On incomplete Cholesky factorizations in half precision arithmetic

Jennifer Scott
1,2*† and Miroslav Tůma³†

1*School of Mathematical, Physical and Computational Sciences,
 University of Reading, Reading RG6 6AQ, UK.
 2STFC Rutherford Appleton Laboratory, Didcot, Oxfordshire,
 OX11 0QX, UK. ORCID iD: 0000-0003-2130-1091.
 3Department of Numerical Mathematics, Faculty of Mathematics and
 Physics, Charles University, Czech Republic. ORCID iD:
 0000-0003-2808-6929.

*Corresponding author(s). E-mail(s): jennifer.scott@reading.ac.uk; Contributing authors: mirektuma@karlin.mff.cuni.cz; †These authors contributed equally to this work.

Abstract

Incomplete factorizations have long been popular general-purpose algebraic preconditioners for solving large sparse linear systems of equations. Guaranteeing the factorization is breakdown free while computing a high quality preconditioner is challenging. A resurgence of interest in using low precision arithmetic makes the search for robustness more important and more challenging. In this paper, we focus on symmetric positive definite problems and explore a number of approaches for preventing and handling breakdowns: prescaling of the system matrix, a look-ahead strategy to anticipate break down as early as possible, the use of global shifts, and a modification of an idea developed in the field of numerical optimization for the complete Cholesky factorization of dense matrices. Our numerical simulations target highly ill-conditioned sparse linear systems with the goal of computing the factors in half precision arithmetic and then achieving double precision accuracy using mixed precision refinement. We also consider the often overlooked issue of growth in the sizes of entries in the factors that can occur when using any precision and can render the computed factors ineffective as preconditioners.

Keywords: half precision arithmetic, preconditioning, incomplete factorizations, iterative methods for linear systems

1 Introduction

Our interest is in solving large-scale symmetric positive definite (SPD) linear systems of equations Ax = b. Incomplete Cholesky (IC) factorizations of the form $A \approx LL^T$, where the factor L is a sparse lower triangular matrix, have long been important and well-used algebraic preconditioners for use with iterative solvers. While they are general purpose and, when compared to sparse direct solvers, require modest computational resources, they do have drawbacks. Their effectiveness can be highly application dependent and, although significant effort has gone into developing a strong theoretical background, most results are limited to model problems. To be useful in practice, their computation and application must be efficient and robust.

Traditionally, matrix factorizations have most often been computed using double precision floating-point arithmetic, which nowadays corresponds to a 64-bit floating-point number format. However, half precision arithmetic is being increasingly supported by modern hardware and because it can offer speed benefits while using less energy and memory, there has been significant interest in recent years in its use in numerical linear algebra; see the comprehensive review [1] and references therein. For linear systems, one strategy that has received attention is GMRES-IR [2]. The idea is to compute the matrix factors in low precision arithmetic and then employ them as preconditioners for GMRES within mixed precision iterative refinement (see also [1, 3, 4] and, for SPD systems, [5]). Using low precision incomplete factors may enable much larger problems to be solved (normally at the cost of more iterations to achieve the requested accuracy). In an initial study [6], we explored this approach, focusing on the safe avoidance of overflows that can occur when computing matrix factors using half precision arithmetic. In the current paper, we again consider half precision IC factorizations and their use in solving ill-conditioned sparse SPD linear systems to double precision accuracy.

When using any precision, breakdown can occur during an incomplete factorization, that is, a pivot may be zero or negative where an exact Cholesky factorisation would have only positive pivots, or a computation within the factorization may overflow. A review is given in the Lapack Working Note [7]. Breakdown is more likely when using low precision arithmetic. This is partly because the initial matrix A must be "squeezed" into half precision, which may mean the resulting matrix is not (sufficiently) positive definite [8]. But, in addition, overflows outside the narrow range of possible numerical values are an ever-present danger. Our interest lies in exploring strategies to prevent breakdown during sparse matrix factorizations. Importantly, these must be robust, inexpensive and not cause serious degradation to the preconditioner quality. We consider and compare the performance in half precision arithmetic of a number of strategies to limit the likelihood of breakdown: prescaling the matrix before it is squeezed, look ahead that checks the diagonal entries of the partially factorized matrix at each major step of the factorization, the use of global shifts, and an approach based on locally modifying the factorization. The latter was originally used to modify approximate (dense) Hessian matrices in the field of numerical optimization. We also demonstrate that, even if double precision is used throughout the computation and breakdown does not occur, it is essential to take action to prevent growth in the factor entries because otherwise, the factors can be ineffective as preconditioners.

The paper is organised as follows. Section 2 looks at the different stages at which breakdown can occur within an incomplete factorization. In Section 3, we present a number of ways to prevent and handle breakdown. Numerical results for a range of highly ill-conditioned linear systems coming from practical applications are presented in Section 4. Finally, in Section 5, our findings and conclusions are summarised.

Terminology. We use high precision (denoted by fp64) to refer to IEEE double precision (64-bit) and low precision (denoted by fp16) for the 1985 IEEE standard 754 half precision (16-bit). Note that bfloat16 is another form of half precision arithmetic but it is not used it in this paper. Table 1 summarises the parameters for different precision arithmetic.

Table 1 Parameters for fp16, fp32, and fp64 arithmetic: the number of bits in the significand and exponent, unit roundoff u, smallest positive (subnormal) number x_{min}^s , smallest normalized positive number x_{min} , and largest finite number x_{max} , all given to three significant figures.

	Signif.	Exp.	u	x_{min}^s	x_{min}	x_{max}
fp16	11	5		5.96×10^{-8}	6.10×10^{-5}	6.55×10^4
fp32	24			1.40×10^{-45}		3.40×10^{38}
fp64	53	11	1.11×10^{-16}	4.94×10^{-324}	2.22×10^{-308}	1.80×10^{308}

2 Possible breakdowns within IC factorizations

A myriad of approaches for computing incomplete factorizations of sparse matrices have been developed, modified and refined over many years. Some combine the factorization with an initial step that discards small entries in A (sparsification). For details of possible variants, we recommend [9, 10], while a comprehensive discussion of early strategies can be found in [11]; see also [12] for a short history and the recent monograph [13] for a broad overview and skeleton algorithms.

Algorithm 1 outlines a basic (right-looking) incomplete Cholesky (IC) factorization of a sparse SPD matrix $A = \{a_{ij}\}$. It assumes a target sparsity pattern $\mathcal{S}\{L\}$ for the incomplete factor $L = \{l_{ij}\}$ is provided, where

$$S{L} = {(i,j) | l_{ij} \neq 0, 1 \leq j \leq i \leq n}.$$

The simplest case $\mathcal{S}\{L\} = \mathcal{S}\{A\}$ is called an IC(0) factorization. Modifications to Algorithm 1 can be made to incorporate threshold dropping strategies and to determine $\mathcal{S}\{L\}$ as the method proceeds. At each major step k, outer product updates are applied to the part of the matrix that has yet to be factored (Lines 7–11).

Unfortunately, unlike a complete Cholesky factorization, there is no guarantee in general that an IC algorithm will not break down or exhibit large growth in the size of the factor entries (even when using double precision arithmetic). This is illustrated

Algorithm 1 Basic right-looking sparse IC factorization

Input: Sparse SPD matrix A and a target sparsity pattern $\mathcal{S}\{L\}$ Output: Incomplete Cholesky factorization $A \approx LL^T$

```
1: l_{ij} = a_{ij} for all (i, j) \in \mathcal{S}\{L\}
 2: for k = 1 : n do
                                                                                        \triangleright Start of k-th major step
          l_{kk} \leftarrow (l_{kk})^{1/2}
                                                                                   ▷ Diagonal entry is the pivot
          for i \in \{i > k \, | \, (i, k) \in \mathcal{S}\{L\}\} do
               l_{ik} \leftarrow l_{ik}/l_{kk}  \triangleright Scale pivot column k of the incomplete factor by the pivot
 5:
                                                                        \triangleright Column k of L has been computed
 6:
          for j \in \{j > k \, | \, (j,k) \in \mathcal{S}\{L\}\} do
 7:
               for i \in \{i \ge k \, | \, (i,k) \in \mathcal{S}\{L\}\} do
 8
                    l_{ij} \leftarrow l_{ij} - l_{ik}l_{jk}
                                                                        \triangleright Update operation on column j > k
 9:
               end for
10:
          end for
12: end for
```

by the following well-conditioned SPD matrix in which $\delta > 0$ is small

$$A = \begin{pmatrix} 3 & -2 & 0 & 2 & 0 \\ -2 & 3 & -2 & c & 0 \\ 0 & -2 & 3 & -2 & 0 \\ 2 & c & -2 & 8 + 2\delta & 2 \\ 0 & 0 & 0 & 2 & 8 \end{pmatrix}.$$

Choosing $\delta \ll 1$ and c=1 results in no growth in the entries of the IC(0) factor and no breakdown. However, if c=0 and entries (2,4) and (4,2) are removed from $\mathcal{S}\{A\}$ then the IC(0) factor becomes

$$\begin{pmatrix} d_1 \\ -2/d_1 & d_2 \\ 0 & -2/d_2 & d_3 \\ 2/d_1 & 0 & -2/d_3 & d_4 \\ 0 & 0 & 0 & 2/d_4 & d_5 \end{pmatrix},$$

with $d_1^2 = 3$, $d_2^2 = 5/3$, $d_3^2 = 3/5$, $d_4^2 = 2\delta$, and $d_5^2 = 8 - 2/\delta$. In this case, if $\delta \ll 1$ then there is large growth in the (5,4) entry and the factorization breaks down because the (5,5) entry is negative (for any working precision).

There are three places in Algorithm 1 where breakdown can occur. Following [6], we refer to these as B1, B2, and B3 breakdowns.

- B1: The diagonal entry l_{kk} may be unacceptably small or negative.
- B2: The column scaling $l_{ik} \leftarrow l_{ik}/l_{kk}$ may overflow.
- B3: The update operation $l_{ij} \leftarrow l_{ij} l_{ik}l_{jk}$ may overflow.

To develop robust IC factorization implementations, breakdowns must either be avoided or they must be detected and handled by restarting the computation with revised data. We seek to avoid breakdowns but, as we cannot guarantee there will be no breakdowns, we still need to monitor for them. A recent study involving multiprecision iterative refinement used the functions offered by MATLAB to check the computed factors for Inf and/or NaN entries and took action if such entries were found [14]. This is not a practical procedure for general use. One possible strategy is to use IEEE-754 floating-point exception handling. This allows overflows to occur, the execution continues until a status flag is checked and, at this point, if overflow has been detected, restarting is initiated; see, for example, [15]. This is straightforward but requires the user to employ the correct compiler flags, which may be challenging, for instance, when a solver is interfaced from other languages. Furthermore, it is likely that non-IEEE arithmetics will gain traction in the future [16]. An alternative and potentially more flexible strategy is to incorporate explicit tests for breakdown into the factorization algorithm. In this case, for an implementation to be robust, the tests employed must only use operations that cannot themselves overflow.

An operation is said to be *safe* in the precision being used if it cannot overflow. To safely detect B1 breakdown it is sufficient to check at Line 3 of Algorithm 1 that $l_{kk} \geq \tau_u$, where the threshold parameter satisfies $\tau_u > 1/x_{max}$. This ensures $(l_{kk})^{-1} < x_{max}$. Typical values are $\tau_u = 10^{-5}$ for half precision factorizations and $\tau_u = 10^{-20}$ for double precision [6]; these are used in our reported experiments (Section 4). B2 breakdown can happen at Line 5. Let l_{kmax} denote the entry below the diagonal in column k of largest absolute value, that is,

$$l_{kmax} = \max_{i>k} \{|l_{ik}| : (i,k) \in \mathcal{S}\{L\}\}.$$
(2.1)

If $l_{kmax} \leq x_{max}$ and $1 \leq l_{kk} \leq x_{max}$ or $l_{kk} \geq l_{kmax}/x_{max}$ then it is safe to compute l_{kmax}/l_{kk} (and thus safe to scale column k). B3 breakdown can occur at Line 9. We give an algorithm for safely detecting B3 breakdown in [6].

Note that although we are focusing on SPD problems and IC factorizations, B1, B2 and B3 breakdowns are also possible during complete or incomplete factorizations of nonsymmetric sparse matrices. Indeed, for non SPD problems, B2 breakdowns in particular are more likely to occur. To illustrate how B2 breakdown can happen, consider the following nonsymmetric matrix, which has some large off-diagonal entries

$$A = \begin{pmatrix} 3 & -2 & 0 & 2 & 2 \\ -2 & 3 & -2 & 0 & 0 \\ 0 & -2 & 3 & -1 & -1 \\ 2 & 0 & -2 & 2.01 & 2.01 \\ 1000 & 1000 & 1000 & 1000 & 100 \end{pmatrix}.$$

The LU factorization of A is given by

$$A = LU = \begin{pmatrix} 1 & & & & \\ -2/3 & 1 & & & \\ 0 & -1.2 & 1 & & \\ 2/3 & 0.8 & -2/3 & 1 & \\ 1000/3 & 1000 & 5000 & -400000 & 1 \end{pmatrix} \begin{pmatrix} 3 & -2 & 2 & 0 & 2 \\ 5/3 & -2 & 4/3 & 4/3 & \\ 0.6 & 0.6 & 0.6 & 0.6 & \\ & & 0.1 & 0.1 & \\ & & & -900 \end{pmatrix}.$$

When using fp16 arithmetic, B2 breakdown occurs on major step 4 because the (5,4) entry overflows (-4000 is divided by 0.01).

3 Preventing and handling breakdown in IC factorizations

While the use of safe tests allows action to be taken before breakdown occurs or the use of IEEE exception handling can capture breakdown, our objective is to reduce the likelihood of breakdown. This will limit the overheads involved in handling breakdowns and the effects on the quality of the computed factorizations through modifications to the data. Breakdown is much more likely to happen when using low precision arithmetic because of the greater likelihood of overflows occurring.

3.1 Avoiding breakdown by prescaling

For both direct and iterative methods for solving systems of equations it is often beneficial to prescale the matrix, that is, to determine diagonal matrices S_r and S_l (with $S_r = S_l$ in the symmetric case) such that the scaled matrix $\widehat{A} = S_r^{-1} A S_l^{-1}$ is "nicer" than the original A. By nicer, we mean that, compared with solving Ax = b, it is easier to solve the system $Ay = S_r^{-1}b$ and then set $x = S_l^{-1}y$. When working in fp16 arithmeters metic, scaling is essential because of the narrow range of the arithmetic (recall Table 1). Numbers of absolute value outside the interval $[x_{min}^s, x_{max}] = [5.96 \times 10^{-8}, 6.55 \times 10^4]$ cannot be represented in fp16 arithmetic and they underflow or overflow when converted to fp16 arithmetic. Moreover, to avoid the performance penalty of handling subnormal numbers, in practice numbers with small absolute values are often flushed to zero. We do this for all entries of absolute value less than 10^{-5} in fp16 arithmetic and 10^{-20} in fp64 arithmetic. When factorizing \widehat{A} in fp16 arithmetic, overflow and underflow may occur during the initial conversion (squeezing) of the matrix into fp16 arithmetic as well as during the factorization. The scaling must be chosen to prevent overflows. For incomplete factorizations, numbers that underflow or are flushed to zero are not necessarily a concern because the factorization is approximate. However, the resulting sparsification may mean that the scaled and squeezed matrix is close to being indefinite.

No single approach to constructing a scaling is universally the best and sparse solvers frequently include a number of options to allow users to experiment to determine the most effective for their applications. Our experience with IC factorizations of SPD matrices is that it is normally sufficient to use simple l_2 -norm scaling (that is, $S_r = S_l = D^{1/2}$ where d_{ii} is the 2-norm of row i of A, is computed in fp64 arithmetic),

resulting in the absolute values of the entries of the scaled matrix \widehat{A} being at most 1. This is used in the current study (but see [17], where equilibration scaling is used and [5] where scaling by the square root of the diagonal is used).

3.2 Preventing breakdown by incorporating look-ahead

Recall that the computation of the diagonal entries of the factor in a (complete or incomplete) Cholesky factorization are based on

$$l_{jj} = a_{jj} - \sum_{i < j} l_{ij}^2.$$

Hence, l_{jj} decreases on each major step k. Thus, to detect potential B1 breakdown as early as possible, look-ahead can be used whereby, for each k the remaining diagonal entries l_{jj} (j > k) are updated (using safe operations) and tested. For the right-looking Algorithm 1, it is straightforward to incorporate testing but, for some IC variants, it may be necessary to hold a copy of the diagonal entries of the factor. Look-ahead is employed in some well-known fp64 arithmetic implementations of IC factorizations e.g., [18, 19]. Algorithm 2 is a modified version of Algorithm 1 that includes checks for breakdown. The safe test for B3 breakdown can be modified so that, ahead of the loop at Line 13, a check is made that the entry of maximum magnitude in column k (that is, l_{kmax} from (2.1)) is less than $(x_{max})^{1/2}$. If it is not, flag = 3 is returned. Otherwise, the multiplication of l_{ik} and l_{jk} is safe and, at Line 17, only the subtraction needs to be checked. If in place of the safe tests, IEEE exception handling is used then the IEEE overflow flag should be tested at the end of each major loop (that is, between Lines 21 and 22).

To illustrate the usefulness of look-ahead, consider the following matrix

$$A = \begin{pmatrix} 3 & -2 & 0 & 1 & 2 \\ -2 & 3 & -2 & 0 & 0 \\ 0 & -2 & 3 & 0 & -2 \\ 1 & 0 & 0 & 5 & 0 \\ 2 & 0 & -2 & 0 & 8 \end{pmatrix}.$$

It is easy to check that A is SPD with condition number $\kappa_2(A) \approx 2*10^6$. If the IC(0) factorization is computed in exact arithmetic then the entry (5,5) of L is zero (B1 breakdown). The look-ahead strategy reveals this at the third step, thus reducing the work performed before breakdown is detected.

A consequence of look-ahead is that, through the early detection of B1 breakdowns and taking action to prevent such breakdowns, B3 breakdowns are indirectly prevented. In our numerical experiments on problems coming from real applications, all breakdowns when using fp16 arithmetic were of type B1 when look-ahead was incorporated. However, B2 and B3 breakdowns remain possible. Consider the following

Algorithm 2 Right-looking IC factorization with safe checks for breakdown

```
Input: SPD matrix A, a target sparsity pattern S\{L\}, parameter \tau_u > 0
Output: Either flag = 0 and A \approx L^T L or flag > 0 (breakdown detected)
 1: l_{ij} = a_{ij} for all (i, j) \in \mathcal{S}\{L\}
 2: flag = 0
 3: if l_{11} < \tau_u then flag = 1 and return
                                                                                        ⊳ B1 breakdown
 4: for k = 1 : n do
                                                                            \triangleright Start of k-th major step
         l_{kk} \leftarrow (l_{kk})^{1/2}
         if l_{kk} \ge 1 or l_{kk} \ge l_{max}/x_{max} then \triangleright l_{max} is largest off-diagonal entry (2.1)
             for i \in \{i > k \mid (i, k) \in \mathcal{S}\{L\}\} do
                  l_{ik} \leftarrow l_{ik}/l_{kk}
                                                                                 ▶ Perform safe scaling
             end for
                                                              \triangleright Column k of L has been computed
 9:
         else
10:
              flag = 2 and return
                                                                                        ▶ B2 breakdown
11:
12:
         end if
         for j \in \{j > k \mid (j, k) \in \mathcal{S}\{L\}\} do
                                                                        \triangleright Update columns j > k of L
13:
             for i \in \{i \ge j \mid (i, j) \in \mathcal{S}\{L\}\} do
14:
                  Test entry (i, j) can be updated safely
                                                                            \triangleright Use Algorithm 2.2 of [6]
15:
                  if not safe to update then flag = 3 and return
                                                                                        \trianglerightB3 breakdown
16:
                  l_{ij} \leftarrow l_{ij} - l_{ik}l_{jk}
                                                                   \triangleright Perform safe update operation
17:
             end for
18:
             if l_{ii} < \tau_u then flag = 1 and return
19:
                                                                                        ▶ B1 breakdown
         end for
20:
21: end for
```

well-conditioned SPD matrix and its complete Cholesky factor (three decimal places):

$$A = \begin{pmatrix} 3 & -2 & 0 & 2 & 0 \\ -2 & 3 & -2 & 0 & 0 \\ 0 & -2 & 3 & -2 & 0 \\ 2 & 0 & -2 & 8.00007 & 550 \\ 0 & 0 & 0 & 550 & 60000 \end{pmatrix}, \qquad L = \begin{pmatrix} 1.732 \\ -1.155 & 1.291 \\ 0 & -1.549 & 0.775 \\ 1.155 & 1.033 & -0.516 & 2.309 \\ 0 & 0 & 0 & 95.254 & 30.414 \end{pmatrix}$$

Observe that the (4,2) entry has filled in. The IC(0) factorization does not allow fill-in and, after four steps, the first four columns of the IC(0) factor of A are given by

$$L_{1:5,1:4} = \begin{pmatrix} 1.732 \\ -1.155 & 1.291 \\ 0 & -1.549 & 0.777 \\ 1.155 & 0 & -2.582 & 0.008 \\ 0 & 0 & 0 & 65738 \end{pmatrix}.$$

In fp16 arithmetic, the (5,4) entry overflows (B3 breakdown). This happens even with look-ahead because the first three entries in row 5 of A are zero and so the (5,4) entry is not updated until after column 4 has been computed. In this example, the (4,4) entry before its square root is taken is greater than τ_u (it is equal to $7*10^{-5}$) and so there is no B1 breakdown in column 4.

3.3 Global shifting to handle breakdown

Once potential breakdown has been detected (either through the B1-B3 tests or using IEEE exception handling) and the factorization halted, a common approach is to modify all the diagonal entries by selecting $\alpha > 0$, replacing the scaled matrix \hat{A} by $A + \alpha I$ and restarting the factorization. There is always an α^* such that for all $\alpha \geq \alpha^*$ the IC factorization of $A + \alpha I$ exists [20]. In practice, α^* is unlikely to be known a priori and it may be necessary to restart the factorization a number of times with ever larger shifts. Algorithm 3 summarizes the global shifting strategy for a SPD matrix held in precision u and for which an IC factorization in precision $u_l \geq u$ is wanted. After each unsuccessful factorization attempt, the shift is doubled [18]. Here $fl_l(\hat{A})$ denotes converting the matrix \widehat{A} from precision u to precision u_l . In our experiments, we use $\alpha_S = 10^{-3}$. The precise choice of the shift is not critical but it should not be unnecessarily large as this may result in the computed factors providing poor quality preconditioners. Note that more sophisticated strategies for changing the shift, which also allow the possibility for a shift to be decreased, are possible [19]. These have been developed for fp64 arithmetic. Our initial experiments suggest it is less clear that there are significant benefits of doing this when using fp16 arithmetic so in our experiments we only report results for using the simple shift doubling strategy.

Algorithm 3 Shifted incomplete IC factorization in precision u_l

8: end for

Input: SPD matrix A in precision u, diagonal scaling matrix S, a target sparsity pattern $S\{L\}$, and initial shift $\alpha_S > 0$

Output: Shift $\alpha \geq 0$ and incomplete Cholesky factorization $S^{-1}AS^{-1} + \alpha I \approx LL^T$ in precision u_l .

```
1: \widehat{A} = S^{-1}AS^{-1} \triangleright Symmetrically scale A
2: A_l = fl_l(\widehat{A}) \triangleright Convert to precision u_l
3: \alpha_0 = 0
4: for k = 0, 1, 2, \dots do
5: A_l + \alpha_k I \approx LL^T in precision u_l \triangleright We use Algorithm 4
6: If successful then set \alpha = \alpha_k and return
7: \alpha_{k+1} = \max(2\alpha_k, \alpha_S)
```

3.4 Local modifications to prevent breakdown

The next strategy is based on seeking to guarantee that the factorization exists by bounding the off-diagonal entries in L. So-called modified Cholesky factorization schemes have been widely used in nonlinear optimization to compute Newton-like directions. Given a symmetric (and possibly indefinite) A, a modified Cholesky algorithm factorizes $A + A_E$, where A_E is termed the correction matrix. The objectives are to compute the correction at minimal additional cost and to ensure $A + A_E$ is SPD and well-conditioned and close to A. A stable approach for dense matrices was originally proposed by Gill and Murray [21] and was subsequently refined by Gill, Murray and Wright (GMW) [22] and others [23–26].

Our GMW variant allows for sparse A and incomplete factorizations. In particular, the incompleteness that can lead to significant growth in the factor is a feature that implies modification of the GMW strategy is necessary. Consider the second example in Section 3.2. It clearly shows that once a diagonal entry is small, but not smaller than τ_u , it may be difficult to get a useful factorization by increasing this diagonal entry by an initially prescribed value that is independent of other entries in its column. In the GMW approach, at the start of major step k of the factorization algorithm, the updated diagonal entry l_{kk} is checked (before its square root is taken). If it is too small compared to the off-diagonal entries in its column then it is modified; a parameter $\beta > 0$ controls the local modification. Specifically, at step k, we set

$$l_{kk} = \max\left\{l_{kk}, \left(\frac{l_{kmax}}{\beta}\right)^2\right\},\tag{3.1}$$

where l_{kmax} is given by (2.1). If $(l_{kmax}/\beta)^2$ overflows (this can be safely checked) then the diagonal entry cannot be modified in this way. We call this a B4 breakdown. If despite the local modification potential breakdown is detected then the factorization is terminated and restarted using a global shift. As the following result shows, the $GMW(\beta)$ strategy limits the size of the off-diagonal entries in L and, for β sufficiently small, it prevents B3 breakdown.

Lemma 1. Let the matrix A be sparse and SPD. Assume that, using the $GMW(\beta)$ strategy, columns 1 to j-1 columns of the IC factor L have been successfully computed in fp16 arithmetic. For $i \geq j$ let nz(i) denote the number of nonzero entries in $L_{i,1:j-1}$. If

$$|a_{ij}| + \min(nz(i), nz(j))\beta^2 \le x_{max} \quad \text{for all} \quad (i, j) \in \mathcal{S}\{L\},$$
 (3.2)

where x_{max} is the largest finite number represented in fp16, then B3 breakdown cannot occur in the j-th step.

Proof. From (3.1), the offdiagonal entries in the first j-1 columns of L satisfy

$$\frac{|l_{ik}|}{(l_{kk})^{1/2}} \le \frac{|l_{ik}|\beta}{l_{kmax}} \le \beta, \quad 1 \le k \le j-1, \ i > k.$$

For any i > j we have

$$l_{ij} = \frac{1}{(l_{jj})^{1/2}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} l_{jk} \right) = \frac{\widetilde{l}_{ij}}{(l_{jj})^{1/2}}.$$
 (3.3)

To avoid breakdown, we require $|\tilde{l}_{ij}| \leq x_{max}$. From (3.2) and (3.3),

$$|\widetilde{l}_{ij}| \le |a_{ij}| + \min(nz(i), nz(j))\beta^2 \le x_{max},$$

and hence B3 breakdown does not occur.

Rules to determine the parameter β for the complete Cholesky factorization of dense matrices (in double precision) are discussed in [21, 22] but for sparse incomplete factorizations in fp16 arithmetic such sophisticated rules are not applicable. Provided β is not very small, its value is not critical to the quality of the preconditioner. Given β , Algorithm 4 incorporates the use of the GMW(β) strategy within the incomplete factorization. Note that the local modifications are not combined with look-ahead.

Algorithm 4 Right-looking IC factorization with safe checks for breakdown and GMW local modifications

```
Input: SPD matrix A, a target sparsity pattern S\{L\}, parameters \tau_u > 0 and \beta > 0
Output: Either flag = 0 and A \approx L^T L or flag > 0 (breakdown detected)
```

```
1: l_{ij} = a_{ij} for all (i, j) \in \mathcal{S}\{L\}
 2: Set flag = 0
 3: for k = 1 : n do
                                                                      \triangleright Start of k-th major step
        if (l_{max}/\beta)^2 does not overflow then \triangleright l_{max} is largest off-diagonal entry (2.1)
            Set l_{kk} = \max\{l_{kk}, (l_{max}/\beta)^2\}.
 5:
 6:
            flag = 4 and return
                                                                                  ⊳ B4 breakdown
 7:
 8:
        if l_{kk} < \tau_u then flag = 1 and return
                                                                                  ▶ B1 breakdown
 9:
        Follow Lines 5–22 of Algorithm 2, with Lines 18–20 (look-ahead) removed.
10:
11: end for
```

3.5 Recovering double precision accuracy

Having computed an incomplete factorization in low precision, we seek to recover double precision accuracy in the computed solution (although in many applications much less accuracy may be sufficient and all that is justified by the accuracy in the data). In their work on using mixed precision for solving general linear systems, Carson and

Higham [2] introduce a variant of iterative refinement that uses GMRES preconditioned by the LU factors of the matrix to solve the correction equation. Carson and Higham use two precisions and this was later extended to allow up to five precisions [3, 4]; see Algorithm 5. In the SPD case, a natural choice is to replace GMRES by the conjugate gradient (CG) method. Unfortunately, the supporting rounding error analysis relies on the backward stability of GMRES and preconditioned CG is not guaranteed to be backward stable [27]. Note, however, that mixed precision results presented in [5, 6] suggest that in practice CG-IR often works as well as GMRES-IR.

Algorithm 5 GMRES-based iterative refinement using five precisions (IC-Krylov-IR)

Input: SPD matrix A and vector b in precision u, five precisions u_r , u_g , u_p , u and u_ℓ , maximum number of outer iterations itmax > 0

Output: Computed solution of the system Ax = b in precision u

- 1: Compute IC factorization of A in precision u_{ℓ}
- 2: Initialize $x_1 = 0$
- 3: **for** i = 1 : itmax or until convergence **do**
- 4: Compute $r_i = b Ax_i$ in precision u_r ; store r_i in precision u
- Use preconditioned GMRES to solve $Ad_i = r_i$ at precision u_g , with preconditioning and products with A in precision u_p ; store d_i in precision u
- 6: Compute $x_{i+1} = x_i + d_i$ in precision u
- 7: end for

4 Numerical experiments

We follow a number of others working on the development of numerical linear algebra algorithms in mixed precision in performing experiments that aim to explore the feasibility of the ideas by using half precision (see, for example, [5, 8, 28, 29]). We want the option to experiment with sparse problems that may be too large for MAT-LAB and have chosen to develop our software in Fortran. We use the NAG compiler (Version 7.1, Build 7118), which is the only Fortran compiler that currently supports the use of fp16 arithmetic and conforms to the IEEE standard. In addition, using the **-roundhreal** option, all half-precision operations are rounded to half precision, both at compile time and runtime. Our numerical experiments are performed on a Windows 11-Pro-based machine with an Intel(R) Core(TM) i5-10505 CPU processor (3.20GHz).

Our test set of SPD matrices is given in Table 1. This set was used in our earlier study [30]. The problems come from a variety of application areas and are of different sizes and densities. As we expect that successfully using fp16 arithmetic will be most challenging for ill-conditioned problems, the problems were chosen because they all have a large estimated condition number (in the range $10^7 - 10^{16}$). Many are initially poorly scaled and some contain entries that overflow in fp16 and thus prescaling of A is essential. The right-hand side vector b is constructed by setting the solution x to be

the vector of 1's. In Table 1, we also report the number of entries in the "scaled and squeezed" matrix A_l (see Line 2 of Algorithm 3). The squeezing discards all entries of the scaled matrix with absolute value less than $\tau_u = 10^{-5}$. We see that this can lead to the loss of a significant number of entries.

Table 1 Statistics for our ill-conditioned test examples. nnz(A) denotes the number of entries in the lower triangular part of A. normA and normb are the infinity norms of A and b. cond2 is a computed estimate of the condition number of A. $nnz(A_l)$ is the number of entries in the lower triangular part of the matrix after scaling and squeezing.

Identifier	n	nnz(A)	normA	normb	cond2	$nnz(A_l)$
Boeing/msc01050	1050	1.51×10^4	2.58×10^{7}	1.90×10^{6}	4.58×10^{15}	4.63×10^{3}
HB/bcsstk11	1473	1.79×10^4	1.21×10^{10}	7.05×10^{8}	2.21×10^{8}	6.73×10^{3}
HB/bcsstk26	1922	1.61×10^4	1.68×10^{11}	8.99×10^{10}	1.66×10^{8}	6.59×10^{3}
HB/bcsstk24	3562	8.17×10^4	5.28×10^{14}	4.21×10^{13}	1.95×10^{11}	3.89×10^4
HB/bcsstk16	4884	1.48×10^{5}	4.12×10^{10}	9.22×10^{8}	4.94×10^{9}	5.24×10^4
Cylshell/s2rmt3m1	5489	1.13×10^{5}	9.84×10^{5}	1.73×10^4	2.50×10^{8}	5.09×10^4
Cylshell/s3rmt3m1	5489	1.13×10^{5}	1.01×10^{5}	1.73×10^{3}	2.48×10^{10}	5.07×10^4
Boeing/bcsstk38	8032	1.82×10^{5}	4.50×10^{11}	4.04×10^{11}	5.52×10^{16}	7.83×10^4
Boeing/msc10848	10848	6.20×10^5	4.58×10^{13}	6.19×10^{11}	9.97×10^{9}	3.02×10^{5}
Oberwolfach/t2dah_e	11445	9.38×10^4	2.20×10^{-5}	1.40×10^{-5}	7.23×10^{8}	4.88×10^4
Boeing/ct20stif	52329	1.38×10^{6}	8.99×10^{11}	8.87×10^{11}	1.18×10^{12}	6.30×10^5
DNVS/shipsec8	114919	3.38×10^{6}	7.31×10^{12}	4.15×10^{11}	2.40×10^{13}	7.70×10^{5}
GHS_psdef/hood	220542	5.49×10^{6}	2.23×10^{9}	1.51×10^{8}	5.35×10^{7}	2.66×10^{6}
Um/offshore	259789	2.25×10^{6}	1.44×10^{15}	1.16×10^{15}	4.26×10^9	1.17×10^{6}

Our results are for the level-based incomplete Cholesky factorization preconditioner $IC(\ell)$ with $\ell=2$ and 3 [31]. We refer to the $IC(\ell)$ factorizations computed using half and double precision arithmetic as fp16- $IC(\ell)$ and fp64- $IC(\ell)$, respectively. The key difference between the two versions is that for the former, during the incomplete factorization, we incorporate the safe checks for the scaling and update operations; for the fp64 version, tests for B1 breakdown are performed (B2 and B3 breakdowns were not encountered in our double precision experiments). The solves with L and L^T require the L factor to be in double precision. This can be done by casting the data into double precision and making an explicit copy of L; this negates the important benefit that half precision offers of reducing memory requirements. Alternatively, the entries can be cast on the fly. This is straightforward to incorporate into a serial triangular solve routine, and only requires a temporary double precision array of length n.

We use two precisions: $u_{\ell} = u_{16}$ for the incomplete factorization and $u_r = u_g = u_p = u_{64}$, where u_{16} and u_{64} denote the unit roundoffs in fp16 and fp64 arithmetic, respectively. That is, we aim to achieve double precision accuracy in the computed solution. The iterative refinement terminates when the normwise backward error for the computed solution satisfies

$$res = \frac{\|b - Ax\|_{\infty}}{\|A\|_{\infty} \|x\|_{\infty} + \|b\|_{\infty}} \le \delta = 10^3 \times u_{64}. \tag{4.1}$$

The implementation of GMRES is taken from the HSL software library [32], and its convergence tolerance is set to $u_{64}^{1/4}$ (see [30] for an explanation of this choice); for each application of GMRES the limit on the number of iterations is 1000.

Our first experiment looks at the effects of incorporating look-ahead. Table 2 presents results with no look-ahead and with look-ahead. Here we only include the test problems for which look-ahead had an effect. We make a number of observations. Incorporating look-ahead can improve robustness, particularly when using fp64 arithmetic. Without look-ahead, in fp64 arithmetic there can be very large growth in the size of some entries in the factors and this goes undetected (no B1 breakdowns occur with $\tau_u=10^{-20}$). With look-ahead, growth did not happen in our tests on ill conditioned problems. In fp16 arithmetic, look-ahead can replace B3 breakdown by B1 breakdown (e.g., HB/bcsstk24). Even if there are no B3 breakdowns, look-ahead can lead to a larger number of B1 breakdowns being flagged (see problem Boeing/msc01050) and hence a larger number of restarts, a larger shift and, consequently, a higher GMRES iteration count. Note that the iteration counts for IC(3) are not guaranteed to be smaller than for IC(2) (although they generally are).

Table 2 Results for IC-GMRES-IR using fp16- $IC(\ell)$ and fp64- $IC(\ell)$ preconditioners $(\ell=2,3)$ with no look-ahead and with look-ahead. its is the total number of GMRES iterations and (n1,n2) are the numbers of times B1 and B3 problems are detected (n2) is nonzero only for fp16- $IC(\ell)$ with no look-ahead). > 1000 indicates the requested accuracy was not obtained within the GMRES iteration limit. ‡ indicates failure to compute useful factors because of enormous growth in the entries.

Identifier	No look-ahead $its (n1, n2)$	With look-ahead $its (n1)$	No look-ahead $its (n1, n2)$	With look-ahead $its (n1)$
	fp16	fp16-IC(3)		
Boeing/msc01050 HB/bcsstk24 Um/offshore	65 (1, 0) 428 (0, 1) 2013 (0, 4)	84 (4) 428 (1) 129 (5)	62 (1, 0) 418 (0, 1) 40 (0, 4)	81 (4) 418 (1) 40 (4)
	fp64	fp64-IC(3)		
Boeing/msc01050 HB/bcsstk11 Cylshell/s3rmt3m1 Boeing/ct20stif GHS_psdef/hood Um/offshore	$\begin{array}{c} 24 \; (0, 0) \\ 201 \; (0, 0) \\ 102 \; (0, 0) \\ > 1000 \; (0, 0) \\ \vdots \; (0, 0) \\ \vdots \; (0, 0) \end{array}$	69 (4) 174 (1) 102 (0) 1940 (2) 568 (5) 128 (5)	$\begin{array}{c} 25 \ (0,0) \\ 29 \ (0,0) \\ > 1000 \ (0,0) \\ 1332 \ (0,0) \\ \vdots \ (0,0) \\ \vdots \ (0,0) \end{array}$	69 (4) 29 (0) 426 (1) 1368 (1) 407 (4) 37 (4)

Table 3 presents results for IC-GMRES-IR using a fp16-IC(2) preconditioner with look-ahead and the GMW(β) strategy for $\beta=0.5$, 10 and 100. B3 breakdown only occurs for GMW(100) (there is a single B3 breakdown for examples HB/bcsstk24 and Boeing/bcsstk38 and for these a global shift is used). B4 breakdown happens only for GMW(10) applied to GHS_psdef/hood (5 occurrences for this example) and GMW(100) applied to HB/bcsstk11 (happens once); again a global shift is used to avoid breakdown. We see that with $\beta=0.5$, for some examples a large number of local modifications (nmod) are made. This leads to the preconditioner being of poorer quality compared to the IC(2) preconditioner with look-ahead. For $\beta=10$, local modifications are only needed for a few problems (HB/bcsstk11, HB/bcsstk24 and Um/offshore). In each case, the resulting preconditioner is not successful. For

GMW(100), local modifications are only made for Um/offshore; for all other test examples, GMW(100) is equivalent to IC(2) with no look-ahead.

Table 3 Results for IC-GMRES-IR using a fp16-IC(2) preconditioner with the GMW(β) strategy and with look-ahead. its is the number of GMRES iterations and (n1, nmod) are the numbers of times B1 breakdown is detected and the number of local modifications made by the GMW strategy. \sharp and * indicate B3 and B4 breakdowns, respectively. > 1000 indicates the requested accuracy was not obtained within the GMRES iteration limit.

Identifier	$\begin{array}{c} \text{GMW}(0.5) \\ its \ (n1, nmod) \end{array}$	$\begin{array}{c} \text{GMW}(10) \\ its \ (n1, nmod) \end{array}$	$GMW(100)$ $its\ (n1, nmod)$	With look-ahead $its (n1)$
Boeing/msc01050	96 (0, 60)	65 (1, 0)	65 (1, 0)	84 (4)
HB/bcsstk11	1092 (0, 476)	> 1000 (0, 310)	205*(0,0)	205 (1)
HB/bcsstk26	786 (0, 476)	111 (1, 0)	111 (1, 0)	87 (1)
HB/bcsstk24	1018 (0, 446)	> 1000 (0, 428)	$428^{\sharp} (0, 0)$	428 (1)
HB/bcsstk16	41 (0, 26)	23(0,0)	23 (0, 0)	23 (0)
Cylshell/s2rmt3m1	787 (0, 584)	155(0,0)	155(0,0)	155 (0)
Cylshell/s3rmt3m1	2017 (1, 710)	630 (2, 0)	630(2,0)	630 (2)
Boeing/bcsstk38	1335 (1, 914)	313 (1, 0)	$313^{\sharp} (0, 0)$	313 (1)
Boeing/msc10848	684 (0, 591)	81 (0, 0)	81 (0, 0)	81 (O)
Oberwolfach/t2dah_e	11 (0, 6)	7(0,0)	7(0,0)	7 (0)
Boeing/ct20stif	2139 (0, 4827)	1900 (2, 0)	1900 (2, 0)	1900 (2)
DNVS/shipsec8	2569(1, 1)	2390 (1, 0)	2390 (1, 0)	1492 (1)
GHS_psdef/hood	2459 (0, 25074)	581* (0, 0)	581 (5, 0)	581 (5)
Um/offshore	> 1000 (0, 3846)	> 1000 (0, 5838)	2013(4, 2)	129 (5)

The sensitivity of the GMW(β) approach to the choice of β is reported on in Table 4 for problem Boeing/bcsstk38. As β increases, the number of local modifications to diagonal entries (nmod) steadily decreases and so too does the GMRES iteration count (its). For this example, for each $\beta \geq 0.4$, B1 breakdown was detected once and a global shift $\alpha = 10^{-3}$ was then employed.

Table 4 Results for problem Boeing/bcsstk38. IC-GMRES-IR is run using a fp16-IC(2) preconditioner computed with the GMW(β) strategy for a range of values of β . nmod and its are the numbers of local modifications made by the GMW strategy and GMRES iterations, respectively.

β	0.1	0.2	0.3	0.4	0.45	0.5	0.6	0.7	0.8	0.9	1.0
nmod	7404	5751	3695	1891	1327	914	621	409	138	8	0
		2634						390	321	313	313

Finally, results for IC-GMRES-IR using a fp64-IC(2) preconditioner are given in Table 5. As we would expect, the number of breakdowns and the iteration counts are often less than for the fp16-IC(2) preconditioner. If $\beta=0.5$, the number of local modifications when using fp64 arithmetic is very similar to the number when using fp16 and the iteration counts are also comparable. For larger β , fp64 can result in a higher quality preconditioner but, as earlier, without look-ahead the computed preconditioner can be ineffective.

All the reported results employed our explicit safe tests for breakdown. We have also run the fp16 arithmetic experiments with the B1 to B4 breakdown tests replaced

Table 5 Results for IC-GMRES-IR using a fp64-IC(2) preconditioner with the GMW(β) strategy and IC(2) with look-ahead. its is the number of GMRES iterations and (n1,nmod) are the numbers of times B1 breakdown is detected and the number of local modifications made by the GMW strategy. For GMW(0.5) and GMW(10), n1=0 for all examples so is omitted. > 1000 indicates the requested accuracy was not obtained within the GMRES iteration limit. ‡ indicates failure to compute useful factors because of enormous growth in the entries.

Identifier	GMW(0.5)	GMW(10)	GMW(100)	With look-ahead
	$its \ (nmod)$	$its \ (nmod)$	$its\ (n1,nmod)$	its (n1)
Boeing/msc01050	78 (60)	24(0)	24 (4, 0)	24(0)
HB/bcsstk11	1087 (476)	201 (0)	201 (0, 0)	232 (0)
HB/bcsstk26	775 (476)	79 (0)	79 (0, 0)	79 (0)
HB/bcsstk24	913 (409)	89 (0)	89 (0, 0)	89 (0)
HB/bcsstk16	41 (26)	22 (0)	22(0,0)	22 (0)
Cylshell/s2rmt3m1	792 (585)	146 (0)	146 (0, 0)	146 (0)
Cylshell/s3rmt3m1	2901 (710)	102 (0)	102(0,0)	102 (0)
Boeing/bcsstk38	1301 (943)	141 (0)	141 (0, 0)	141 (0)
Boeing/msc10848	790 (600)	68 (0)	68 (0, 0)	68 (0)
Oberwolfach/t2dah_e	14 (6)	6 (0)	6 (0, 0)	6 (0)
Boeing/ct20stif	2122 (4847)	2036 (40)	> 1000 (0, 0)	1940 (2)
DNVS/shipsec8	701 (4658)	354 (0)	354 (0, 55)	354 (0)
GHS_psdef/hood	2480 (25054)	> 1000 (2013)	> 1000 (0, 11998)	568 (5)
Um/offshore	> 1000 (4094)	> 1000 (6327)	‡(4, 4730)	128 (5)

by IEEE exception handling. As expected, because in fp16 arithmetic $\tau_u = 10^{-5}$ and $x_{min} = \mathcal{O}(10^{-5})$, this led to the same number of restarts and hence the same iteration counts. However, by only testing the exception flag at the end of each major step, this approach did not distinguish between the different types of breakdown. For the experiments using fp64 arithmetic, IEEE exception handling did not detect any problems and consequently, for some examples, this led to growth in the factor entries (exactly as in the case of no look-ahead).

5 Concluding remarks

Following on from our earlier study [30], in this paper we have again illustrated the potential for using half precision arithmetic to compute incomplete factorization preconditioners that can be used to obtain double precision accuracy in the solution of highly ill conditioned symmetric positive definite linear systems. In fp16 arithmetic, the danger of breakdown during the factorization of a sparse matrix is imminent and we must employ strategies that force computational robustness. To avoid breakdown, we have looked at global strategies plus a local modification scheme based on the GMW approach that has been used for dense matrices within the field of optimization. This strategy employs a parameter β . Choosing a small β prevents breakdown during the factorization (in both fp16 and fp64 arithmetic) and there is no need to employ a global shift. However, the penalty for avoiding the need to restart the factorization when possible breakdown is detected is a preconditioner that is of poorer quality than that which is obtained by employing a simple global shifting approach.

When using higher precision arithmetic, the potential dangers within an incomplete factorization algorithm can be hidden. As our experiments have demonstrated, a standard IC factorization using fp64 arithmetic without look-ahead can lead to an ineffective preconditioner because of growth in the size of the entries in the factors.

Without careful monitoring (which is not routinely done), this growth may be unobserved but when subsequently applying the preconditioner, the triangular solves can overflow, resulting in the computation aborting.

Finally, we reiterate that, although our focus has been on symmetric positive definite systems, breakdown and/or large growth in factor entries is also an issue for the incomplete factorization of general sparse matrices. Again, safe checks (or the use of IEEE exception handling) need to be built into the algorithms and their implementations to guarantee robustness.

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