

Reducing the Amount of Pivoting in Symmetric Indefinite Systems

Dulcenea Becker¹, Marc Baboulin⁴, and Jack Dongarra^{1,2,3}

¹ University of Tennessee, USA

{dbecker7,dongarra}@eecs.utk.edu

² Oak Ridge National Laboratory, USA

³ University of Manchester, United Kingdom

⁴ INRIA / Université Paris-Sud, France

marc.baboulin@inria.fr

Abstract. This paper illustrates how the communication due to pivoting in the solution of symmetric indefinite linear systems can be reduced by considering innovative approaches that are different from pivoting strategies implemented in current linear algebra libraries. First a tiled algorithm where pivoting is performed within a tile is described and then an alternative to pivoting is proposed. The latter considers a symmetric randomization of the original matrix using the so-called recursive butterfly matrices. In numerical experiments, the accuracy of tile-wise pivoting and of the randomization approach is compared with the accuracy of the Bunch-Kaufman algorithm.

Keywords: dense linear algebra, symmetric indefinite systems, LDL^T factorization, pivoting, tiled algorithms, randomization.

1 Introduction

A symmetric matrix A is called indefinite when the quadratic form $x^T Ax$ can take on both positive and negative values. By extension, a linear system $Ax = b$ is called symmetric indefinite when A is symmetric indefinite. These types of linear systems are commonly encountered in optimization problems coming from physics of structures, acoustics, and electromagnetism, among others. Symmetric indefinite systems also result from linear least squares problems when they are solved via the augmented system method [7, p. 77].

To ensure stability in solving such linear systems, the classical method used is called the diagonal pivoting method [9] where a block- LDL^T factorization¹ is obtained such as

$$PAP^T = LDL^T \quad (1)$$

where P is a permutation matrix, A is a symmetric square matrix, L is unit lower triangular and D is block-diagonal, with blocks of size 1×1 or 2×2 ;

¹ Another factorization method is for example the Aasen's method [13, p.163]: $PAP^T = LTL^T$ where L is unit lower triangular and T is tridiagonal.

all matrices are of size $n \times n$. If no pivoting is applied, *i.e.* $P = I$, D becomes diagonal. The solution x can be computed by successively solving the triangular or block-diagonal systems $Lz = Pb$, $Dw = z$, $L^T y = w$, and ultimately we have $x = P^T y$.

There are several pivoting techniques that can be applied to determine P . These methods involve different numbers of comparisons to find the pivot and have various stability properties. As for the LU factorization, the *complete pivoting* method (also called *Bunch-Parlett* algorithm [9]) is the most stable pivoting strategy. It guarantees a satisfying growth factor bound [14, p. 216] but also requires up to $\mathcal{O}(n^3)$ comparisons. The well-known *partial pivoting* method, based on the *Bunch-Kaufman* algorithm [8], is implemented in LAPACK [1] and requires at each step of the factorization the exploration of two columns, resulting in a total of $\mathcal{O}(n^2)$ comparisons. This algorithm has good stability properties [14, p. 219] but in certain cases $\|L\|$ may be unbounded, which is a cause for possible instability [3], leading to a modified algorithm referred to as *rook pivoting* or *bounded Bunch-Kaufman pivoting*. The latter involves between $\mathcal{O}(n^2)$ and $\mathcal{O}(n^3)$ comparisons depending on the number of 2×2 pivots. Another pivoting strategy, called *Fast Bunch-Parlett* strategy (see [3, p. 525] for a description of the algorithm), searches for a local maximum in the current lower triangular part. It is as stable as the rook pivoting but it also requires between $\mathcal{O}(n^2)$ and $\mathcal{O}(n^3)$ comparisons.

With the advent of architectures such as multicore processors [19] and Graphics Processing Units (GPU), the growing gap between communication and computation efficiency made the communication overhead due to pivoting more critical. These new architectures prompted the need for developing algorithms that lend themselves to parallel execution. A class of such algorithms for shared memory architectures, called *Tiled Algorithms*, has been developed for one-sided dense factorizations² [10,11] and made available as part of the PLASMA library [12].

Tiled algorithms are based on decomposing the computation into small tasks in order to overcome the sequential nature of the algorithms implemented in LAPACK. These tasks can be executed out of order, as long as dependencies are observed, rendering parallelism. Furthermore, tiled algorithms make use of a tile data-layout where data is stored in contiguous blocks, which differs from the column-wise layout used by LAPACK, for instance. The tile data-layout allows the computation to be performed on small blocks of data that fit into cache, and hence exploits cache locality and re-use. However, it does not lend itself straightforwardly for pivoting, as this requires a search for pivots and permutations over full columns/rows. For symmetric matrices, the difficulties are even greater since symmetric pivoting requires interchange of both rows and columns. The search for pivots outside a given tile curtails memory locality and increases data dependence between tiles (or tasks). The former has a direct impact on the performance of serial kernels and the latter on parallel performance [18].

In this paper, the possibility of eliminating the overhead due to pivoting by considering randomization techniques is investigated. These techniques were

² LDL^T is still under development and shall be available in the future [6].

initially proposed in [16] and modified approaches were studied in [4,5] for the LU factorization. In this context, they are applied to the case of symmetric indefinite systems. According to this random transformation, the original matrix A is transformed into a matrix that would be sufficiently “random” so that, with a probability close to 1, pivoting is not needed. This transformation is a multiplicative preconditioning by means of random matrices called *recursive butterfly matrices*. The LDL^T factorization without pivoting is then applied to the preconditioned matrix. One observes that two levels of recursion for butterfly matrices are enough to obtain an accuracy close to that of LDL^T with either partial (Bunch-Kaufman) or rook pivoting on a collection of matrices. The overhead is reduced to $\sim 8n^2$ operations, which is negligible when compared to the cost of pivoting.

2 Tile-Wise Pivoting

Given Equation (1), the tiled algorithm starts by decomposing A in $nt \times nt$ tiles³ (blocks), where each A_{ij} is a tile of size $nb \times nb$. The same decomposition can be applied to L and D . For instance, for $nt = 3$:

$$\begin{bmatrix} A_{11} & A_{21}^T & A_{31}^T \\ A_{21} & A_{22} & A_{32}^T \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} L_{11} & & \\ L_{21} & L_{22} & \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} D_{11} & & \\ & D_{22} & \\ & & D_{33} \end{bmatrix} \begin{bmatrix} L_{11}^T & L_{21}^T & L_{31}^T \\ & L_{22}^T & L_{32}^T \\ & & L_{33}^T \end{bmatrix} \quad (2)$$

Upon this decomposition and using the same principle as the Schur complement, a series of tasks can be set to calculate each L_{ij} and D_{ii} :

$$[L_{11}, D_{11}] = \text{LDL}(A_{11}) \quad (3)$$

$$L_{21} = A_{21}^T (D_{11} L_{11}^T)^{-1} \quad (4)$$

$$L_{31} = A_{31}^T (D_{11} L_{11}^T)^{-1} \quad (5)$$

$$\tilde{A}_{22} = A_{22} - L_{21} D_{11} L_{21}^T \quad (6)$$

$$\tilde{A}_{32} = A_{32} - L_{31} D_{11} L_{21}^T \quad (7)$$

$$[L_{22}, D_{22}] = \text{LDL}(\tilde{A}_{22}) \quad (8)$$

$$L_{32} = \tilde{A}_{32} (D_{22} L_{22}^T)^{-1} \quad (9)$$

$$\tilde{A}_{33} = A_{33} - L_{31} D_{11} L_{31}^T - L_{32} D_{22} L_{32}^T \quad (10)$$

$$[L_{33}, D_{33}] = \text{LDL}(\tilde{A}_{33}) \quad (11)$$

$\text{LDL}(X_{kk})$ at Equations (3), (8) and (11) means the actual LDL^T factorization of tile X_{kk} . These tasks can be executed out of order, as long as dependencies are observed, rendering parallelism (see [6] for more details).

Following the same approach, for $PAP^T = \text{LDL}^T$, and given

$$P = \begin{bmatrix} P_{11} & & \\ & \ddots & \\ & & P_{nt,nt} \end{bmatrix} \quad (12)$$

³ For rectangular matrices, A is decomposed into $mt \times nt$ tiles.

the tasks for $nt = 3$ may be described as:

$$[L_{11}, D_{11}, P_{11}] = \text{LDL}(A_{11}) \quad (13)$$

$$L_{21} = P_{22}A_{21}P_{11}^T(D_{11}L_{11}^T)^{-1} \quad (14)$$

$$L_{31} = P_{33}A_{31}P_{11}^T(D_{11}L_{11}^T)^{-1} \quad (15)$$

$$\tilde{A}_{22} = A_{22} - (P_{22}^T L_{21})D_{11}(P_{22}^T L_{21})^T \quad (16)$$

$$\tilde{A}_{32} = A_{32} - (P_{33}^T L_{31})D_{11}(P_{33}^T L_{31})^T \quad (17)$$

$$[L_{22}, D_{22}, P_{22}] = \text{LDL}(\tilde{A}_{22}) \quad (18)$$

$$L_{32} = P_{33}\tilde{A}_{32}P_{22}^T(D_{22}L_{22}^T)^{-1} \quad (19)$$

$$\tilde{A}_{33} = A_{33} - (P_{33}^T L_{31})D_{11}(P_{33}^T L_{31})^T - (P_{33}^T L_{32})D_{22}(P_{33}^T L_{32})^T \quad (20)$$

$$[L_{33}, D_{33}, P_{33}] = \text{LDL}(\tilde{A}_{33}) \quad (21)$$

Equations (13) to (21) are similar to Equations (3) to (11), except that the permutation matrix P_{kk} has been added. This permutation matrix P_{kk} generates a circular dependence between equations, which is not an issue when pivoting is not used. For instance, in order to calculate

$$L_{21} = P_{22}A_{21}P_{11}^T(D_{11}L_{11}^T)^{-1} \quad (22)$$

P_{22} is required. However, to calculate

$$[L_{22}, D_{22}, P_{22}] = \text{LDL}(A_{22} - (P_{22}^T L_{21})D_{11}(P_{22}^T L_{21})^T) \quad (23)$$

L_{21} is required. To overcome this circular dependence, instead of actually calculating L_{21} , $P_{22}^T L_{21}$ is calculated, since the equations can be rearranged such as $P_{22}^T L_{21}$ is always used and therefore L_{21} is not needed. Hence, Equations (14), (15) and (19) become, in a general form,

$$P_{ii}^T L_{ij} = A_{ij}P_{jj}^T(D_{jj}L_{jj}^T)^{-1} \quad (24)$$

After P_{ii} is known, L_{ij} , for $1 \geq j \geq i - 1$, can be calculated such as

$$L_{ij} = P_{ii}L_{ij} \quad (25)$$

This procedure may be described as in Algorithm 1, where A is a symmetric matrix of size $n \times n$ split in $nt \times nt$ tiles A_{ij} , each of size $nb \times nb$.

The permutation matrices P_{kk} of Algorithm 1 are computed during the factorization of tile A_{kk} . If pivots were searched only inside tile A_{ii} , the factorization would depend only and exclusively on A_{kk} . However, for most pivoting techniques, pivots are searched throughout columns, which make the design of efficient parallel algorithm very difficult [18].

The tile-wise pivoting restricts the search of pivots to the tile A_{kk} when factorizing it, *i.e.* if LAPACK [1] routine xSYTRF was chosen to perform the factorization, it could be used as it is. In other words, the same procedure used to

Algorithm 1. Tiled LDL^T Factorization with Tile-wise Pivoting

```

1: for  $k = 1$  to  $nt$  do
2:    $[L_{kk}, D_{kk}, P_{kk}] = \text{LDL}(A_{kk})$ 
3:   for  $j = k + 1$  to  $nt$  do
4:      $L_{jk} = A_{jk} P_{jj}^T (D_{kk} L_{kk}^T)^{-1}$ 
5:   end for
6:   for  $i = k + 1$  to  $nt$  do
7:      $A_{ii} = A_{ii} - L_{ik} D_{kk} L_{ik}^T$ 
8:     for  $j = k + 1$  to  $i - 1$  do
9:        $A_{ij} = A_{ij} - L_{ik} D_{kk} L_{jk}^T$ 
10:    end for
11:  end for
12:  for  $i = 1$  to  $j - 1$  do
13:     $L_{ki} = P_{kk} L_{ki}$ 
14:  end for
15: end for
    
```

factorize an entire matrix A is used to factorize the tile A_{kk} . This approach does not guarantee the accuracy of the solution; it strongly depends on the matrix to be factorized and how the pivots are distributed. However, it guarantees numerical stability of the factorization of each tile A_{kk} , as long as an appropriate pivoting technique is applied. For instance, LDL^T without pivoting fails as soon as a zero is found on the diagonal, while the tile-wise pivoted LDL^T does not, as shown in Section 4. Note that pivoting is applied as part of a sequential kernel, which means that the pivot search and hence the permutations are also serial.

3 An Alternative to Pivoting in Symmetric Systems

A randomization technique that allows pivoting to be avoided in the LDL^T factorization is described. This technique was initially proposed in [16] in the context of general linear systems where the randomization is referred to as Random Butterfly Transformation (RBT). It is shown in [16] that, with probability 1, Gaussian Elimination can operate without pivoting on the randomized matrix. Then a modified approach has been described in [5] for the LU factorization of general dense matrices and we propose here to adapt this technique specifically to symmetric indefinite systems. It consists of a multiplicative preconditioning $U^T A U$ where the matrix U is chosen among a particular class of random matrices called *recursive butterfly matrices*. Then LDL^T factorization without pivoting is performed on the symmetric matrix $U^T A U$ and, to solve $Ax = b$, $(U^T A U)y = U^T b$ is solved instead, followed by $x = Uy$. We study the random transformation with *recursive butterfly matrices*, and minimize the number of recursion steps required to get a satisfying accuracy. The resulting transformation will be called Symmetric Random Butterfly Transformation (SRBT). We define two types of matrices that will be used in the symmetric random transformation. These definitions are inspired from [16] in the particular case of real-valued matrices.

Definition 1. A butterfly matrix is defined as any $n \times n$ matrix of the form:

$$B = \frac{1}{\sqrt{2}} \begin{pmatrix} R_0 & R_1 \\ R_0 & -R_1 \end{pmatrix}$$

where $n \geq 2$ and R_0 and R_1 are random diagonal and nonsingular $\frac{n}{2} \times \frac{n}{2}$ matrices.

Definition 2. A recursive butterfly matrix of size n and depth d is a product of the form

$$W^{<n,d>} = \begin{pmatrix} B_1^{<n/2^{d-1}>} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & B_{2^{d-1}}^{<n/2^{d-1}>} \end{pmatrix} \times \dots \times \begin{pmatrix} B_1^{<n/2>} & 0 \\ 0 & B_2^{<n/2>} \end{pmatrix} \times B_1^{<n>}$$

where $B_i^{<n/2^{k-1}>}$ are butterfly matrices of size $n/2^{k-1}$ with $1 \leq k \leq d$.

Note that this definition requires n to be a multiple of 2^{d-1} which can always be obtained by ‘‘augmenting’’ the matrix A with additional 1’s on the diagonal. Note also that Definition 2 differs from the definition of a recursive butterfly matrix given in [16], which corresponds to the special case where $d = \log_2 n + 1$, *i.e.* the first term of the product expressing $W^{<n,d>}$ is a diagonal matrix of size n . For instance, if $n = 4$ and $d = 2$, the recursive butterfly matrix $W^{<4,2>}$ is defined by

$$\begin{aligned} W^{<4,2>} &= \begin{pmatrix} B_1^{<2>} & 0 \\ 0 & B_2^{<2>} \end{pmatrix} \times B^{<4>} \\ &= \frac{1}{2} \begin{pmatrix} r_1^{<2>} & r_2^{<2>} & 0 & 0 \\ r_1^{<2>} & -r_2^{<2>} & 0 & 0 \\ 0 & 0 & r_3^{<2>} & r_4^{<2>} \\ 0 & 0 & r_3^{<2>} & -r_4^{<2>} \end{pmatrix} \begin{pmatrix} r_1^{<4>} & 0 & r_3^{<4>} & 0 \\ 0 & r_2^{<4>} & 0 & r_4^{<4>} \\ r_1^{<4>} & 0 & -r_3^{<4>} & 0 \\ 0 & r_2^{<4>} & 0 & -r_4^{<4>} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} r_1^{<2>} r_1^{<4>} & r_2^{<2>} r_2^{<4>} & r_1^{<2>} r_3^{<4>} & r_2^{<2>} r_4^{<4>} \\ r_1^{<2>} r_1^{<4>} & -r_2^{<2>} r_2^{<4>} & r_1^{<2>} r_3^{<4>} & -r_2^{<2>} r_4^{<4>} \\ r_3^{<2>} r_1^{<4>} & r_4^{<2>} r_2^{<4>} & -r_3^{<2>} r_3^{<4>} & -r_4^{<2>} r_4^{<4>} \\ r_3^{<2>} r_1^{<4>} & -r_4^{<2>} r_2^{<4>} & -r_3^{<2>} r_3^{<4>} & r_4^{<2>} r_4^{<4>} \end{pmatrix}, \end{aligned}$$

where $r_i^{<j>}$ are real random entries.

The objective here is to minimize the computational cost of the RBT defined in [16] by considering a number of recursions d such that $d < \log_2 n \ll n$, resulting in the transformation defined as follows.

Definition 3. A symmetric random butterfly transformation (SRBT) of depth d of a square matrix A is the product:

$$A_r = U^T A U$$

where U is a recursive butterfly matrix of depth d .

Remark 1. Let A be a square matrix of size n , the computational cost of a multiplication $B^T AB$ with B butterfly of size n is $M(n) = 4n^2$. Then the number of operations involved in the computation of A_r by an SRBT of depth d is

$$\begin{aligned} C(n, d) &= \sum_{k=1}^d ((2^{k-1})^2 \times M(n/2^{k-1})) = \sum_{k=1}^d ((2^{k-1})^2 \times 4(n/2^{k-1})^2) \\ &= \sum_{k=1}^d (4n^2) = 4dn^2 \end{aligned}$$

Note that the maximum cost in the case of an RBT as described in [16] is

$$C(n, \log_2 n + 1) \simeq 4n^2 \log_2 n.$$

We can find in [16] details on how RBT might affect the growth factor, and in [5] we can find more information concerning the practical computation of A_r as well as a packed storage description and a condition number analysis. Note that, since we know that we do not pivot when using SRBT, the LDL^T factorization without pivoting can be performed with a very efficient tiled algorithm [6].

4 Numerical Experiments

Experiments to measure the accuracy of each procedure described in the previous sections were carried out using Matlab version 7.12 (R2011a) on a machine with a precision of $2.22 \cdot 10^{-16}$. Table 1 presents accuracy comparisons of linear systems solved using the factors of A calculated by LDL^T with: no pivoting (NP), partial pivoting (PP), tile-wise pivoting (TP), and the Symmetric Random Butterfly Transformation followed by no pivoting (SRBT NP) and tile-wise pivoting (SRBT TP). For tile-wise pivoting (TP), the matrices have 64 tiles (8×8). The partial pivoting corresponds to the Bunch-Kaufman algorithm as it is implemented in LAPACK. Note that for all experiments the rook pivoting achieves the same accuracy as the partial pivoting and therefore is not listed.

All matrices are of size 1024×1024 , either belonging to the Matlab gallery or the Higham's Matrix Computation Toolbox [14] or generated using Matlab function `rand`. Matrices `|i - j|`, `max(i, j)` and `Hadamard` are defined in the experiments performed in [16]. Matrices `rand1` and `rand2` correspond to random matrices with entries uniformly distributed in $[0, 1]$ with all and $1/4$ of the diagonal elements set to 0, respectively. Matrices `rand0` and `rand3` are also random matrices, where the latter has its diagonal elements scaled by $1/1000$.

For all test matrices, we suppose that the exact solution is $x = [1 \ 1 \dots 1]^T$ and we set the right-hand side $b = Ax$. In Table 1, the 2-norm condition number of each matrix is listed. Note that we also computed the condition number of the randomized matrix which, similarly to [5], is of same order of magnitude as $\text{cond } A$ and therefore is not listed. For each LDL^T solver, the component-wise backward error is reported. The latter is defined in [15] and expressed as

$$\omega = \max_i \frac{|A\hat{x} - b|_i}{(|A| \cdot |\hat{x}| + |b|)_i},$$

Table 1. Component-wise backward error for LDL^T solvers on a set of test matrices of size 1024×1024 and 64 tiles (8×8) when applicable

Matrix	Cond A	NP	PP	TP	SRBT	
					NP (IR)	TP (IR)
<code>condex</code>	$1 \cdot 10^2$	$5 \cdot 10^{-15}$	$6 \cdot 10^{-15}$	$7 \cdot 10^{-15}$	$6 \cdot 10^{-15}$ (0)	$4 \cdot 10^{-15}$ (0)
<code>fiedler</code>	$7 \cdot 10^5$	Fail	$2 \cdot 10^{-15}$	$7 \cdot 10^{-15}$	$9 \cdot 10^{-15}$ (0)	$1 \cdot 10^{-15}$ (0)
<code>orthog</code>	$1 \cdot 10^0$	$8 \cdot 10^{-1}$	$1 \cdot 10^{-14}$	$5 \cdot 10^{-1}$	$3 \cdot 10^{-16}$ (1)	$4 \cdot 10^{-16}$ (1)
<code>randcorr</code>	$3 \cdot 10^3$	$4 \cdot 10^{-16}$	$3 \cdot 10^{-16}$	$4 \cdot 10^{-16}$	$5 \cdot 10^{-16}$ (0)	$3 \cdot 10^{-16}$ (0)
<code>augment</code>	$5 \cdot 10^4$	$7 \cdot 10^{-15}$	$4 \cdot 10^{-15}$	$8 \cdot 10^{-15}$	$2 \cdot 10^{-16}$ (1)	$5 \cdot 10^{-15}$ (0)
<code>prolate</code>	$6 \cdot 10^{18}$	$8 \cdot 10^{-15}$	$8 \cdot 10^{-16}$	$2 \cdot 10^{-15}$	$2 \cdot 10^{-15}$ (0)	$1 \cdot 10^{-15}$ (0)
<code>toepfd</code>	$1 \cdot 10^7$	$5 \cdot 10^{-16}$	$7 \cdot 10^{-16}$	$6 \cdot 10^{-16}$	$2 \cdot 10^{-16}$ (0)	$1 \cdot 10^{-16}$ (0)
<code>ris</code>	$4 \cdot 10^0$	Fail	$3 \cdot 10^{-15}$	$8 \cdot 10^{-1}$	$6 \cdot 10^{-1}$ (10)	$6 \cdot 10^{-1}$ (10)
<code> i - j </code>	$7 \cdot 10^5$	$2 \cdot 10^{-15}$	$2 \cdot 10^{-15}$	$7 \cdot 10^{-15}$	$1 \cdot 10^{-14}$ (0)	$1 \cdot 10^{-15}$ (0)
<code>max(i, j)</code>	$3 \cdot 10^6$	$2 \cdot 10^{-14}$	$2 \cdot 10^{-15}$	$5 \cdot 10^{-15}$	$1 \cdot 10^{-14}$ (0)	$1 \cdot 10^{-15}$ (0)
<code>Hadamard</code>	$1 \cdot 10^0$	0	0	0	$7 \cdot 10^{-15}$ (0)	$4 \cdot 10^{-15}$ (0)
<code>rand0</code>	$2 \cdot 10^5$	$1 \cdot 10^{-12}$	$7 \cdot 10^{-14}$	$1 \cdot 10^{-13}$	$1 \cdot 10^{-15}$ (1)	$1 \cdot 10^{-15}$ (0)
<code>rand1</code>	$2 \cdot 10^5$	Fail	$1 \cdot 10^{-13}$	$2 \cdot 10^{-11}$	$1 \cdot 10^{-15}$ (1)	$1 \cdot 10^{-15}$ (0)
<code>rand2</code>	$1 \cdot 10^5$	Fail	$5 \cdot 10^{-14}$	$6 \cdot 10^{-13}$	$1 \cdot 10^{-15}$ (1)	$2 \cdot 10^{-15}$ (0)
<code>rand3</code>	$8 \cdot 10^4$	$4 \cdot 10^{-13}$	$7 \cdot 10^{-14}$	$4 \cdot 10^{-13}$	$1 \cdot 10^{-15}$ (1)	$1 \cdot 10^{-15}$ (0)

NP: LDL^T with No PivotingPP: LDL^T with Partial PivotingTP: LDL^T with Tile-wise Pivoting

SRBT: Symmetric Random Butterfly Transformation

followed by LDL^T without pivoting

IR: Iterative refinement number of iterations

where \hat{x} is the computed solution.

Similarly to [16], the random diagonal matrices used to generate the butterfly matrices described in Definition 1 have diagonal values $\exp(\frac{r}{10})$ where r is randomly chosen in $[-\frac{1}{2}, \frac{1}{2}]$ (matlab instruction `rand`). The number of recursions used in the SRBT algorithm (parameter d in Definition 3) has been set to 2. Hence, the resulting cost of SRBT is $\sim 8n^2$ operations (see Remark 1). To improve the stability, iterative refinement (in the working precision) is added when SRBT is used. Similarly to [2,17], the iterative refinement algorithm is called while $\omega > (n + 1)u$, where u is the machine precision. The number of iterations (IR) in the iterative refinement process is also reported in Table 1.

For all matrices, except `orthog` and `ris` with TP and `ris` with SRBT, the factorization with both tile-wise pivoting and randomization achieves satisfactory results. Iterative refinement turns out to be necessary in a few cases when using SRBT but with never more than one iteration (except for `ris` for which neither TP nor SRBT have achieved accurate results). SRBT TP shows slightly better results than SRBT NP. The former only requires iterative refinement for one of the test cases while the latter for a few. For matrix `prolate`, all methods result in a small backward error. However, the solution cannot be accurate at all due to the large condition number. Note that when matrices are orthogonal (`orthog`) or proportional to an orthogonal matrix (`Hadamard`), LDL^T must

not be used. Also, `toeppd` is positive definite and would normally be solved by Cholesky and not LDL^T . These three test cases have been used only for testing purposes. In the case of the integer-valued matrix `Hadamard`, SRBT destroys the integer structure and transforms the initial matrix into a real-valued one. For the four random matrices, TP achieves results slightly less accurate than SRBT. However, in these cases iterative refinement added to TP would enable us to achieve an accuracy similar to SRBT.

TP and SRBT are always more accurate than NP but they both failed to produce results as accurate as PP for at least one of the test matrices. Nevertheless, despite the reduced number of test cases, they cover a reasonable range of matrices, including those with zeros on the diagonal. Test case `rand1` has only zeros on the diagonal and was accurately solved by both techniques. This case fails at the very first step of the LDL^T method without pivoting. Test case `orthog` has been solved accurately with SRBT but not with TP. For this particular case, when the pivot search is applied on the full matrix, rows/columns 1 and n are permuted, then rows/columns 2 and $n - 1$ are permuted, and so forth. In others, the pivots are spread far apart and the tile-wise pivoting cannot reach them, *i.e.* there are not *good enough* pivots within each tile.

5 Conclusion and Future Work

A tiled LDL^T factorization with tile-wise pivoting and a randomization technique to avoid pivoting in the LDL^T factorization have been presented. The tile-wise pivoting consists of choosing a pivoting strategy and restraining the pivot search to the tile being factored. The randomization technique, called Symmetric Random Butterfly Transformation (SRBT), involves a multiplicative preconditioning which is computationally very affordable and negligible compared to the communication overhead due to classical pivoting algorithms.

Both techniques give accurate results on most test cases considered in this paper, including pathological ones. However, further development of the tile-wise pivoting is required in order to increase its robustness. In particular, techniques such as search by pairs of tiles, also called incremental pivoting, have to be investigated for symmetric indefinite factorizations. Also, to improve stability, the solution obtained after randomization should be systematically followed by iterative refinement in fixed precision (one iteration is sufficient in general). The algorithms presented in this paper shall be integrated into PLASMA, which will allow performance comparisons of the LDL^T solvers and more extensive testing using the matrices available as part of LAPACK.

References

1. Anderson, E., Bai, Z., Bischof, C., Blackford, S., Demmel, J., Dongarra, J., Croz, J.D., Greenbaum, A., Hammarling, S., McKenney, A., Sorensen, D.: LAPACK User's Guide, 3rd edn. SIAM (1999)

2. Arioli, M., Demmel, J.W., Duff, I.S.: Solving sparse linear systems with sparse backward error. *SIAM J. Matrix Anal. and Appl.* 10(2), 165–190 (1989)
3. Ashcraft, C., Grimes, R.G., Lewis, J.G.: Accurate symmetric indefinite linear equation solvers. *SIAM J. Matrix Anal. and Appl.* 20(2), 513–561 (1998)
4. Baboulin, M., Dongarra, J., Tomov, S.: Some issues in dense linear algebra for multicore and special purpose architectures. In: *Proceedings of the 9th International Workshop on State-of-the-Art in Scientific and Parallel Computing, PARA 2008* (2008)
5. Baboulin, M., Dongarra, J., Herrmann, J., Tomov, S.: Accelerating linear system solutions using randomization techniques. *Lapack Working Note 246 and INRIA Research Report 7616* (May 2011)
6. Becker, D., Faverge, M., Dongarra, J.: Towards a Parallel Tile LDL Factorization for Multicore Architectures. Technical Report ICL-UT-11-03, Innovative Computing Laboratory, University of Tennessee, Knoxville, TN, USA (April 2011)
7. Björck, Å.: *Numerical Methods for Least Squares Problems*. Society for Industrial and Applied Mathematics (1996)
8. Bunch, J.R., Kaufman, L.: Some stable methods for calculating inertia and solving symmetric linear systems. *Math. Comput.* 31, 163–179 (1977)
9. Bunch, J.R., Parlett, B.N.: Direct methods for solving symmetric indefinite systems of linear equations. *SIAM J. Numerical Analysis* 8, 639–655 (1971)
10. Buttari, A., Langou, J., Kurzak, J., Dongarra, J.: Parallel tiled QR factorization for multicore architectures. *Concurrency Computat.: Pract. Exper.* 20(13), 1573–1590 (2008)
11. Buttari, A., Langou, J., Kurzak, J., Dongarra, J.: A class of parallel tiled linear algebra algorithms for multicore architectures. *Parallel Comput. Syst. Appl.* 35, 38–53 (2009)
12. Dongarra, J., Kurzak, J., Langou, J., Langou, J., Ltaief, H., Luszczek, P., YarKhan, A., Alvaro, W., Faverge, M., Haidar, A., Hoffman, J., Agullo, E., Buttari, A., Hadri, B.: *PLASMA Users’ Guide, Version 2.3*. Technical Report, Electrical Engineering and Computer Science Department, University of Tennessee, Knoxville, TN (September 2010)
13. Golub, G.H., van Loan, C.F.: *Matrix Computations*, 3rd edn. The Johns Hopkins University Press (1996)
14. Higham, N.J.: *Accuracy and Stability of Numerical Algorithms*, 2nd edn. SIAM (2002)
15. Oettli, W., Prager, W.: Compatibility of approximate solution of linear equations with given error bounds for coefficients and right-hand sides. *Numerische Mathematik* 6, 405–409 (1964)
16. Parker, D.S.: Random butterfly transformations with applications in computational linear algebra. Technical Report CSD-950023, Computer Science Department, UCLA (1995)
17. Skeel, R.D.: Iterative refinement implies numerical stability for Gaussian elimination. *Math. Comput.* 35, 817–832 (1980)
18. Strazdins, P.E.: Issues in the Design of Scalable Out-of-Core Dense Symmetric Indefinite Factorization Algorithms. In: Sloot, P.M.A., Abramson, D., Bogdanov, A.V., Gorbachev, Y.E., Dongarra, J., Zomaya, A.Y. (eds.) *ICCS 2003, Part III*. LNCS, vol. 2659, pp. 715–724. Springer, Heidelberg (2003)
19. Sutter, H.: The Free Lunch Is Over: A Fundamental Turn Toward Concurrency in Software. *Dr. Dobbs’s Journal* 30(3) (2005)