LU factorization and its communication avoiding version

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Plan

LU factorization

Block LU factorization

Communication avoiding LU factorization

Norms and other notations

$$||A||_{F} = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^{2}}$$

$$||A||_{2} = \sigma_{max}(A)$$

$$||A||_{\infty} = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$$

$$||A||_{1} = \max_{1 \le j \le n} \sum_{i=1}^{n} |a_{ij}|$$

Inequalities $|x| \le |y|$ and $|A| \le |B|$ hold componentwise.

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Algebra of the LU factorization

LU factorization

Compute the factorization PA = LU

Example

Given the matrix

$$A = \begin{pmatrix} 3 & 1 & 3 \\ 6 & 7 & 3 \\ 9 & 12 & 3 \end{pmatrix}$$

Let

$$M_1 = \begin{pmatrix} 1 & & \\ -2 & 1 & \\ -3 & & 1 \end{pmatrix}, \quad M_1 A = \begin{pmatrix} 3 & 1 & 3 \\ 0 & 5 & -3 \\ 0 & 9 & -6 \end{pmatrix}$$

Algebra of the LU factorization

In general

where e_k is the k-th unit vector, $m_k = (0, \dots, 0, 1, m_{k+1,k}, \dots, m_{n,k})^T$, $e_i^T m_k = 0, \forall i \leq k$

The factorization can be written as

$$M_{n-1} \dots M_1 A = A^{(n)} = U$$

Algebra of the LU factorization

We obtain

$$A = M_{1}^{-1} \dots M_{n-1}^{-1} U$$

$$= (I + m_{1}e_{1}^{T}) \dots (I + m_{n-1}e_{n-1}^{T}) U$$

$$= \left(I + \sum_{i=1}^{n-1} m_{i}e_{i}^{T}\right) U$$

$$= \begin{pmatrix} 1 \\ m_{21} & 1 \\ \vdots & \vdots & \ddots \\ m_{n1} & m_{n2} & \dots & 1 \end{pmatrix} U = LU$$

The need for pivoting

- For stability, avoid division by small diagonal elements
- For example

$$A = \begin{pmatrix} 0 & 3 & 3 \\ 3 & 1 & 3 \\ 6 & 2 & 3 \end{pmatrix} \tag{1}$$

has an LU factorization if we permute the rows of matrix A

$$PA = \begin{pmatrix} 6 & 2 & 3 \\ 0 & 3 & 3 \\ 3 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & & \\ & 1 & \\ 0.5 & & 1 \end{pmatrix} \cdot \begin{pmatrix} 6 & 2 & 3 \\ & 3 & 3 \\ & & 1.5 \end{pmatrix} \tag{2}$$

- lacksquare Partial pivoting allows to bound the multipliers $m_{ik} \leq 1$ and hence $|L| \leq 1$
- Factorization referred to as LU with partial pivoting (LUPP) or also Gaussian elimination with partial pivoting GEPP

Wilkinson's backward error stability result

Growth factor g_W defined as

$$g_W = \frac{\max_{i,j,k} |a_{ij}^k|}{\max_{i,j} |a_{ij}|}$$

Note that

$$|u_{ij}|=|a_{ij}^i|\leq g_W\max_{i,j}|a_{ij}|$$

Theorem (Wilkinson's backward error stability result, see also [N.J.Higham, 2002] for more details)

Let $A \in \mathbb{R}^{n \times n}$ and let \hat{x} be the computed solution of Ax = b obtained by using GEPP. Then

$$(A + \Delta A)\hat{x} = b, \qquad \|\Delta A\|_{\infty} \le n^2 \gamma_{3n} g_W(n) \|A\|_{\infty},$$

where $\gamma_n = nu/(1 - nu)$, u is machine precision and assuming nu < 1.

The growth factor

- The LU factorization is backward stable if the growth factor is small (grows linearly with n).
- For partial pivoting, the growth factor $g(n) \le 2^{n-1}$, and this bound is attainable.
- In practice it is on the order of $n^{2/3} n^{1/2}$

Exponential growth factor for Wilkinson matrix

$$A = diag(\pm 1) \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 1 \\ -1 & 1 & 0 & \dots & 0 & 1 \\ -1 & -1 & 1 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 & 1 \\ -1 & -1 & \cdots & -1 & 1 & 1 \\ -1 & -1 & \cdots & -1 & -1 & 1 \end{bmatrix}$$

Experimental results for special matrices

Several error bounds for GEPP, the normwise backward error η and the componentwise backward error w (r = b - Ax).

$$\eta = \frac{||r||_1}{||A||_1 ||x||_1 + ||b||_1},
w = \max_i \frac{|r_i|}{(|A||x| + |b|)_i}.$$

matrix	cond(A,2)	gw	L 1	cond(U,1)	$\frac{ PA-LU _F}{ A _F}$	η	w _b
hadamard	1.0E+0	4.1E+3	4.1E+3	5.3E+5	0.0E+0	3.3E-16	4.6E-15
randsvd	6.7E+7	4.7E+0	9.9E+2	1.4E+10	5.6E-15	3.4E-16	2.0E-15
chebvand	3.8E+19	2.0E+2	2.2E+3	4.8E+22	5.1E-14	3.3E-17	2.6E-16
frank	1.7E+20	1.0E+0	2.0E+0	1.9E+30	2.2E-18	4.9E-27	1.2E-23
hilb	8.0E+21	1.0E+0	3.1E+3	2.2E+22	2.2E-16	5.5E-19	2.0E-17

- Two reasons considered to be important for the average case stability [Trefethen and Schreiber, 90]:
 - the multipliers in L are small
 - $\ \square$ the correction introduced at each elimination step is of rank 1

Plan

LU factorization

Block LU factorization

Communication avoiding LU factorization

Block formulation of the LU factorization

Partitioning of matrix A of size $n \times n$

$$A = \left[\begin{array}{cc} A_{11} & A_{12} \\ A_{21} & A_{22} \end{array} \right]$$

where A_{11} is of size $b \times b$, A_{21} is of size $(m-b) \times b$, A_{12} is of size $b \times (n-b)$ and A_{22} is of size $(m-b) \times (n-b)$.

Block LU algebra

The first iteration computes the factorization:

$$P_1^T A = \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} = \begin{bmatrix} L_{11} \\ L_{21} & I_{n-b} \end{bmatrix} \cdot \begin{bmatrix} U_{11} & U_{12} \\ & A^1 \end{bmatrix}$$

The algorithm continues recursively on the trailing matrix A^1 .

Block LU factorization - the algorithm

 Compute the LU factorization with partial pivoting of the first block column

$$P_1\begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} = \begin{pmatrix} L_{11} \\ L_{21} \end{pmatrix} U_{11}$$

2. Pivot by applying the permutation matrix P_1^T on the entire matrix,

$$\bar{A} = P_1^T A.$$

3. Solve the triangular system

$$L_{11}U_{12}=\bar{A}_{12}$$

4. Update the trailing matrix,

$$A^1 = \bar{A}_{22} - L_{21}U_{12}$$

5. Compute recursively the block LU factorization of A^1 .

LU Factorization as in ScaLAPACK

LU factorization on a $P = Pr \times Pc$ grid of processors

For ib = 1 to n-1 step b A(ib) = A(ib : n, ib : n)

- 1. Compute panel factorization
 - □ find pivot in each column, swap rows
- 2. Apply all row permutations
 - broadcast pivot information along the rows
 - swap rows at left and right
- 3. Compute block row of U
 - broadcast right diagonal block of L of current panel
- 4. Update trailing matrix
 - broadcast right block column of L
 - broadcast down block row of U









Cost of LU Factorization in ScaLAPACK

LU factorization on a $P = Pr \times Pc$ grid of processors

For ib = 1 to n-1 step b

$$A(ib) = A(ib : n, ib : n)$$

- 1. Compute panel factorization
 - \square #messages = $O(n \log_2 P_r)$
- 2. Apply all row permutations
 - $\square \#messages = O(n/b(\log_2 P_r + \log_2 P_c))$
- 3. Compute block row of U
 - $\square \#messages = O(n/b \log_2 P_c)$
- 4. Update trailing matrix
 - $\square \#messages = O(n/b(\log_2 P_r + \log_2 P_c))$









Cost of parallel block LU

Consider that we have a $\sqrt{P} \times \sqrt{P}$ grid, block size b

$$\gamma \cdot \left(\frac{2/3n^3}{P} + \frac{n^2b}{\sqrt{P}}\right) + \beta \cdot \frac{n^2 \log P}{\sqrt{P}} + \alpha \cdot \left(1.5n \log P + \frac{3.5n}{b} \log P\right).$$

Plan

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Block LU factorization

Communication avoiding LU factorization

The LU factorization of a tall skinny matrix

First try the obvious generalization of TSQR.

$$W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} = \begin{pmatrix} \Pi_{00} L_{00} U_{00} \\ \Pi_{10} L_{10} U_{10} \\ \Pi_{20} L_{20} U_{20} \\ \Pi_{30} L_{30} U_{30} \end{pmatrix}$$

$$= \begin{pmatrix} \Pi_{00} \\ \Pi_{10} \\ \Pi_{20} \\ \Pi_{30} \end{pmatrix} \begin{pmatrix} L_{00} \\ L_{10} \\ L_{20} \\ L_{30} \end{pmatrix} \begin{pmatrix} U_{00} \\ U_{10} \\ U_{20} \\ U_{30} \end{pmatrix} = \Pi_0 L_0 \begin{pmatrix} U_{00} \\ U_{10} \\ U_{20} \\ U_{30} \end{pmatrix}$$

$$\begin{pmatrix} U_{00} \\ U_{10} \\ U_{20} \\ U_{30} \end{pmatrix} = \begin{pmatrix} \Pi_{01} L_{01} U_{01} \\ \Pi_{11} L_{11} U_{11} \end{pmatrix} = \begin{pmatrix} \Pi_{01} \\ \Pi_{11} \end{pmatrix} \begin{pmatrix} L_{01} \\ \Pi_{11} \end{pmatrix} \begin{pmatrix} U_{01} \\ U_{11} \end{pmatrix} = \Pi_1 L_1 \begin{pmatrix} U_{01} \\ U_{11} \end{pmatrix}$$

$$\begin{pmatrix} U_{01} \\ U_{11} \end{pmatrix} = \Pi_{02} \cdot L_{02} \cdot U_{02}$$

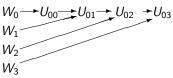
The final factorization is:

$$W = \Pi_0 L_0 \Pi_1 L_1 \Pi_{02} L_{02} U_{02}$$

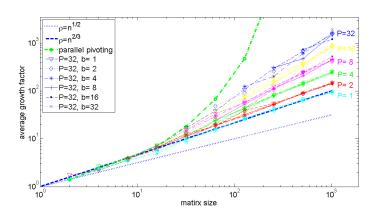
Obvious generalization of TSQR to LU

Block parallel pivoting:

- Block pairwise pivoting:
 - uses a flat tree and is optimal in the sequential case
 - introduced by Barron and Swinnerton-Dyer, 1960: block LU factorization used to solve a system with 100 equations on EDSAC 2 computer using an auxiliary magnetic-tape
 - used in PLASMA for multicore architectures and FLAME for out-of-core algorithms and for multicore architectures

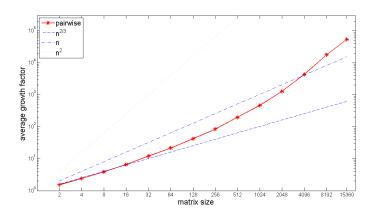


Block parallel pivoting



- Unstable for large number of processors P
- When P=number rows, it corresponds to parallel pivoting, known to be unstable (Trefethen and Schreiber, 90)

Block pairwise pivoting



- Results shown for random matrices
- Will become unstable for large matrices

Tournament pivoting - the overall idea

At each iteration of a block algorithm

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$
 where $W = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix}$

where A_{11} is of size $b \times b$, A_{21} is of size $(m-b) \times b$, A_{12} is of size $b \times (n-b)$ and A_{22} is of size $(m-b) \times (n-b)$.

- \square Preprocess W to find at low communication cost good pivots for the LU factorization of W, return a permutation matrix P
- ☐ Permute the pivots to top, ie compute *PA*
- \square Compute LU with no pivoting of W, update trailing matrix, obtain

$$PA = \begin{pmatrix} L_{11} & & & \\ L_{21} & I_{n-b} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & & \\ & A_{22} - L_{21}U_{12} \end{pmatrix}$$

For details see [Grigori et al., 2011]

Tournament pivoting for a tall skinny matrix

1. Compute GEPP factorization of each W_i , find permutation Π_0

$$W = A(:,1:b) = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} = \begin{pmatrix} \Pi_{00} L_{00} U_{00} \\ \Pi_{10} L_{10} U_{10} \\ \Pi_{20} L_{20} U_{20} \\ \Pi_{30} L_{30} U_{30} \end{pmatrix}, \begin{array}{l} \text{Pick b pivot rows, form } A_{00} \\ \text{Same for } A_{10} \\ \text{Same for } A_{20} \\ \text{Same for } A_{30} \\ \end{array}$$

2. Perform $\log_2 P$ times GEPP factorization of selected $2b \times b$ rows, find permutations Π_1, Π_2

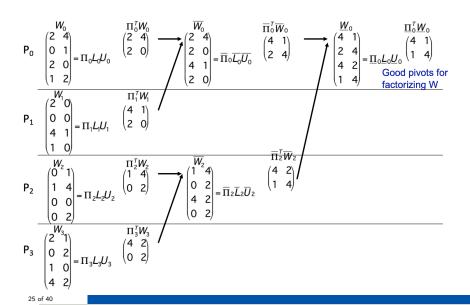
$$\begin{pmatrix} A_{00} \\ A_{10} \\ A_{20} \\ A_{30} \end{pmatrix} = \begin{pmatrix} \Pi_{01} L_{01} U_{01} \\ \Pi_{11} L_{11} U_{11} \end{pmatrix}, \text{ Pick b pivot rows, form } A_{01}$$
 Same for A_{11}

$$\begin{pmatrix} A_{01} \\ A_{11} \end{pmatrix} = \begin{pmatrix} \Pi_{02} L_{02} U_{02} \end{pmatrix}, \quad \begin{array}{l} \text{Pick b pivot rows that will} \\ \text{be used as pivots to factor } W \end{array}$$

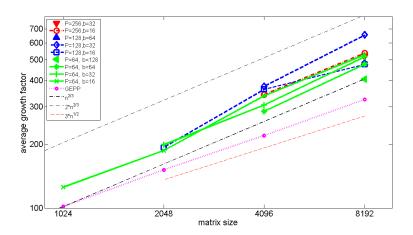
3. Perform LU factorization with no pivoting of the permuted matrix

$$\Pi_2^T \Pi_1^T \Pi_0^T W = LU$$

Tournament pivoting



Growth factor for binary tree based CALU



- Random matrices from a normal distribution
- Same behaviour for all matrices in our test, and $|L| \le 4.2$

Our "proof of stability" for CALU

- CALU as stable as GEPP in following sense: In exact arithmetic, CALU process on a matrix A is equivalent to GEPP process on a larger matrix G whose entries are blocks of A and zeros.
- Example of one step of tournament pivoting:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \\ A_{31} & A_{32} \end{pmatrix},$$

$$\begin{array}{c}
A_{11} \longrightarrow \bar{A}_{11} \\
A_{21} \longrightarrow A_{21}
\end{array}$$

$$G = \begin{pmatrix} \bar{A}_{11} & \bar{A}_{12} \\ A_{21} & A_{21} \\ -A_{31} & A_{32} \end{pmatrix}$$

 Proof possible by using original rows of A during tournament pivoting (not the computed rows of *U*).

Outline of "proof of stability"

• After the factorization of first panel by CALU, A_{32}^s (the Schur complement of A_{32}) is not bounded as in GEPP,

$$\begin{pmatrix} \Pi_{11} & \Pi_{12} \\ \Pi_{21} & \Pi_{22} \\ & I \end{pmatrix} \cdot \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \\ A_{31} & A_{32} \end{pmatrix} \quad = \quad \begin{pmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \\ A_{31} & A_{32} \end{pmatrix} = \begin{pmatrix} \bar{L}_{11} & & & \\ \bar{L}_{21} & I_b & & \\ \bar{L}_{31} & & I_{m-2b} \end{pmatrix} \cdot \begin{pmatrix} \bar{U}_{11} & \bar{U}_{12} \\ \bar{A}_{22}^{\sharp} \\ A_{32}^{\sharp} \end{pmatrix}$$

• but A_{32}^s can be obtained by GEPP on larger matrix G formed from blocks of A

$$G = \begin{pmatrix} \bar{A}_{11} & \bar{A}_{12} \\ A_{21} & A_{21} \\ -A_{31} & A_{32} \end{pmatrix} = \begin{pmatrix} \bar{L}_{11} & & & \\ A_{21}\bar{U}_{11}^{-1} & L_{21} & & \\ & -L_{31} & I_{m-2b} \end{pmatrix} \begin{pmatrix} \bar{U}_{11} & & \bar{U}_{12} \\ & U_{21} & -L_{21}^{-1}A_{21}\bar{U}_{11}^{-1}\bar{U}_{12} \\ & A_{32}^{*} \end{pmatrix}$$

GEPP on G does not permute and

$$\begin{array}{lcl} L_{31}L_{21}^{-1}A_{21}\bar{U}_{11}^{-1}\bar{U}_{12} + A_{32}^{\mathfrak{s}} & = & L_{31}U_{21}\bar{U}_{11}^{-1}\bar{U}_{12} + A_{32}^{\mathfrak{s}} = A_{31}\bar{U}_{11}^{-1}\bar{U}_{12} + A_{32}^{\mathfrak{s}} \\ & = & \bar{L}_{31}\bar{U}_{12} + A_{32}^{\mathfrak{s}} = A_{32} \end{array}$$

Growth factor in exact arithmetic

- Matrix of size m-by-n, reduction tree of height $H = log_2(P)$
- In practice growth factor for GEPP and CALU is on the order of $n^{2/3} -n^{1/2}$

	matrix of size $m imes (b+1)$						
	TSLU	GEPP					
	upper bound	attained	upper bound				
L	2 ^{bH}	$2^{(b-2)H-(b-1)}$	1				
gw	$2^{b(H+1)}$	2 ^b	2 ^b				
	matrix of size $m \times n$						
	CAL	GEPP					
	upper bound	attained	upper bound				
L	2 ^{bH}	$2^{(b-2)H-(b-1)}$	1				
gw	$2^{n(H+1)-1}$	2^{n-1}	2^{n-1}				

Cost of LU Factorization in ScaLAPACK

LU factorization on a $P = Pr \times Pc$ grid of processors

For ib = 1 to n-1 step b

$$A(ib) = A(ib : n, ib : n)$$

- 1. Compute panel factorization
 - $\square \#messages = O(n/b \log_2 P_r)$
- 2. Apply all row permutations
 - $\square \#messages = O(n/b(\log_2 P_r + \log_2 P_c))$
- 3. Compute block row of U
 - $\square \#messages = O(n/b\log_2 P_c)$
- 4. Update trailing matrix
 - $\square \#messages = O(n/b(\log_2 P_r + \log_2 P_c))$









CALU based on TSLU

Cost of CALU vs ScaLAPACK's PDGETRF

- $n \times n$ matrix on $\sqrt{P} \times \sqrt{P}$ processor grid, block size b
- Flops: $(2/3)n^3/P + 3/2n^2b\log_2 P/\sqrt{P}$ vs $(2/3)n^3/P + n^2b/P^{1/2}$
- Bandwidth: $n^2 \log_2 P / \sqrt{P}$ vs same
- Latency: $3n \log_2 P/b$ vs $1.5n \log_2 P$

Close to optimal (modulo log P factors)

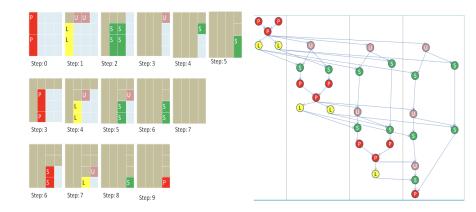
- Assume $O(n^2/P)$ memory/processor, $O(n^3)$ algorithm
- Choose b near n/\sqrt{P} (its upper bound)
- Bandwidth lower bound: $\Omega(n^2/\sqrt{P})$ just $\log_2 P$ smaller
- Latency lower bound: $\Omega(\sqrt{P})$ just polylog(P) smaller

Performance vs ScaLAPACK

- Parallel TSLU (LU on tall-skinny matrix) □ IBM Power 5 Up to 4.37x faster (16 procs, $1M \times 150$) Cray XT4 Up to 5.52x faster (8 procs, $1M \times 150$) Parallel CALU (LU on general matrices) □ Intel Xeon (two socket, quad core) Up to 2.3x faster (8 cores, $10^6 \times 500$) □ IBM Power 5 Up to 2.29x faster (64 procs, 1000×1000) Cray XT4 Up to 1.81x faster (64 procs, 1000×1000)
- Details in SuperComputing'08 (LG, Demmel, Xiang), IPDPS'10 (S. Donfack, LG).

CALU and its task dependency graph

- The matrix is partitioned into blocks of size $T \times b$
- The computation of each block is associated with a task.



Scheduling CALU's Task Dependency Graph

- Static scheduling
 - + Good locality of data

Ignores noise



- Dynamic scheduling
 - + Keeps cores busy

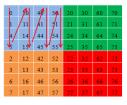
- Poor usage of data locality
- Can have large dequeue overhead



Lightweight scheduling

- Emerging complexities of multi- and mani-core processors suggest a need for self-adaptive strategies
 - One example is work stealing
- Goal
 - Design a tunable strategy that is able to provide a good trade-off between load balance, data locality, and dequeue overhead
 - □ Provide performance consistency
- Approach: combine static and dynamic scheduling
 - □ Shown to be efficient for regular mesh computation [B. Gropp and V. Kale]

Possible data layouts



Block cyclic layout (BCL)



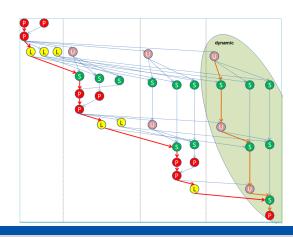
Two level block layout (2I-BL)

Data layout/scheduling	Static	Dynamic	Static(%dynamic)	
Column Major Layout (CM)		Х		
Block Cyclic Layout (BCL)	X	Х	X	
2-level Block Cyclic Layout (2I-BL)	X	Х	X	

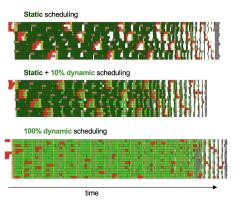
Lightweight scheduling

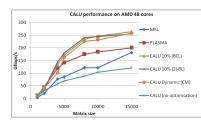
- A self-adaptive strategy to provide
 - $\hfill \square$ A good trade-off between load balance, data locality, and dequeue overhead.
 - □ Performance consistency
 - □ Shown to be efficient for regular mesh computation [B. Gropp and V. Kale]

- Combined static/dynamic scheduling
 - A thread executes in priority its statically assigned tasks
 - When no task ready, it picks a ready task from the dynamic part
 - The size of the dynamic part is guided by a performance model



Best performance of CALU on multicore architectures





Reported performance for PLASMA uses LU with block pairwise pivoting

Acknowledgement

Some of the examples taken from [Golub and Van Loan, 1996]

References (1)

- Golub, G. H. and Van Loan, C. F. (1996).

 Matrix Computations (3rd Ed.).

 Johns Hopkins University Press, Baltimore, MD, USA.
- Grigori, L., Demmel, J., and Xiang, H. (2011).
 CALU: a communication optimal LU factorization algorithm.

 SIAM Journal on Matrix Analysis and Applications, 32:1317–1350.
- N.J.Higham (2002).

 Accuracy and Stability of Numerical Algorithms.

 SIAM, second edition.