \hat{\mathbf{F}} \\ \hat{\mathbf{E}} & \hat{\mathbf{C}} \end{bmatrix} \approx \hat{\mathbf{M}} = \begin{bmatrix} \tilde{\mathbf{B}} & \tilde{\mathbf{F}} \\ \tilde{\mathbf{E}} & \tilde{\mathbf{C}} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_B & \mathbf{0} \\ \mathbf{L}_E & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{D}_B & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_C \end{bmatrix} \begin{bmatrix} \mathbf{U}_B & \mathbf{U}_F \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \quad (2.3)$$

where $\hat{\mathbf{B}} \approx \tilde{\mathbf{B}} = \mathbf{L}_B \mathbf{D}_B \mathbf{U}_B$, $\hat{\mathbf{E}} \approx \tilde{\mathbf{E}} = \mathbf{L}_E \mathbf{D}_B \mathbf{U}_B$, $\hat{\mathbf{F}} \approx \tilde{\mathbf{F}} = \mathbf{L}_B \mathbf{D}_B \mathbf{U}_F$, and $\mathbf{S}_C = \hat{\mathbf{C}} - \mathbf{L}_E \mathbf{D}_B \mathbf{U}_F$ is the *Schur complement*. If \mathbf{S}_C is further approximated recursively using such a block factorization, one obtains a *multilevel ILU* ($MLILU$) [10, 11, 84, 90, 109, 86, 22, 74], also known as *multilevel block factorization* [105].

Given a block vector $\mathbf{u} = \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}$, then $\hat{\mathbf{M}}^{-1} \mathbf{u}$ can be computed as

$$\hat{\mathbf{M}}^{-1} \mathbf{u} = \begin{bmatrix} \tilde{\mathbf{B}}^{-1} \mathbf{u}_1 \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} -\tilde{\mathbf{B}}^{-1} \tilde{\mathbf{F}} \\ \mathbf{I} \end{bmatrix} \mathbf{S}_C^{-1} (\mathbf{u}_2 - \tilde{\mathbf{E}} \tilde{\mathbf{B}}^{-1} \mathbf{u}_1). \quad (2.4)$$

There are several motivations to use multilevel ILU. One of them is to expose parallelism, such as in ILUM and BILUTM [84, 90]. The idea is to permute \mathbf{A} so that $\tilde{\mathbf{B}}$ in (2.3) is a block diagonal matrix, of which each block can then be factorized independently. This approach was inspired by the domain-decomposition (such as additive Schwarz) methods [94], but ILUM factorizes the Schur complement recursively instead of resolving the overlapping regions of subdomains iteratively. Another motivation of multilevel ILU is to construct an algebraic analogy of multigrid methods [80, 108]; see e.g. [10, 11, 12]. However, the fine-coarse grid relationship in multilevel ILU is quite different from the geometric [80, 25] and algebraic multigrid methods [54, 103, 102]. More recently, multilevel ILU has been used successfully in improving the robustness of ILU as a preconditioner; see e.g. [22, 86, 74, 109]. In this work, we strive to improve the robustness of multilevel ILU further along with its efficiency.

2.1.3 Criteria of ILU

When developing ILU methods, one must answer the following question: *what is a good incomplete factorization?* Intuitively, \mathbf{M} in (2.2) or $\hat{\mathbf{M}}$ in (2.3) should be as “close” to $\mathbf{P}^T \mathbf{A} \mathbf{Q}$. However, more precise definitions are needed for analysis and derivations. In the following, we consider the robustness and efficiency issues separately. For simplicity, we will omit \mathbf{P} and \mathbf{Q} in the discussions.

Criteria for stability and accuracy For ILU to be a “robust” preconditioner, it should be accurate and stable. In [29], Chow and Saad consider these issues from an algorithmic point of view. Most notably, they emphasized the importance of avoiding small pivots. In [18], Bollhöfer pointed out the importance of monitoring \mathbf{L}^{-1} and \mathbf{U}^{-1} , of which the norms can be estimated incrementally as in [55]. Based on this idea,

Bollhöfer and Saad developed a robust multilevel ILU approach [22], which dynamically defers the rows and columns that lead to large $\|\mathbf{L}^{-1}\|_\infty$ and $\|\mathbf{U}^{-1}\|_1$.

From an empirical point view, Benzi [13] measured the stability and accuracy of a preconditioner \mathbf{M} using $\|\mathbf{A}\mathbf{M}^{-1} - \mathbf{I}\|_F$ and $\|\mathbf{A} - \mathbf{M}\|_F$, respectively. The Frobenius norm is used probably due to its ease of computation. These measures work well for SPD systems, but the correlation between a small $\|\mathbf{A} - \mathbf{M}\|_F$ and a good preconditioner is weaker for general matrices. In this work, we use an alternative measure based on the spectral radius of $\mathbf{A}\mathbf{M}^{-1} - \mathbf{I}$.

Definition 1. A preconditioner \mathbf{M} is *accurate* for \mathbf{A} if $\rho(\mathbf{A}\mathbf{M}^{-1} - \mathbf{I}) \leq \rho_0$ for some $\rho_0 \lesssim 1$; the smaller the spectral radius, the more accurate the preconditioner.

This measure of the spectral radius is relevant to preconditioning because

$$|\lambda_i(\mathbf{A}\mathbf{M}^{-1}) - \lambda_j(\mathbf{A}\mathbf{M}^{-1})| \leq 2\rho_0 \quad (2.5)$$

for $1 \leq i, j \leq n$. Hence, the smaller ρ_0 is, the better the eigenvalues of $\mathbf{A}\mathbf{M}^{-1}$ are clustered, and the better the preconditioned KSP method may converge. Note that it is unnecessary for ρ_0 to be less than 1 for the convergence of a KSP method. However, a small ρ_0 imposes constraints on stability. In addition, if $\rho_0 < 1$, then \mathbf{M} can be used in place of a stationary iterative method as a smoother in multigrid methods [108], which can further accelerate convergence. Hence, we will use the approximate minimization of $\rho(\mathbf{A}\mathbf{M}^{-1} - \mathbf{I})$ in our derivation.

In the context of multilevel ILU, the accuracy and stability of the preconditioner is more complicated. For a two-level incomplete factorization of an SPD system, Notay [76, Theorem 2] showed that the stability requires both the leading block and the Schur complement (i.e., $\tilde{\mathbf{B}}$ and \mathbf{S}_C in (2.3)) to be well-conditioned. In addition, the Cauchy–Bunyakovski–Schwarz (CBS) constant [8, Chapter 9] should be (far) smaller than 1; assuming $\tilde{\mathbf{E}} = \tilde{\mathbf{F}}^T$ in (2.3), this condition requires that

$$\sup_{\mathbf{u}_1 \neq \mathbf{0}, \mathbf{u}_2 \neq \mathbf{0}} \frac{\mathbf{u}_1^T \tilde{\mathbf{E}} \mathbf{u}_2}{\sqrt{\mathbf{u}_1^T \tilde{\mathbf{B}} \mathbf{u}_1} \sqrt{\mathbf{u}_2^T \hat{\mathbf{C}} \mathbf{u}_2}} \ll 1. \quad (2.6)$$

These conditions are specific to SPD systems. As a heuristic for general matrices, we may argue that the leading blocks must be well conditioned at each level, and it is advantageous for the off-diagonal blocks to be as small as possible.

An unfortunate aspect of Notay’s analysis is that it demands well conditioned Schur complement, which is impractical for matrices from elliptic PDEs or second-order systems of PDEs, because the condition numbers are $\mathcal{O}(h^{-2})$ as the mesh resolution h tends to zero [41, 62]. Fortunately, in multilevel ILU, some preprocessing (such as equilibration [99, 34]) can be applied to the Schur complement, which can improve the condition number and in turn improve stability. In [22], Bollhöfer and Saad emphasized the accuracy of the Schur complement, who suggested to use a formulation due to Tismenetsky [98], which unfortunately often leads to excessive fills. A simpler alternative is to tighten the dropping thresholds for the Schur complement, as used in [20, 74, 88, 109]. In this work, we use a more elaborate version of the latter strategy, which we refer to *hierarchical dual thresholding*.

Criteria for efficiency Traditionally, the efficiency of ILU is equated to the “sparsity” of the \mathbf{L} and \mathbf{U} factors [29]. In this work, we give a more strict definition.

Definition 2. A preconditioner \mathbf{M} is *efficient* if it can be constructed in (nearly) linear time in the number of nonzeros in the input matrix \mathbf{A} , and $\mathbf{M}^{-1}\mathbf{u}$ can be computed in (nearly) linear time for any $\mathbf{u} \in \mathbb{R}^n$.

For ILU, this definition requires not only the number of nonzeros in \mathbf{L} and \mathbf{U} , but also the computational time of the factorization, to be (approximately) proportional to the number of nonzeros in \mathbf{A} . For linear systems arising from finite differences or finite elements for PDEs, the number of nonzeros per row is typically bounded by a constant. For such systems, Definition 2 requires (near) linear time complexity of ILU in the number of unknowns. In addition, the efficiency requirement must be satisfied under the constraint of the accuracy of \mathbf{M} . This is admittedly a tall order because a direct sparse solver has superlinear time complexity

for matrices from 2D and 3D PDEs [52]. To the best of our knowledge, none of the existing ILU technique achieved this efficiency goal under the accuracy constraint. Although ILU0 and a simple ILUT meet this criterion of efficiency, they do not satisfy the stability constraint in general. Note that our efficiency objective is similar to that of Hackbusch’s hierarchical matrices [51]. However, Hackbusch measures the accuracy by some norm of $\mathbf{A} - \mathbf{M}$, but we measure it using $\mathbf{A}\mathbf{M}^{-1} - \mathbf{I}$, which is more appropriate for preconditioning [13].

2.2 Dropping strategies

For ILU, the dropping strategies are important for both robustness and efficiency. Most modern ILU techniques use some form of “dual thresholding” [82], which combines a dropping strategy based on numerical values along with another dropping strategy based on some combinatorial (or symbolic) properties, such as the level of the elimination tree or the number of fills in rows or columns. For the former, the dropping is controlled by a parameter known as *drop tolerance* (or in short, *droptol* or τ). Different weighting schemes can be applied to numerical values. Let \mathbf{L}_k and \mathbf{U}_k denote the L and U factors of the ILU of the $k \times k$ leading block of \mathbf{A} . In [18], Bollhöfer proposed to use $\|\mathbf{L}_k^{-1}\|_\infty$ and $\|\mathbf{U}_k^{-1}\|_1$ as weights for the entries in the k th column of \mathbf{L} and the k th row of \mathbf{U} , respectively. Li et al. adopted it in [64] and referred to it as *dropping based on condition number estimation*. In [22, Theorem 6], Bollhöfer and Saad proposed a much more strict dropping strategy, which weights the values with a user-specified threshold, which corresponds to an upper bound of $\|\mathbf{L}_k^{-1}\|_\infty \|\mathbf{U}_k^{-1}\|_1$. To distinguish the two variants, we refer to the former as *variable inverse-based dropping* and the latter as *fixed inverse-based dropping*. In [72], Mayer proposed to weigh the values in the i th column of \mathbf{L} with some norm of the i th row of \mathbf{U} and vice versa. In this work, we use a modified inverse-based dropping, which we derive based on Definition 1. We also introduce a scalability-oriented dropping to achieve near linear-time complexity.

We note two concepts closely related to dropping. The first is the *Crout version of ILU* (or *ILUC*) [64], also known as the *left-looking ILU* for symmetric matrices [38]. Unlike the typically *ijk*-ordered Gaussian elimination, at the k th step, the Crout ILU computes the i th column of \mathbf{L} (i.e., ℓ_k) by left looking, and analogously for the k th row of \mathbf{U} (denoted by \mathbf{u}_k^T). In this way, the numerical values in ℓ_k and \mathbf{u}_k^T are updated as late as possible, so it allows more accurate dropping compared to right-looking algorithms. In addition, $\|\mathbf{L}_k^{-1}\|_\infty$ and $\|\mathbf{U}_k^{-1}\|_1$ can be estimated incrementally for the inverse-based dropping in Crout ILU. The second concept is *modified ILU* (*MILU*) [85], introduced by Dupont et al. [37] and also by Gustafsson [50] for elliptic PDEs. MILU modifies the diagonal entries to compensate the discarded entries so that the sum of each row is preserved. This strategy improves the accuracy for certain applications [39], and it is adopted in SuperLU [67]. We do not use it in HILUCSI, because it was ineffective for general linear systems in our testing.

2.3 Pivoting versus deferring

It is well known that small pivots can make Gaussian elimination unstable [47], and similar for ILU [29]. Analogous to LU and LDL^T factorizations, small pivots in ILU can be mitigated by using some variant of partial pivoting for unsymmetric matrices (such as column pivoting in ILUP and ILUTP [81, 85], row pivoting in SuperLU [67], and “dual pivoting” in [71]) and by using Bunch-Kauffman pivots [26, 47] for symmetric indefinite matrices (such as in ILDUC-BKP [63] and in ILUPACK [91]). The pivoting strategies may be *dynamic* in that they are determined at each step. However, unlike complete factorization, dynamic pivoting cannot guarantee the stability of the factorization, even for nonsingular systems. To overcome this issue, Saad [86] advocated *static pivoting*, which permutes the matrix in a preprocessing step. Saad’s work was motivated by that of Olschowa and Neumaier [77], who showed that any structurally nonsingular matrix can be permuted and scaled to obtain an *I-matrix*, whose diagonal entries have magnitude 1 and whose off-diagonal entries have a magnitude less than or equal to 1. To this end, Saad proposed a permutation strategy called ddPQ to achieve some weak diagonal dominance of a leading block, which he then used as the leading block in multilevel ILU without further permutation. However, the weak diagonal dominance from ddPQ cannot guarantee good pivots. In our testing, ddPQ is quite sensitive to the input matrix.

Instead of pivoting, Bollhöfer and Saad [22] proposed to defer the rows and columns to the next level dynamically if they lead to too large norms of \mathbf{L}^{-1} or \mathbf{U}^{-1} . Such a strategy naturally leads to a dynamic

Table 1: Comparison of pivoting and deferring in different ILU methods.

	pivoting			deferring	
	partial	static	Bunch-Kauffman	dynamic	static
HILUCSI				✓	✓
ARMS [88]		✓			
ILUPACK [22, 91]			✓ (sym. inf.)	✓	
SuperLU [67]	✓				
ILU++ [74]	✓ (dual)				

construction of multilevel structure. In this work, we use deferring to bound the norms of both \mathbf{D}^{-1} and the inverse triangular factors, so that it would also achieve the same goal as pivoting in avoiding small pivots, in addition to controlling the triangular factors. Analogous to dynamic pivoting, we refer to these deferring strategies as *dynamic deferring*. An advantage of dynamic deferring versus dynamic pivoting is that the former allows using more efficient data structures, as will explain in Section 4. In addition, we introduce *static deferring* for (nearly) symmetric saddle-point problems that have many zeros in the diagonal, as we will describe in Section 3. In Table 1, we compare different ILU methods in terms of pivoting and deferring.

2.4 Reordering and equilibration

Reordering is an effective preprocessing technique for complete and incomplete factorizations. Some commonly used reordering methods include reverse Cuthill-McKee (RCM) [70], approximate minimum degree (AMD) [5], nested dissection (ND) [45], etc. Among these techniques, RCM aims to reduce the bandwidth, and it is widely used for (nearly) SPD systems [15, 49]. In contrast, AMD aims to reduce fills, and it is effective in improving the quality of droppings, especially for general unsymmetric matrices. Both ILUPACK and SuperLU use some variants of AMD as the default reordering strategy.

While reordering is concerned with sparsity patterns, equilibration focuses on numerical properties. A simple equilibration technique is to scale rows and columns [47, 99]. A more sophisticated technique, known as *Hungarian scaling* in [56], combines scaling with column permutation of \mathbf{A} , so that $\mathbf{D}_r \mathbf{A} \mathbf{P}_c \mathbf{D}_c$ is an I-matrix [77]. Motivated by the work of Olschowka and Neumaier, Duff and Koster [34, 35] developed similar strategies for sparse matrices, which were implemented in the MC64 routine of the HSL library [60]. The strategy was adopted by several packages, including ILUPACK, SuperLU, PARDISO, MUMPS [6], MATLAB R2019a [97], etc. An I-matrix can reduce the condition number; in addition, an I-matrix has a weak diagonal dominance like ddPQ [86]. MC64 was designed for unsymmetric matrices. A sophisticated equilibration for symmetric indefinite systems was developed by Duff and Pralet [36]. A simple symmetrization strategy was described used in the routine HSL_MC64 in the HSL library, which applies a post-processing step after calling MC64, by setting $\mathbf{P}_r = \mathbf{P}_c$ and $\tilde{\mathbf{D}}_r = \tilde{\mathbf{D}}_c = \sqrt{\mathbf{D}_r \mathbf{D}_c}$, so that $\tilde{\mathbf{D}}_r \mathbf{P}_r \mathbf{A} \mathbf{P}_c \tilde{\mathbf{D}}_c$ preserves symmetry. We adopt the latter approach in this work.

3 Algorithmic Components for Robustness

To achieve robustness, we must take into account all the aspects reviewed in the previous section. At the same time, to keep the algorithm as simple as possible, we integrate only the essential components that have some mathematical or heuristic justifications, and we modify (and sometimes simplify) the techniques used in the state-of-the-art ILU techniques. Through mathematical analysis and extensive numerical experimentation, we reach at the factorization procedure in HILUCSI as sketched in Figure 3.1. In the following, we focus on four of its algorithmic components.

3.1 Mixed symmetric and unsymmetric preprocessing

Like ILUPACK, HILUCSI leverages some preprocessing techniques, including reordering and equilibration, at each level of multilevel ILU. A novelty of HILUCSI is that it mixes the preprocessing techniques for symmetric and unsymmetric matrices in a hierarchical fashion. In particular, for nearly and partially symmetric

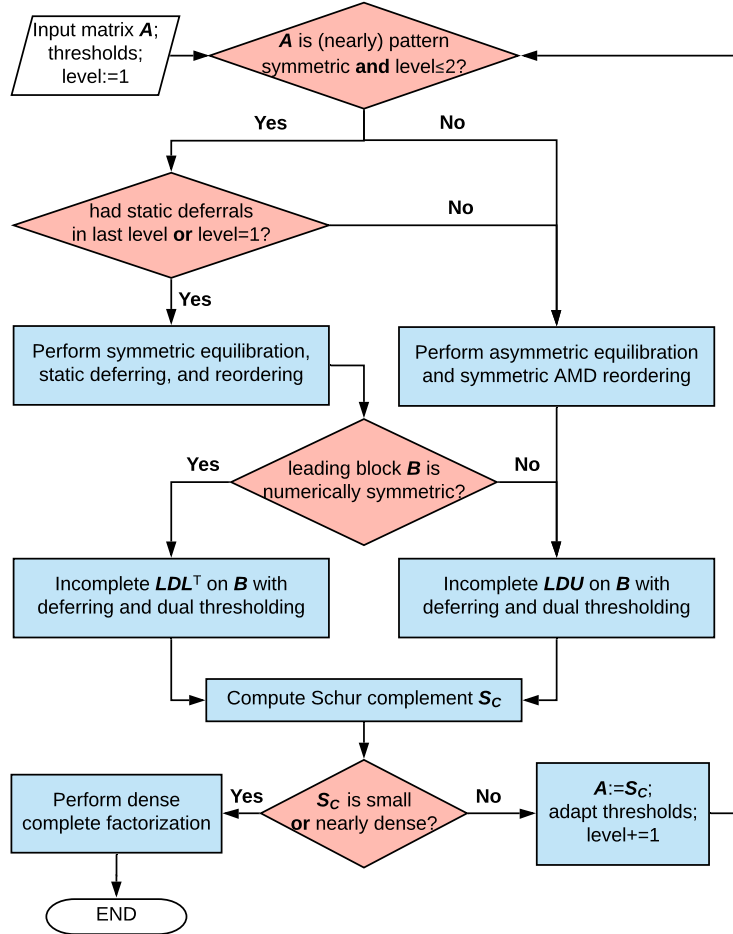


Figure 3.1: Flowchart of the multilevel ILDU factorization in HILUCSI.

matrices, we apply symmetric equilibration (similar to that in HSL_MC64 [60] as described in Section 2.4) and RCM reordering in the first level, and we apply unsymmetric equilibration and AMD reordering on $\text{nzp}(\mathbf{A}) + \text{nzp}(\mathbf{A}^T)$ at lower levels, where nzp denotes the *nonzero pattern*. In addition, after equilibration, we perform a post-processing to defer zero (or tiny) diagonal entries to the next level, as we describe in Section 3.2; in this case, we apply symmetric equilibration and AMD reordering on the second level.

The mixed preprocessing requires some justification. First, we observe that equilibration is particularly important in multilevel ILU. Besides stabilizing the factorization of the Schur complement, after scaling, the norm of the leading block (i.e., $\|\tilde{\mathbf{B}}\|$) is well bounded. Due to the Cauchy-Schwarz inequality,

$$\|\tilde{\mathbf{B}}^{-1}\| \leq \|\mathbf{L}_B^{-1}\| \|\mathbf{D}_B^{-1}\| \|\mathbf{U}_B^{-1}\|, \quad (3.1)$$

so bounding norms of \mathbf{L}_B^{-1} , \mathbf{D}_B^{-1} , and \mathbf{U}_B^{-1} allows controlling $\kappa(\mathbf{B})$, which Notay [76] showed to be important for SPD systems. In Section 3.2, we will give another simple argument to show that it is desirable to bound the norms of \mathbf{L}_B^{-1} , \mathbf{D}_B^{-1} and \mathbf{U}_B^{-1} for unsymmetric matrices.

Second, we observe that the symmetric equilibration is often more effective than unsymmetric equilibration for nearly symmetric matrices arising from systems of PDEs, especially when used in conjunction with RCM. This behavior is probably because those matrices may have some block diagonal dominance as defined in [44], which may be destroyed by unsymmetric equilibration. Symmetric equilibration with RCM reordering permutes the dominant block diagonal within a narrower band, so that it may preserve block diagonal dominance more effectively. In addition, for SPD matrices, RCM tends to lead to smaller off-diagonal blocks and in turn a smaller CBS constant in (2.6), which also improves the quality of the preconditioner. In our experiments, the combination of symmetric equilibration with RCM reordering at the top level significantly improves both robustness and efficiency for nearly symmetric matrices. However, if the sparsity pattern is unsymmetric or highly irregular, unsymmetric equilibration and AMD reordering tend to be more robust; see Section 5.3 for some comparisons.

Note that unlike MC64, symmetric equilibration does not produce I-matrices. Indeed, any zeros in the diagonal of the input matrix would remain in the diagonal after symmetric equilibration. The zero or tiny diagonal entries require some special attention, which we address using static deferring.

3.2 Static and dynamic deferring

As shown in Table 1, HILUCSI differs from the other ILU techniques in that it avoids small pivots and ill-conditioned triangular factors using static and dynamic deferring. During static deferring, we symmetrically permute the zero and tiny diagonal entries to the lower-right corner of the matrix, to be factorized in the next level. During dynamic deferring, we also symmetrically permute a row and column to the lower-right corner if the diagonal is smaller than a threshold (κ_D) or the estimated norms $\|\mathbf{L}^{-1}\|_\infty$ and $\|\mathbf{U}^{-1}\|_1$ exceed some threshold (κ_L and κ_U). In practice, we use the threshold κ for κ_D , κ_L , and κ_U , and a value of 3 or 5 is very robust.

Our strategy requires some justification. First, unlike the Bollobás-Saad dynamic deferring [22], our dynamic deferring considers not only $\|\mathbf{L}^{-1}\|_\infty$ and $\|\mathbf{U}^{-1}\|_1$ but also $\|\mathbf{D}\|$ and $\|\mathbf{D}^{-1}\|$. Bounding norms of \mathbf{D}^{-1} , \mathbf{L}^{-1} , and \mathbf{U}^{-1} can be justified from Definition 1, in that

$$\rho(\mathbf{A}\mathbf{M}^{-1} - \mathbf{I}) = \rho(\delta_A \mathbf{M}^{-1}) \leq \|\delta_A \mathbf{M}^{-1}\| \leq \|\mathbf{M}^{-1}\| \|\delta_A\|. \quad (3.2)$$

Hence, given an “accurate” preconditioner \mathbf{M} , it is important that $\|\mathbf{M}^{-1}\|$ is bounded, which can be achieved computationally by bounding norms of \mathbf{D}^{-1} , \mathbf{L}^{-1} , and \mathbf{U}^{-1} . In contrast, bounding $\|\mathbf{L}^{-1}\|$ and $\|\mathbf{U}^{-1}\|$ alone, as done in [22], is insufficient. We attribute to this difference as the key factor in improved robustness of HILUCSI compared to ILUPACK.

Second, note that dynamic deferring can effectively resolve zero or tiny pivots in most cases. However, our experiments show that it is advantageous to perform a static deferring, because zero or tiny pivots tend to lead to fast growth of $\|\mathbf{L}^{-1}\|_\infty$ and $\|\mathbf{U}^{-1}\|_1$, which tends to lead to poorer-quality preconditioners. The static deferring also eliminates the need of Bunch-Kaufman pivoting, which not only simplifies the implementation but also improves robustness and efficiency in our comparison, especially for (nearly) symmetric saddle-point problems. Finally, note that in the extreme case, a matrix may have all zero diagonals, which does not introduce complications because HILUCSI switches to unsymmetric equilibration in the next level.

3.3 Hierarchical dual thresholding

HILUCSI uses a combination of numerical and combinatorial dropping strategies, analogous to other “dual thresholding.”

3.3.1 Modified inverse-based dropping

For numerical dropping, we use a modified inverse-based thresholding. In particular, unlike the variable and fixed inverse-based thresholding in [18] and [22], we use $\kappa_D \|\mathbf{L}_k^{-1}\|_\infty$ and $\kappa_D \|\mathbf{U}_k^{-1}\|_1$ as weights for dropping in the k th column in \mathbf{L} and k th row in \mathbf{U} , respectively, where κ_D is a use-specified upper bound of $\|\mathbf{D}^{-1}\|_\infty$ during dynamic deferring.

We motivate the modified inverse-based thresholding based on Definition 1. Let $\delta_A = \mathbf{A} - \mathbf{M}$, where $\mathbf{M} = \mathbf{L}\mathbf{D}\mathbf{U}$, and $\mathbf{A} = (\mathbf{L} + \delta_L)(\mathbf{D} + \delta_D)(\mathbf{U} + \delta_U)$, where δ_L , δ_D , and δ_U denote the perturbations to \mathbf{L} , \mathbf{D} , and \mathbf{U} , respectively. Hence,

$$\begin{aligned}\delta_A &= (\mathbf{L} + \delta_L)(\mathbf{D} + \delta_D)(\mathbf{U} + \delta_U) - \mathbf{L}\mathbf{D}\mathbf{U} \\ &= \delta_L\mathbf{D}\mathbf{U} + \mathbf{L}\delta_D\mathbf{U} + \mathbf{L}\mathbf{D}\delta_U + \text{h.o.t.},\end{aligned}$$

where we omit the higher-order terms that involve more than one δ matrix. Hence,

$$\begin{aligned}\rho(\mathbf{A}\mathbf{M}^{-1} - \mathbf{I}) &= \rho\left(\sqrt{\mathbf{D}^{-1}}\mathbf{L}^{-1}\delta_A\mathbf{M}^{-1}\mathbf{L}\sqrt{\mathbf{D}}\right) \\ &\approx \rho\left(\sqrt{\mathbf{D}^{-1}}(\mathbf{L}^{-1}\delta_L + \delta_D\mathbf{D}^{-1})\sqrt{\mathbf{D}} + \sqrt{\mathbf{D}}\delta_U\mathbf{U}^{-1}\sqrt{\mathbf{D}^{-1}}\right) \\ &\leq \sqrt{\kappa(\mathbf{D})}(\|\mathbf{L}^{-1}\delta_L\| + \|\delta_D\mathbf{D}^{-1}\| + \|\delta_U\mathbf{U}^{-1}\|).\end{aligned}\tag{3.3}$$

Note that if we omit the $\sqrt{\kappa(\mathbf{D})}$ factor and we bound $\|\mathbf{L}^{-1}\delta_L\|$ and $\|\delta_U\mathbf{U}^{-1}\|$ using their ∞ -norm and 1-norm, respectively, we would obtain the variable inverse-based dropping in [18] and [64]; we refer readers to these references for the details on estimating $\|\mathbf{L}_k^{-1}\|_\infty$ and $\|\mathbf{U}_k^{-1}\|_1$. However, the dropping strategy in [18] and [64] omitted the conditioning of the diagonal matrix, because their analysis was not based on $\rho(\mathbf{A}\mathbf{M}^{-1} - \mathbf{I})$. In dynamic deferring, we restrict the magnitude of the diagonal entries to be no smaller than $1/\kappa_D$, and we estimate the maximum magnitudes to be approximately κ_D . Hence, $\sqrt{\kappa(\mathbf{D})}$ can be bounded approximately by κ_D , which leads to our modified inverse-based dropping. Like the original inverse-based dropping, the modified version can be easily incorporated into Crout ILU.

3.3.2 Scalability-oriented dropping

For combinatorial dropping, we introduce a *scalability-oriented dropping*. The basic idea is to limit the number of nonzeros (nnz) in the k th column of \mathbf{L} , namely ℓ_k , by a factor of the input matrix, i.e.,

$$\text{nnz}(\ell_k) \leq \alpha \max\{\text{nnz}(\mathbf{a}_j), 0.85 \overline{\text{nnz}(\mathbf{a}_*)}\},\tag{3.4}$$

where $\overline{\text{nnz}(\mathbf{a}_*)}$ denotes the average number of nonzeros in the columns of \mathbf{A} and is introduced to avoid excessive dropping for small columns in a highly nonuniform matrix. We limit the nnz in the rows of \mathbf{U} in a symmetric fashion. In the multilevel setting, we limit the rows and columns in all the levels based on the original input matrix, instead of based on the Schur complement from the previous level. This strategy is important for the scalability analysis. Furthermore, before computing the Schur complement, we apply dropping to limit the nonzeros in each column in \mathbf{U}_F based on the right-hand side of (3.4), and similarly for the rows in \mathbf{L}_E . In Section 4, we will show that with this strategy, HILUCSI achieves near linear-time complexity.

3.3.3 Hierarchical dual thresholding

In HILUCSI, the numerical dropping is controlled by τ and κ , and the combinatorial dropping is controlled by α . In practice, we found that the combination $\tau = 10^{-4}$, $\kappa = 3$, and $\alpha = 10$ is very robust for almost all the systems we have tested, while $\tau = 10^{-2}$, $\kappa = 5$, and $\alpha = 3$ work well for most problems from systems of

PDEs. In addition, we observe that the accuracy of the factorization of the second level is often the most critical because it corresponds to factorizing the largest Schur complement. For this reason, we refine the thresholds for level 2 by reducing τ by a factor of 10, reducing κ by up to a factor of 2 (while restricting $\kappa \geq 2$), and doubling α . For lower levels, however, we revert α back for efficiency but use the refined τ and κ for stability and accuracy.

4 Achieving efficiency and scalability

In this section, we focus on the efficiency issues of HILUCSI for large-scale linear systems.

4.1 Linear time complexity

We show that HILUCSI meets the efficiency requirement in Definition 2, especially for those arising from systems of PDEs.

Proposition 3. *If the input matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ has a constant number of nonzeros per row and per column, excluding the preprocessing step, the total cost of HILUCSI on each level is linear in n .*

We outline the proof for the first level. Given a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, let $\mathbf{P} \in \mathbb{N}^{n \times n}$, $\mathbf{Q} \in \mathbb{N}^{n \times n}$, $\mathbf{L} \in \mathbb{R}^{n \times m}$, $\mathbf{D} \in \mathbb{R}^{m \times m}$ and $\mathbf{U} \in \mathbb{R}^{m \times n}$ be the output of the factorization of the current level. Omitting dynamic deferring and thresholding, it is easy to show that the number of floating point operations in Crout ILU is bounded by

$$\mathcal{O} \left(\text{nnz}(\mathbf{L} + \mathbf{U}) \left(\max_{i \leq m} \{\text{nnz}(\mathbf{a}_i^T)\} + \max_{j \leq m} \{\text{nnz}(\mathbf{a}_j)\} \right) \right), \quad (4.1)$$

where \mathbf{a}_i^T and \mathbf{a}_j denote the i th row and j th column of $\mathbf{P}^T \mathbf{A} \mathbf{Q}$, respectively. Given an efficient data structure, the floating-point operations in dynamic deferring is proportional to Crout ILU. Furthermore, in the scalability-oriented dropping, we use quick select, which has an expected linear time complexity, to find the largest nonzeros, followed by quick sort after dropping. Hence, the asymptotic complexity of dropping is lower than that of Crout update. Assuming there is a constant number of nonzeros in each row and column,

$$\max_{i \leq n} \{\text{nnz}(\mathbf{a}_i^T)\} + \max_{j \leq n} \{\text{nnz}(\mathbf{a}_j)\} = \mathcal{O}(1), \quad (4.2)$$

and $\text{nnz}(\mathbf{L} + \mathbf{U}) = \text{nnz}(\mathbf{A}) = \mathcal{O}(n)$. Hence, Crout ILU with deferring takes linear time. Finally, by ensuring the nonzeros in each row of \mathbf{L}_E and in each column of \mathbf{U}_F are bounded by a constant, the Schur component can be computed in linear time. The above analysis also applies to the other levels. Finally, HILUCSI uses a dense factorization in the last level if its size is $\mathcal{O}(n^{1/3})$, so its cost is also linear in $\mathcal{O}(n)$.

Note that the overall time complexity of HILUCSI may be slightly superlinear because the worst-case complexities of some preprocessing components (including MC64 and AMD [53, 35]) are superlinear. However, MC64 has an expected linear-time complexity under our assumptions [35], and the cost of AMD is typically negligible. In addition, the number of levels may not be a constant in the worst case, but it is typically small. Hence, by design HILUCSI is expected to deliver nearly linear-time complexity. In Section 5, we will show that HILUCSI indeed scales better than both ILUPACK and SuperLU, and its near linear complexity makes its performance competitive with highly optimized direct solvers for large systems.

4.2 Implementation details

To realize the near linear-time complexity in Proposition 3, we need an efficient data structure for sparse matrices. In particular, the data structure must support efficient sequential access of the k th row of \mathbf{L} along with all the rows in $\mathbf{U}_{1:k-1, k:n}$, and similarly for \mathbf{U} and $\mathbf{L}_{k:n, 1:k-1}$, as required by the k th step of the Crout ILU. In addition, it must support efficient static and dynamic deferring. The standard storage formats, such as CSR (Compressed Sparse Row), CSC (Compressed Sparse Column), or AIJ, are insufficient. We use a bi-index data structure, similar to that proposed by Jones and Plassmann [59] for the row-version of

incomplete Cholesky factorization and that used in Crout version of ILU without pivoting for unsymmetric matrices by Li, Saad, and Chow in [29, 64].

For simplicity, let us first consider the data structure in [64] for \mathbf{U} without deferring. Because \mathbf{U} is constructed row by row, we store it using the CSR format, in which the column indices for each row are sorted in ascending order. We then augment it using two size- n arrays: `Ufirst` and `Ulist`, where the former stores the index of the first nonzero in each row of $\mathbf{U}_{1:k-1,k:n}$ in CSR, and the latter maintains the linked lists of the entries in `Ufirst` by columns. At the k th step, all the nonzero entries in the k th column of \mathbf{U} must be in `Ufirst`. Hence, we can access a complete linked list of the entries in the k th columns in \mathbf{U} through `Ulist`. The same holds for \mathbf{L} , except that we use CSC as the base for storing \mathbf{L} .

The data structure in [64] does not support deferring or pivoting. We extend it to support deferring. For simplicity, we describe the procedure for \mathbf{U} as follows. At the k th step, suppose there have been $d - 1$ deferrals and the current column in \mathbf{U} is going to be the d th deferral. We move the current column in \mathbf{U} to the $(n + d)$ th position. By induction, there will be a gap of d for the column indices in \mathbf{U} . Hence, before processing the k th column, we move column $k + d + 1$ to the k th position in \mathbf{U} , which eliminates the gap in a “just-in-time” fashion for \mathbf{U}_B . For the indices in \mathbf{U}_F , we eliminate the gap at the end of the Crout ILU for the current level. The processing of \mathbf{L} is symmetric to that of \mathbf{U} . To implement this efficiently, we enlarge some size- n arrays (e.g., the permutation vectors, `Llist`, and `Ulist`) to size $2n$. This memory overhead is negligible, and it enables us to preserve the amortized constant time per nonzero. In contrast, for Crout ILU with dynamic pivoting, such as those in [63] and [74], the data structure needs to support efficient sequential access to all the rows and columns in \mathbf{U} , and similarly for \mathbf{L} . That requirement would double the storage and also incur significantly more data movement. Note that ILUPACK [20] also extended the data structures in [64] to support deferring, but we were unable to find its implementation details for comparison.

5 Numerical results

We have implemented HILUCSI using the C++-11 standard. In this section, we assess the robustness and efficiency of our implementation for some challenging benchmark problems and compare its performance against some state-of-the-art packages. In particular, we chose ILUPACK v2.4 [20, 23] as the representative of multilevel ILU, partially because HILUCSI is based on the same Crout-version of multilevel ILU as in ILUPACK, and more importantly, ILUPACK has been optimized for both unsymmetric and symmetric matrices. In comparison with other packages, our tests showed that ILUPACK outperformed ARMS in ITSOL v2 [88] by up to an order of magnitude for larger unsymmetric systems, and the gap is even larger for symmetric systems; ILUPACK is significantly more robust than ILU++ [73, 74]. In addition, we chose the supernodal ILUTP in SuperLU v5.2.1 [65, 67] as a representative of single-level ILU, because of its efficient supernodal implementation. In all of our tests, we used right-preconditioning for restarted GMRES(30), which limits the dimension of the Krylov subspace to 30. We used 10^{-6} for the convergence criteria of GMRES and limited the number of iterations to 500. For HILUCSI and ILUPACK, we used our own implementation of flexible GMRES; for SuperLU, we used the GMRES implementation in the latest PETSc v3.11.3. Furthermore, we also compare HILUCSI against the multithreaded direct solvers in MUMPS 5.2.0 [6], MKL PARDISO v2018/3.222, and PARDISO 6.0 [79, 92].

We conducted our tests on a single node of a cluster running CentOS 7.4 with two 2.5 GHz Intel Xeon CPU E5-2680v3 processors and 64 GB of RAM. We compiled HILUCSI, SuperLU and PETSc all using GCC 4.8.5 with the optimization option `-O3`, and we used the binary release of ILUPACK v2.4 for GNU64. We accessed ILUPACK through its MATLAB mex functions, of which the overhead is negligible. For accurate timing, both turbo and power saving modes were turned off for the processors.

5.1 Robustness as “black-box” preconditioners

We have tested HILUCSI using more than 60 challenging, larger-scale benchmark problems that were highlighted in the ILU literature. These matrices were mostly from the SuiteSparse Matrix Collections [33] and the Matrix Market [17], representing a wide range of applications. In our tests, HILUCSI succeeded for all the nonsingular real linear systems and most singular systems with a low-dimensional null space and

a meaningful right-hand side.¹ We present results on select benchmark problems from some highlighted problems in [22], [67], and [110], together with two larger unsymmetric systems for Navier-Stokes (N-S) equations. Table 2 summarizes these unsymmetric matrices, including their application areas, types, sizes, and estimated condition numbers. Note that PR02R is a singular system with a meaningful right-hand side.

In addition, we generated two sets of symmetric saddle-point problems using FEniCS v2017.1.0 [4] by discretizing the 3D Stokes equation and the mixed formulation of the Poisson equation. These equations have a wide range of applications in CFD, solid mechanics, heat transfer, etc. We discretized the former using Taylor–Hood elements [95], and discretized the latter using a mixture of linear Brezzi-Douglas-Marini (BDM) elements [24] and degree-0 discontinuous Galerkin elements [31]. These problems are challenging in that the matrices have some implicit and nonuniform block structures, and they have many zeros in the diagonals. To facilitate scalability study, for each set, we generated three linear systems using meshes of different resolutions. Note that the matrices generated by FEniCS do not enforce symmetry exactly and contain some nearly zero values due to rounding errors. We manually filtered out the small values that are close to machine precision and then enforced symmetry using $(\mathbf{A} + \mathbf{A}^T)/2$.

We first assess the robustness of HILUCSI versus ILUPACK and SuperLU for GMRES(30). In this test, we treat ILU as nearly a “black-box” preconditioner. We used a fixed droptol $\tau = 10^{-4}$ for all the codes, as in [67], and used the recommended defaults for the other parameters for most problems. In particular, for ILUPACK, we used MC64 matching, AMD ordering, and condest (i.e., κ) 5. For SuperLU, when using its default options, we only solved four problems. We doubled its fill factor from 10 to 20, which allowed SuperLU to solve another five problems. For HILUCSI, we used our default values $\kappa = 3$ and $\alpha = 10$ for most cases, except that we used $\alpha = 15$ for twotone, which is not a PDE-based problem.

In Table 2, we report the overall runtimes (including both factorization and solve times) for each code, and the fastest runtime for each case is highlighted in bold. HILUCSI had a 100% success rate for these problems, and it was the fastest for 70% of the cases. In contrast, ILUPACK solved 85% of cases and it was the fastest for 5% of the cases. Among the successful cases, ILUPACK ran out of the 64GB of main memory for RM07R and it used about 30GB of swap space, so the timing result was unreliable. For the symmetric problems, ILUPACK automatically detects symmetric matrices and then applies ILDL^T factorization with mixed 1×1 and 2×2 pivots automatically. This optimization in ILUPACK benefitted its timing for those problems but hurt its robustness for the two larger systems from Stokes equations, which we could solve only by explicitly forcing ILUPACK to use unsymmetric ILU. In addition, ILUPACK was unable to solve PR02R, regardless of how we tuned condest. SuperLU was the least robust among the three: it solved only 45% of cases² and it was the fastest for 25% of cases. Note that for the largest system solved by all the codes, namely atmosmodl, HILUCSI outperformed ILUPACK and SuperLU by a factor of 6 and 9, respectively. On the other hand, for a medium-sized problem, namely e40r5000, SuperLU outperformed HILUCSI and ILUPACK by a factor of 7.5 and 15, respectively. This result shows that SuperLU is efficient for its excellent cache performance, but its ILUTP is fragile compared to multilevel ILU in ILUPACK and HILUCSI. Overall, HILUCSI delivered the best robustness and efficiency.

5.2 Efficiency with optimized parameters

The default parameters in the preceding comparison are robust for general problems, but they may be too strict for linear systems from specific classes of PDEs. We now compare the software for some saddle-point problems arising from PDEs, including some nearly symmetric indefinite systems and symmetric saddle-point problems.

5.2.1 Nearly symmetric, indefinite systems

For nearly symmetric matrices, we use six PDE-based problems in Table 2, which are from different types of equations in CFD, including 2D Euler, 3D Navier-Stokes equations, and Helmholtz equations. Table 3 shows the comparison of HILUCSI, ILUPACK, and SuperLU for these systems in terms of the factorization times, total times, GMRES iterations, and nonzero ratios. We highlighted the fastest runtimes in bold.

¹HILUCSI failed for the system invextr1_new used in [110], where all their tested methods failed it as well. The problem is challenging because it has a large null-space dimension of 2,910.

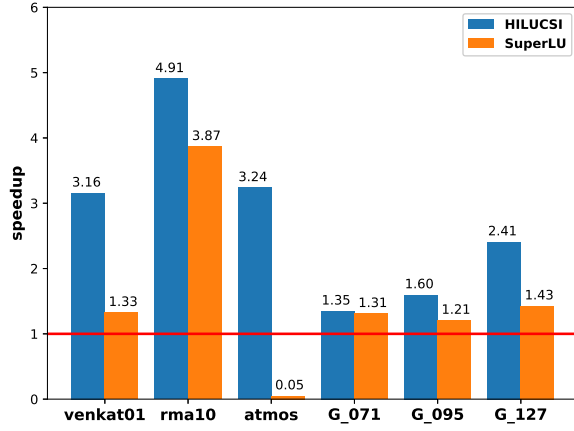
²In [67], SuperLU had a higher success rate using GMRES(50) and unlimited fill factor, but we used GMRES(30) (the default in PETSc [9]) and a fill factor 10 (the default in SuperLU) or 20.

Table 2: Comparison of robustness of HILUCSI, ILUPACK, and SuperLU, denoted as H, I, and S, respectively, using robust, unoptimized parameters (droptol 10^{-4} for all codes and $\alpha = 10$ for HILUCSI). For HILUCSI, ‘*’ indicates enlarging α to 15; for ILUPACK, ‘*’ indicates out of the 64GB main memory; for SuperLU, ‘*’ indicates doubling fill-factor. \times , and $-$ indicate failed factorization and stagnation of GMRES(30), respectively. The overall leaders are in bold.

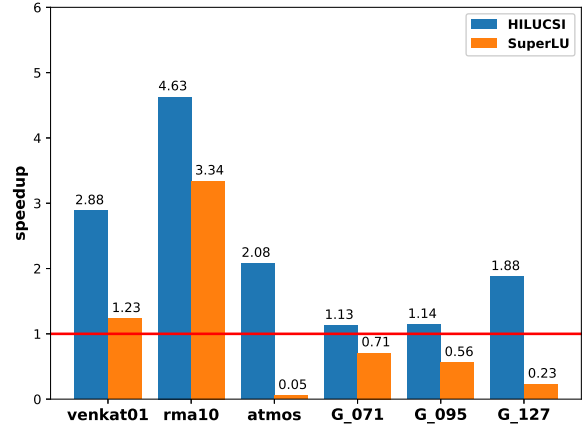
Matrix	Appl.	n	nnz	Cond.	total time (sec.)		
					H	I	S
(nearly) pattern-symmetric, indefinite systems from PDEs							
venkat01	2D Euler	62,424	1,717,792	2.5e6	6.81	8.40	5.91
rma10	3D CFD	46,835	2,374,001	4.4e10	10.6	31.7	4.73
mixtank_new		29,957	1,995,041	2.2e11	40.2	128	-
Goodwin_071	3D	56,021	1,797,934	1.4e7	20.8	15.5	16.3
Goodwin_095	Navier-Stokes (N-S)	100,037	3,226,066	3.4e7	39.9	42.6	21.1*
Goodwin_127		178,437	5,778,545	8.2e7	75.1	95.1	65.0*
RM07R		381,689	37,464,962	2.2e11	3.3e3	~3e4*	×
PR02R	2D N-S	161,070	8,185,136	1.1e21	261	—	—
e40r5000		17,281	553,956	2.5e10	18.7	36.8	2.4*
xeono2	materials	157,464	3,866,688	1.4e5	44.8	198	—
atmosmodl	Helmholtz	1,489,752	10,319,760	1.5e3	85.1	502	718
other unsymmetric systems							
onetone1	circuit	36,057	335,552	9.4e6	0.44	1.12	—
twotone	simulation	120,750	1,224,224	4.5e9	7.71*	18.5	—
bbmat	2D airfoil	38,744	1,771,722	5.4e8	31.9	36.5	59.0*
symmetric, saddle-point problems from PDEs							
S3D1	3D Stokes	18,037	434,673	1.2e7	1.63	6.56	9.90*
S3D2		121,164	3,821,793	8.9e7	80.7	×	×
S3D3		853,376	31,067,368	6.3e8	781	×	×
M3D1	3D	29,404	522,024	1.7e5	6.66	8.31	—
M3D2	mixed	211,948	4,109,496	2.3e6	67.1	127	×
M3D3	Poisson	1,565,908	31,826,184	3.8e7	599	1.3e3	×
success rate					100%	85%	45%
leader rate					70%	5%	25%

Table 3: Comparison of HILUCSI (denoted as H) versus ILUPACK (I) and SuperLU (S) for nearly pattern-symmetric, indefinite problems with optimized parameters (drop tolerance 10^{-2} for all and $\alpha = 3$ for HILUCSI). \times indicates failed factorization. The fastest times are in bold.

Matrix	factor. time (sec.)			total time (sec.)			GMRES iters.			nnz ratio		
	H	I	S	H	I	S	H	I	S	H	I	S
venkat01	1.11	3.50	2.64	1.25	3.62	2.94	7	5	7	3.0	2.8	2.4
rma10	2.31	11.3	2.93	2.47	11.4	3.43	9	4	9	2.0	3.8	2.8
atmosmodl	10.5	33.8	686	19.8	41.0	748	33	22	75	2.9	4.0	6.2
Goodwin_071	4.01	5.40	4.12	4.99	5.63	7.95	41	12	52	4.8	3.5	5.0
Goodwin_095	7.36	11.8	9.74	10.7	12.3	21.9	78	14	84	4.8	3.9	5.7
Goodwin_127	13.3	32.1	22.5	17.7	33.3	146	56	16	449	4.8	5.0	6.1



(a) Relative speedup of factorization time.



(b) Relative speedup of total time.

Figure 5.1: Speedups of (a) factorization and (b) total times of HILUCSI and SuperLU versus ILUPACK for nearly pattern-symmetric, indefinite problems with optimized parameters. Higher is better. G stands for Goodwin in the horizontal axis.

For a fair comparison, we used $\tau = 0.01$ for all the codes, used $\kappa = 5$ for both HILUCSI and ILUPACK, and used $\alpha = 3$ for HILUCSI. It can be seen that HILUCSI was the fastest for all the cases in terms of both factorization and total times. HILUCSI required more GMRES iterations than ILUPACK, while SuperLU required significantly more iterations for the largest systems. In addition, we note that HILUCSI could solve all the problems with $\alpha = 2$, which would further improve the factorization time but at the cost of more GMRES iterations for some systems.

Figure 5.1 shows the relative speedups of HILUCSI and SuperLU versus ILUPACK in terms of factorization and solve times. It can be seen that HILUCSI outperformed ILUPACK for all six cases by a factor between 1.1 and 4.9. For the Goodwin problems, it is clear that the relative speedup increased as the problem sizes increased, thanks to the near linear-time complexity of HILUCSI as shown in Proposition 3. We note that ILUPACK has a parameter `elbow` for controlling the size of reserved memory, but the parameter made no difference in our testing. ILUPACK also has another parameter `lfil` for space-based dropping, but its use is discouraged in its documentation, so we did not use it by default. Our tests showed that using a small `lfil` in ILUPACK decreases its robustness, while its time complexity still remained higher than HILUCSI.

In addition, we observe that although SuperLU outperformed ILUPACK in terms of factorization times for all the Goodwin problems, it underperformed in terms of the overall times for these problems, because its solve time was significantly larger due to too many GMRES iterations. This again shows the superior robustness of multilevel ILU in HILUCSI and ILUPACK versus the ILUTP in SuperLU.

Table 4: Comparison of HILUCSI (denoted as H) with unsymmetric and symmetric ILUPACK (denoted by IU and IS, respectively) for symmetric saddle-point systems with droptol 10^{-2} for all and $\alpha = 3$ for HILUCSI. \times indicates failed factorization.

Matrix	HILUCSI		GMRES iters.			nnz ratio			#levels		
	factor.	total	H	IU	IS	H	IU	IS	H	IU	IS
S3D1	0.44	0.45	4	3	7	2.0	4.6	6.4	3	6	5
S3D2	5.56	5.83	7	3	\times	2.5	6.3	\times	3	6	\times
S3D3	61.7	64.1	7	4	\times	2.7	8.4	\times	4	9	\times
M3D1	0.69	0.78	14	6	11	2.7	7.9	5.8	4	8	5
M3D2	6.25	7.75	26	11	29	2.6	9.5	7.3	5	10	5
M3D3	52.9	76.8	53	24	62	2.6	10	7.2	6	15	5

5.2.2 Symmetric saddle-point problems

We now assess the robustness and efficiency of HILUCSI as the problem sizes increase. To this end, we use the symmetric saddle-point problems and compare HILUCSI with two different solvers in ILUPACK for symmetric and unsymmetric matrices, respectively. Because SuperLU v5.2.1 failed for most of these problems, we do not include it in this comparison. For these saddle-point problems, because there are static deferring, our algorithm enabled symmetric matching in HILUCSI on the first two levels, and we applied RCM ordering for the first level and applied AMD ordering for all the other levels. For ILUPACK, we used AMD ordering, as recommended by ILUPACK’s documentation.

Table 4 shows the comparison of HILUCSI with ILUPACK in terms of the numbers of GMRES iterations, the nonzero ratios, and the numbers of levels, along with the runtimes of HILUCSI. Figure 5.2 shows the relative speedups of HILUCSI and symmetric ILUPACK relative to the unsymmetric ILUPACK. It can be seen that HILUCSI outperformed the unsymmetric ILUPACK by a factor of four to ten for these problems. The improvement was mostly due to the improved dropping in HILUCSI; in addition, HILUCSI also had fewer levels than unsymmetric ILUPACK. In contrast, the symmetric ILUPACK failed for the two larger systems for the Stokes equations due to encountering a structurally singular system during preprocessing. For the two larger cases for the mixed formulation of the Poisson equation, symmetric ILUPACK was notably less robust and required many more GMRES iterations. Among the four solved problems, symmetric ILUPACK improved the runtimes of unsymmetric ILUPACK by a factor of 1.2 to 2.6, due to performing computations only on the lower triangular part and different dropping strategies. Finally, note that the improvement from symmetric ILUPACK cannot be achieved if we did not explicit symmetrize the matrices or force ILUPACK to use the symmetric solver. In contrast, since HILUCSI treats the pattern symmetric matrices as nearly symmetric, it delivers more consistent performance even if the matrix is slightly unsymmetric due to rounding or truncation errors. Note that the timing results in Table 4 for HILUCSI did not take advantage of numerical symmetry. Using a symmetric kernel in the first two levels would further improve its performance by 10–20%. Hence, the penalty of losing numerical symmetric is relatively small when using HILUCSI. In addition, we observe that in Figure 5.2, the relative speedup of HILUCSI versus ILUPACK improves significantly as the size of the problem grows, similar to what we observed for unsymmetric systems.

5.3 Benefits of mixed processing

To assess the effectiveness of mixing symmetric and unsymmetric preprocessing for HILUCSI, we applied symmetric preprocessing on zero, one, and two levels. Table 5 shows a comparison of the factorization times, total times, GMRES iterations, and nnz ratios for three different classes of problems. It can be seen that for matrices with fully unsymmetric structures, using symmetric preprocessing did not improve robustness and decreased efficiency. However, for many unsymmetric matrices with nearly symmetric structures, using symmetric preprocessing on the first level significantly improved robustness and efficiency. Furthermore, when static deferring is invoked in (nearly) symmetric saddle-point problems, using two levels of symmetric preprocessing further reduced the factorizations times, but the total runtime remained about the same.

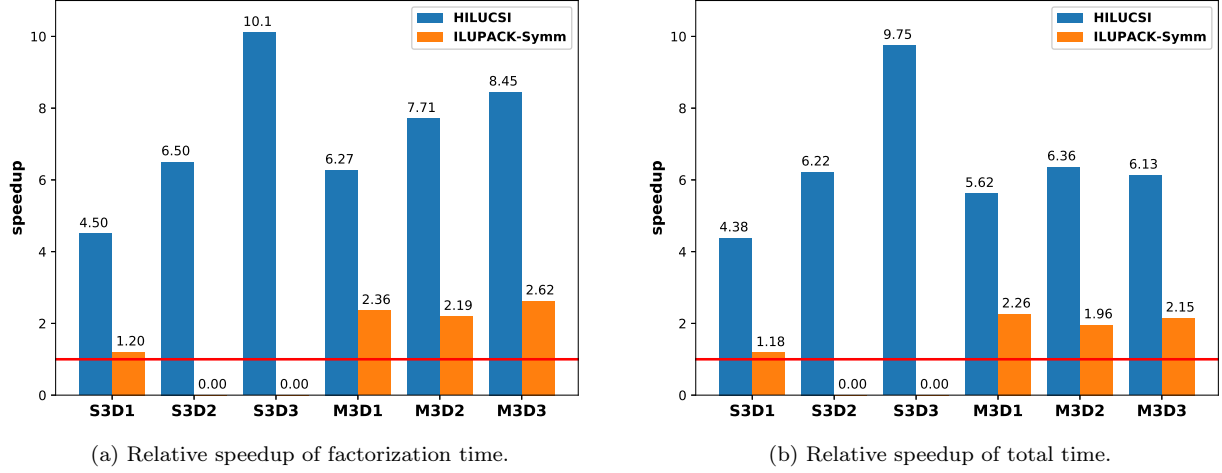


Figure 5.2: Speedups of (a) factorization and (b) total times of HILUCSI and symmetric factorization in ILUPACK versus unsymmetric ILUPACK for symmetric saddle-point problems. Higher is better.

Table 5: Effect of mixing symmetric and unsymmetric processing in HILUCSI. H0, H1 and H2 denote using zero, one, and two levels of symmetric preprocessing.

Matrix	factor. time			total time			GMRES iters.			nnz ratio		
	H0	H1	H2	H0	H1	H2	H0	H1	H2	H0	H1	H2
general unsymmetric systems												
bbmat	31.4	45.5	55.2	31.9	46.3	55.9	9	11	9	17	25	32
(nearly) pattern symmetric systems												
rma10	4.85	2.31	2.53	5.02	2.47	2.69	67	9	9	3.4	2.0	2.3
PR02R	—	256	293	—	261	300	—	14	15	—	28	32
symmetric, saddle-point problems												
M3D3	—	53.6	52.9	—	77.3	76.8	—	52	53	—	2.6	2.6
M3D2	8.06	6.37	6.25	16.1	7.69	7.75	120	23	26	4.0	2.6	2.6

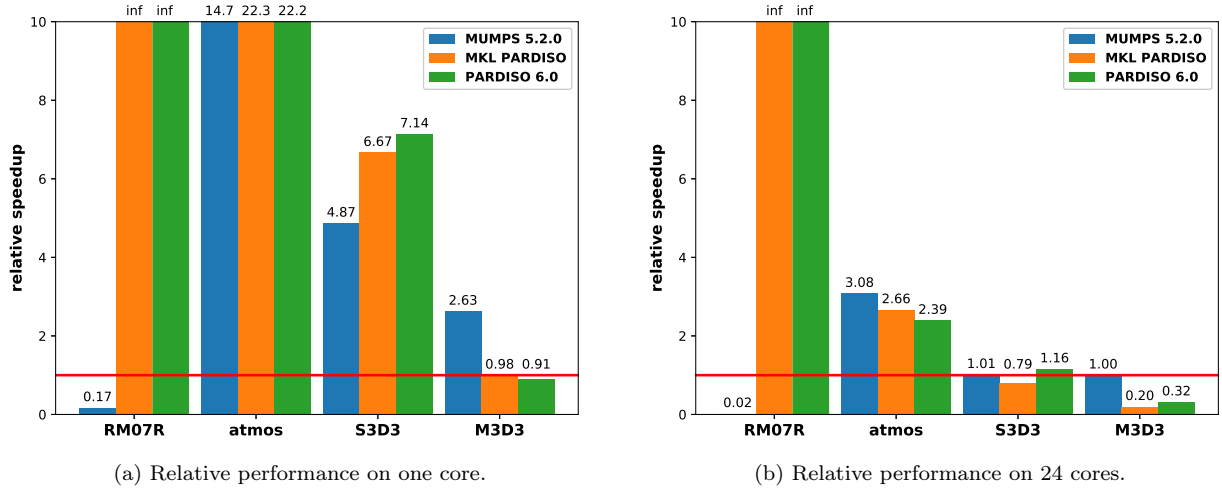


Figure 5.3: Relative performance HILUCSI versus MUMPS, MKL PARDISO, and PARDISO 6 for larger systems. Higher is better for HILUCSI.

5.4 Comparison with multithreaded solvers

Our comparisons above showed that HILUCSI improved the robustness and efficiency compared to the state-of-the-art ILU preconditioners for iterative solvers. In recent years, significant research has been devoted to developing parallel solvers, such as PETSc [9], hypre [43], SuperLU_MT/SuperLU_Dist [65], pARMS [68], MUMPS [6], PARDISO [79, 92], fine-grained ILU [28], etc. Since most computers nowadays have multiple cores, it is therefore a natural question to ask how well HILUCSI performs compared to parallel solvers when using all the cores on a desktop in a way “transparent” to the end-user. Hence, we compare our serial HILUCSI against three state-of-the-art multithreaded solvers, including MUMPS 5.2.0, MKL PARDISO v2018/3.222, and PARDISO 6.0. Although these are all branded as direct solvers, MKL PARDISO and PARDISO trade stability for performance by pivoting within supernode only and replacing tiny pivots by a small epsilon, similar to that in [66]. In addition, PARDISO 6 has an implementation of multilevel ILU for symmetric indefinite systems based on ILUPACK [91], but its overall performance was worse than the direct solver in PARDISO 6, so we only report the comparison with the direct solvers.

First, we compare the robustness. MUMPS solved all the problems in Table 2. In contrast, both versions of PARDISO failed for RM07R and PR02R with the default settings, which have iterative refinements enabled, resulting in a success rate of 90%, which is comparable to ILUPACK but worse than HILUCSI. The failures were due to encountering too many tiny or zero pivots within supernodes, which “rendered the factorization well-defined but essentially useless” [92] for these linear systems.

Next, we assess the performance for larger systems. We focus on the four largest systems in Table 2. Figure 5.3 shows the relative speed of HILUCSI (including its timing for RM07R in Table 2 and its timing for the others in Tables 3 and 4) versus those three packages. For the three larger problems, namely atmosmodl, S3D3, and M3D3, which had approximately one million unknowns, HILUCSI outperformed MUMPS and both versions of PARDISO on a single core. In addition, the serial HILUCSI is competitive with the parallel performance of MUMPS and PARDISO on 24 cores. However, for RM07R, which is relatively small, MUMPS outperformed HILUCSI significantly both in serial and in parallel. Overall, HILUCSI was highly competitive for large systems with more than one million unknowns when using optimized parameters.

6 Conclusions and Future Work

In this paper, we described a multilevel incomplete LU factorization technique, called HILUCSI. HILUCSI is sophisticated in that it mixes the equilibration and reordering techniques for symmetric and unsymmetric matrices, and it also introduces static pivoting, modified inverse-based dynamic deferring, and hierarchical

dual thresholding. Nevertheless, compared to some of the advanced ILU packages, such as ILUPACK and SuperLU, HILUCSI is relatively simple in that it does not require partial or Bunch-Kaufman pivoting for stability. We showed that HILUCSI achieved robustness and efficiency for a wide range of linear systems, especially for problems arising from systems of PDEs. Those systems are often challenging when using only symmetric or unsymmetric techniques alone. We demonstrated the robustness of HILUCSI as a right-preconditioner of restarted GMRES for symmetric and unsymmetric saddle-point problems from mixed Poisson, Stokes, and Navier-Stokes equations as well as some non-PDE problems. Our results showed that HILUCSI outperforms ILUPACK by a factor of four to ten for medium to large problems. Because HILUCSI scales better as the number of unknowns increases, its performance advantage would become even wider for larger problems.

In its current form, HILUCSI has several limitations. First, if the memory is very limited, there may be too many scalability-oriented droppings and the preconditioner may lose robustness. We plan to optimize HILUCSI further for limited-memory situations. Second, for vector-valued PDEs, the matrices may exhibit block structures. It is worthwhile to explore such block structures to improve cache performance, similar to that in [67] and [49]. Finally, HILUCSI is presently sequential. Although its serial performance is competitive with the parallel performance of MUMPS on 24 cores for large systems, it is desirable to speed up HILUCSI via parallelization.

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