

NUMERICAL STABILITY OF SYMMETRIC INDEFINITE SOLVERS: DIRECT METHODS

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Outline

Introduction

Bunch-Kaufmann factorization

Parlett-Reid reduction

Aasen's factorization

Numerical stability

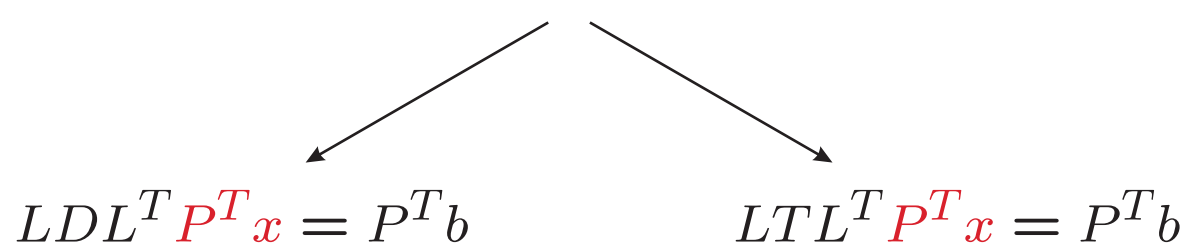
Conclusions

Solution of a symmetric indefinite system of linear equations

$$Ax = b$$

A is symmetric (indefinite)

$$P^T A P \textcolor{red}{P}^T x = P^T b$$


$$LDL^T \textcolor{red}{P}^T x = P^T b$$

$$LTL^T \textcolor{red}{P}^T x = P^T b$$

Block Bunch-Kaufmann factorization

$$P^T A P = L D L^T$$

The diagram illustrates the Block Bunch-Kaufmann factorization. On the left is a purple square matrix labeled $P^T A P$. This is followed by an equals sign. To the right of the equals sign are three matrices: a green lower triangular matrix labeled L , a blue block diagonal matrix labeled D , and a green upper triangular matrix labeled L^T . The L matrix has a green lower triangle and a white upper triangle. The D matrix has blue blocks along its diagonal. The L^T matrix has a green upper triangle and a white lower triangle.

A is symmetric (definite or indefinite)

L is **unit** lower triangular

D is **symmetric block diagonal** with 1x1, 2x2 blocks

P is a **permutation** matrix

Bunch-Kaufmann factorization

1		
0	1	
		I_{n-2}

L_2

		A

$P_2 A P_2^T$

1	0	
	1	
		I_{n-2}

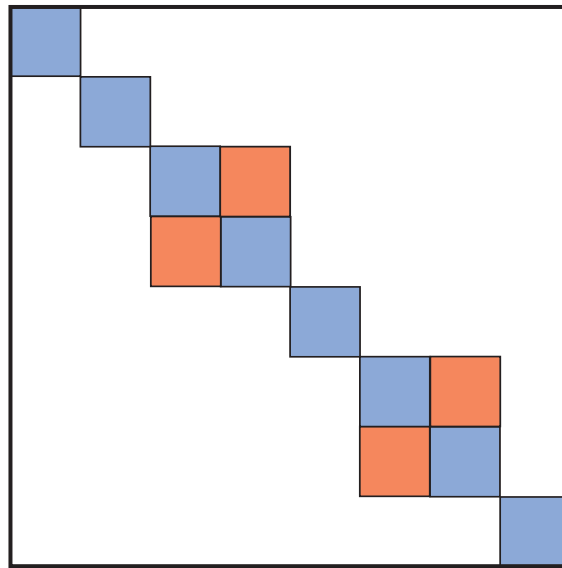
L_2^T

=

		0
		0
0	0	C

$L_2 P_2 A P_2^T L_2$

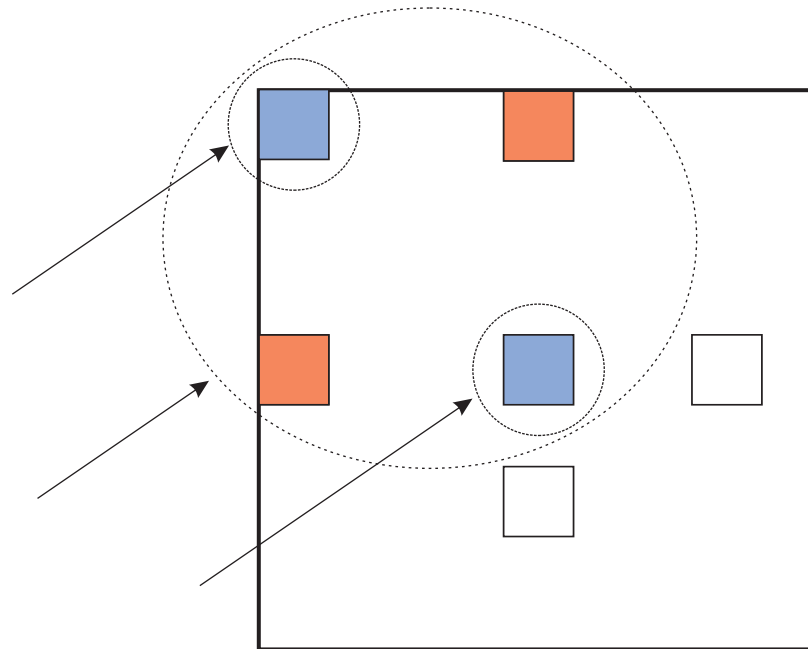
Bunch-Kaufmann factorization



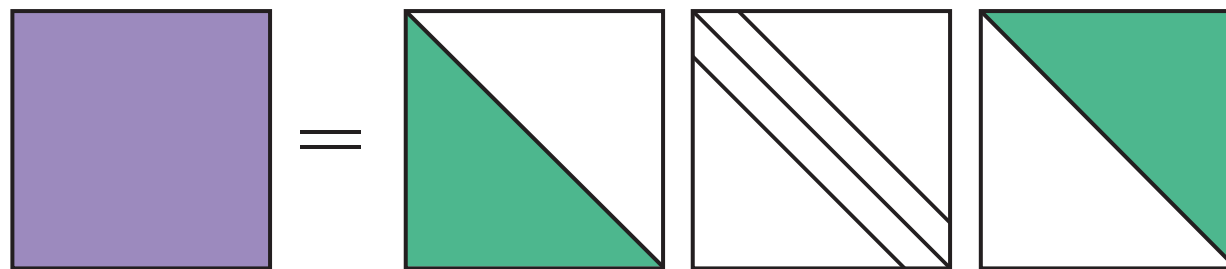
$$\underbrace{L_{n-1}P_{n-1} \dots L_2P_2L_1P_1AP_1^T L_1^T P_2^T L_2^T \dots P_{n-1}^T L_{n-1}^T}_D$$

Bunch-Kaufmann pivoting strategy

- complete pivoting $O(n^3)$ comparisons Bunch, Parlett
- partial pivoting $O(n^2)$ comparisons implemented in LINPACK, LAPACK



Triangular tridiagonalization


$$P^T A P = L T L^T$$

The diagram illustrates the triangular tridiagonalization of a symmetric matrix A . The equation is $P^T A P = L T L^T$. The matrices are represented as follows:

- $P^T A P$: A solid purple square, representing a symmetric matrix.
- L : A green lower triangular matrix, representing a unit lower triangular matrix.
- T : A white square with three black diagonal lines, representing a symmetric tridiagonal matrix.
- L^T : A green upper triangular matrix, representing the transpose of L .

A is symmetric (definite or indefinite)

L is **unit** lower triangular

T is **symmetric** tridiagonal

P is a **permutation** matrix

Parlett - Reid reduction

1		
0	1	
0	$-\frac{\nu}{\alpha}$	I_{n-2}

L_2

$A_{1,1}$	α	ν^T
α	$A_{2:n,2:n}$	
ν		

$P_2^T A P_2^T$

1	0	0
	1	$-\nu/\alpha$
		I_{n-2}

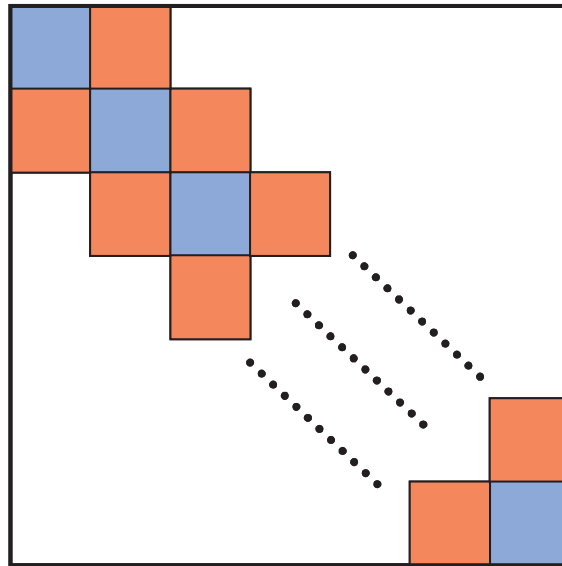
L_2^T

=

$A_{1,1}$	α	0
α	C	
0		

$L_2 P_2^T A P_2^T L_2^T$

Parlett - Reid reduction



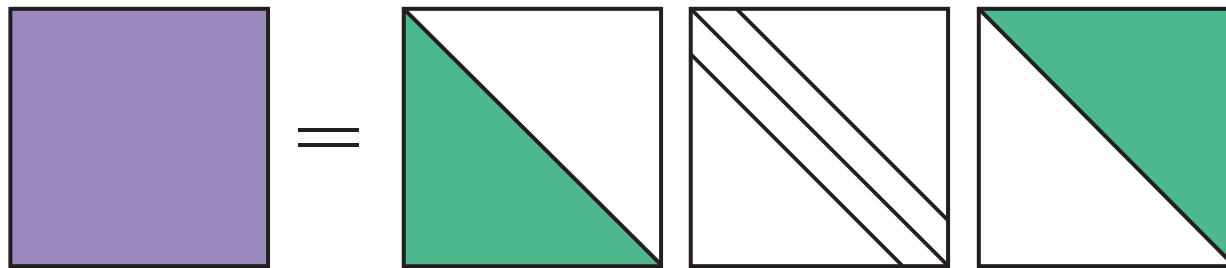
$$\underbrace{L_{n-1}P_{n-1} \dots L_3P_3L_2P_2AP_2^T L_2^T P_3^T L_3^T \dots P_{n-1}^T L_{n-1}^T}_{L^{-1}P^T} \underbrace{P L^{-T}}_{T}$$

Parlett - Reid reduction

- The reduced matrix remains symmetric during reduction, the updates are performed on a half of the matrix
- Complexity: at each step two rank-one updates on half a matrix $2(n-1)^2$; $O(n)$ other operations; total $2/3n^3 + O(n^2)$

→ Aasen's factorization

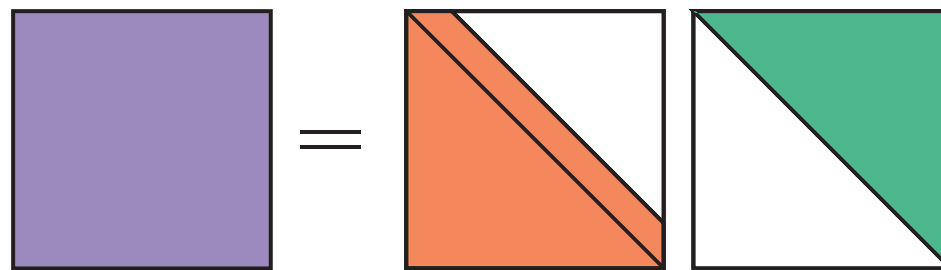
Parlett - Reid reduction



The diagram illustrates the Parlett-Reid reduction of a symmetric matrix $P^T A P$. It is shown as a product of three matrices: L , T , and L^T . The matrix L is a unit lower triangular matrix, represented by a square with a green lower triangular region. The matrix T is a symmetric tridiagonal matrix, represented by a square with three parallel diagonal lines. The matrix L^T is the transpose of L , represented by a square with a green upper triangular region.

$$P^T A P = L T L^T$$

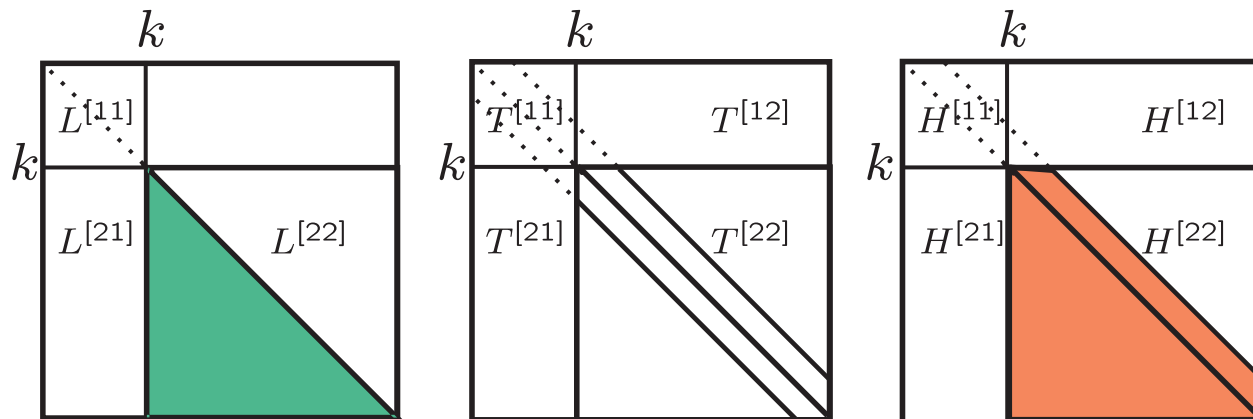
Aasen's factorization



The diagram illustrates Aasen's factorization of a symmetric matrix $P^T A P$. It is shown as a product of two matrices: $H = LT$ and L^T . The matrix $H = LT$ is a unit upper triangular matrix, represented by a square with an orange upper triangular region. The matrix L^T is a unit lower triangular matrix, represented by a square with a green lower triangular region.

$$P^T A P = H L^T$$

Notation



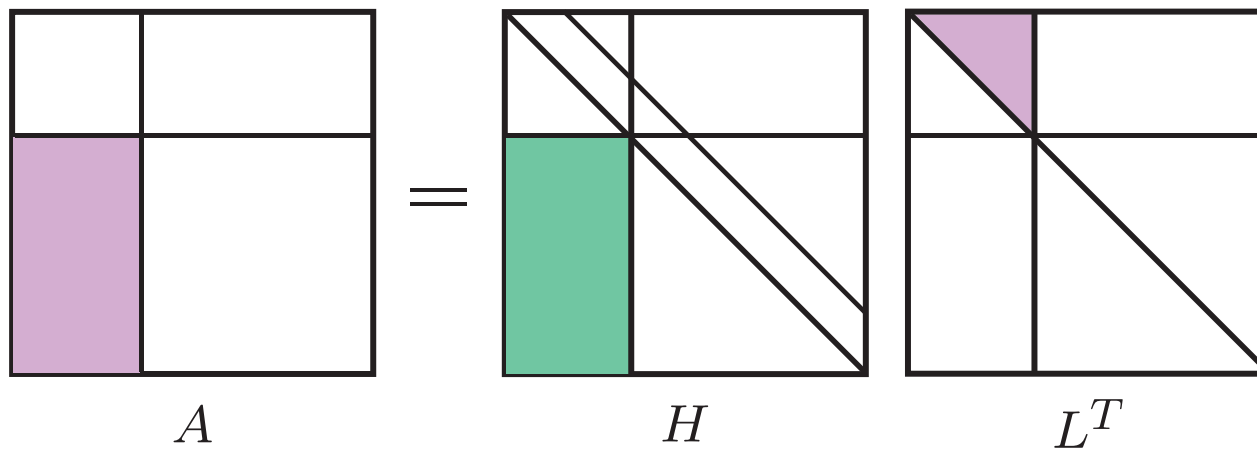
Parlett - Reid reduction

works on $L^{[22]}T^{[22]}(L^{[22]})^T$

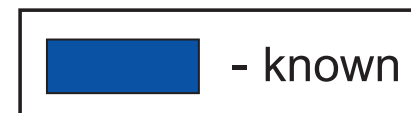
Aasen's factorization

- * for $k > 1$ $L^{[22]}T^{[22]}(L^{[22]})^T \neq H^{[22]}(L^{[22]})^T$
- * update of $A^{[22]}$
compute $(k+1)$ -th column L and k -th column of T and H
- * pivoting strategy

Aasen's factorization – Phase 1

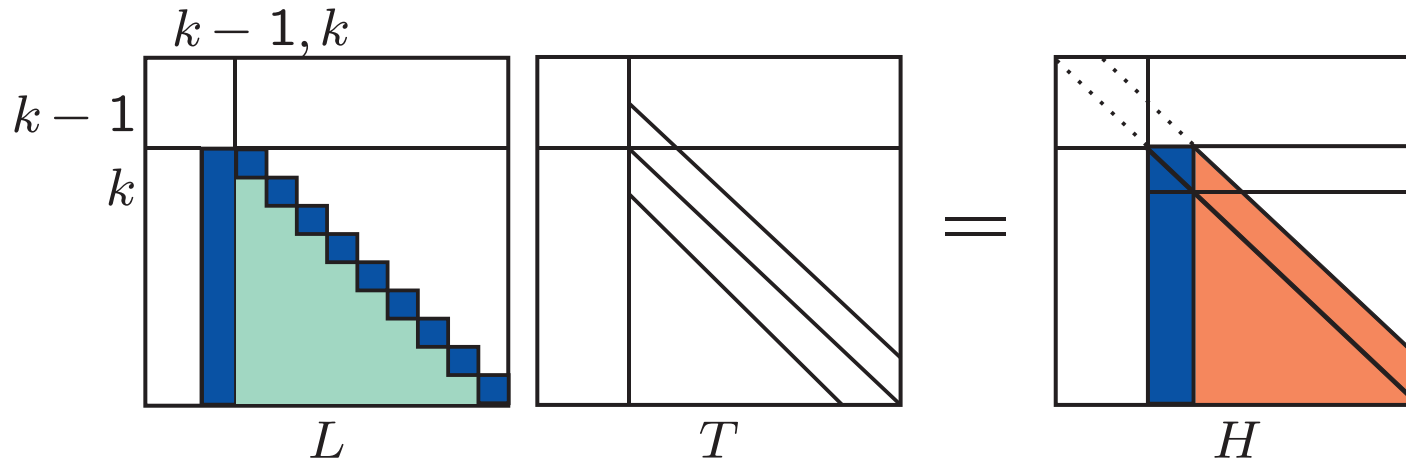


Compute i -th column of $H^{[21]}$ from i -th column of $A^{[21]}$ and previous columns of $H^{[21]}$ and $L^{[11]}$



Aasen's factorization – Phase 2

Second phase – extract the first column of $L^{[22]}T^{[22]}$

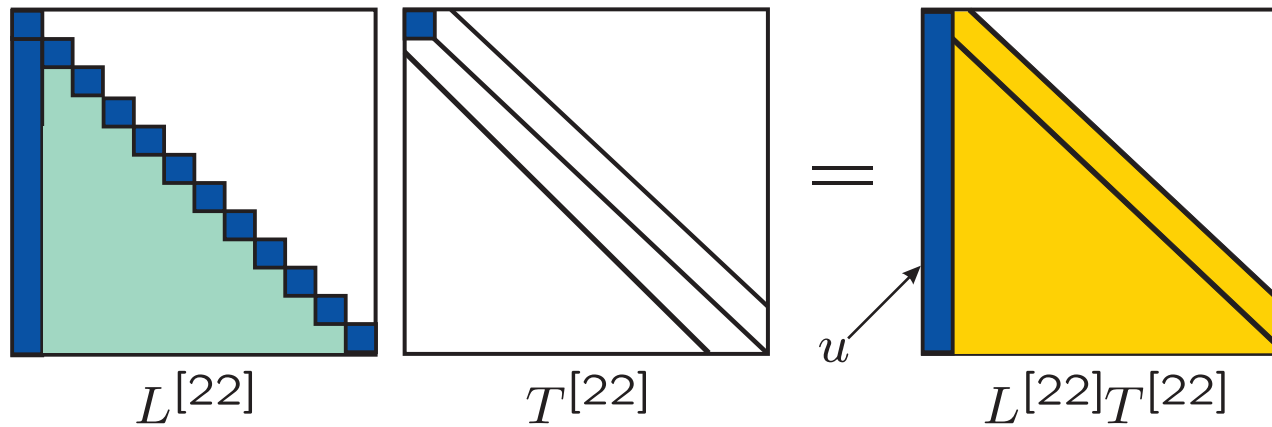


$$u \leftarrow H_{1,1:\text{last}}^{[22]} - L_{1:\text{last},k-1} T_{k,k-1}$$

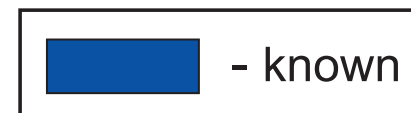


Aasen's factorization – Phase 3

Third phase – extract $T_{1,1}^{[22]}$

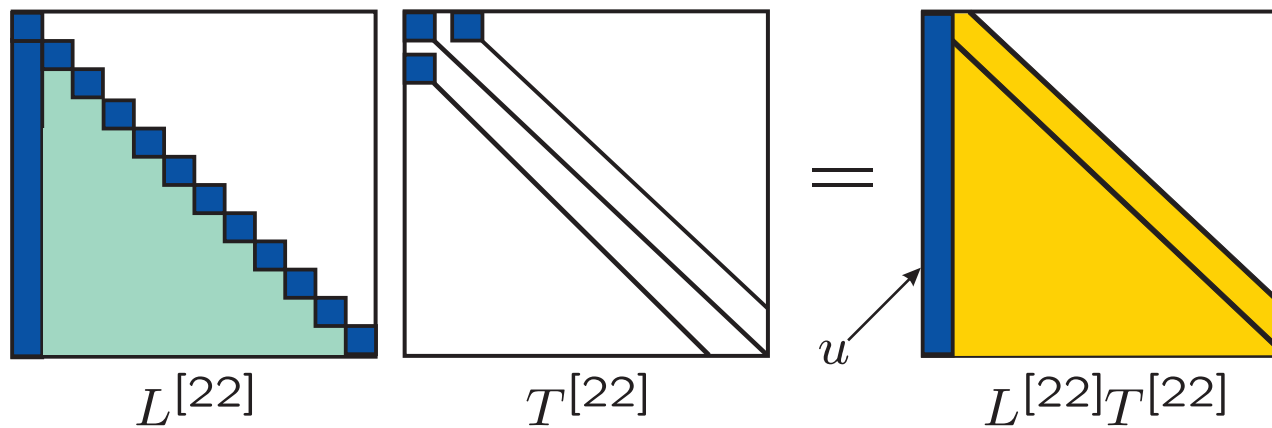


$$T_{1,1}^{[22]} = u_1$$



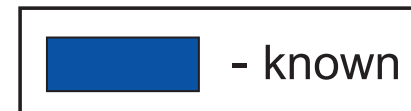
Aasen's factorization – Phase 4

Fourth phase – extract $T_{1,2}^{[22]}$ and $L_{2:\text{last},2}^{[22]}$



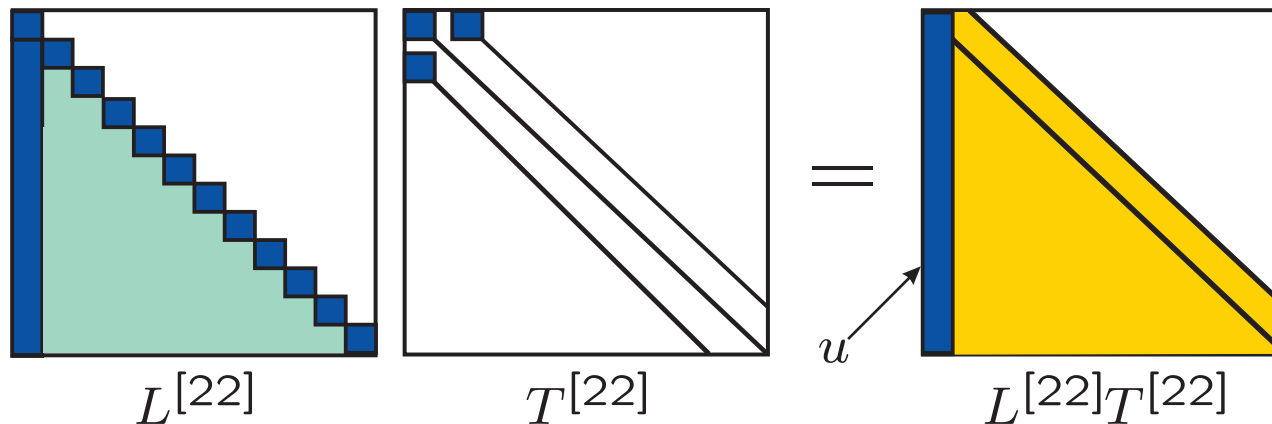
$$u_{2:\text{last}} = T_{1,1}^{[22]} L_{2:\text{last},1}^{[22]} + T_{1,2}^{[22]} L_{2:\text{last},2}^{[22]}$$

$$\boxed{T_{1,2}^{[22]}} \boxed{L_{2:\text{last},2}^{[22]}} = u_{2:\text{last}} - T_{1,1}^{[22]} L_{2:\text{last},1}^{[22]}$$



Aasen's factorization – pivoting strategy

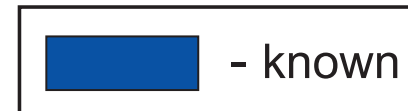
Fourth phase – extract $T_{1,2}^{[22]}$ and $L_{2:\text{last},2}^{[22]}$



$$u_{2:\text{last}} = T_{1,1}^{[22]} L_{2:\text{last},1}^{[22]} + T_{1,2}^{[22]} L_{2:\text{last},2}^{[22]}$$

$$\boxed{T_{1,2}^{[22]}} \boxed{L_{2:\text{last},2}^{[22]}} = \underbrace{u_{2:\text{last}} - T_{1,1}^{[22]} L_{2:\text{last},1}^{[22]}}$$

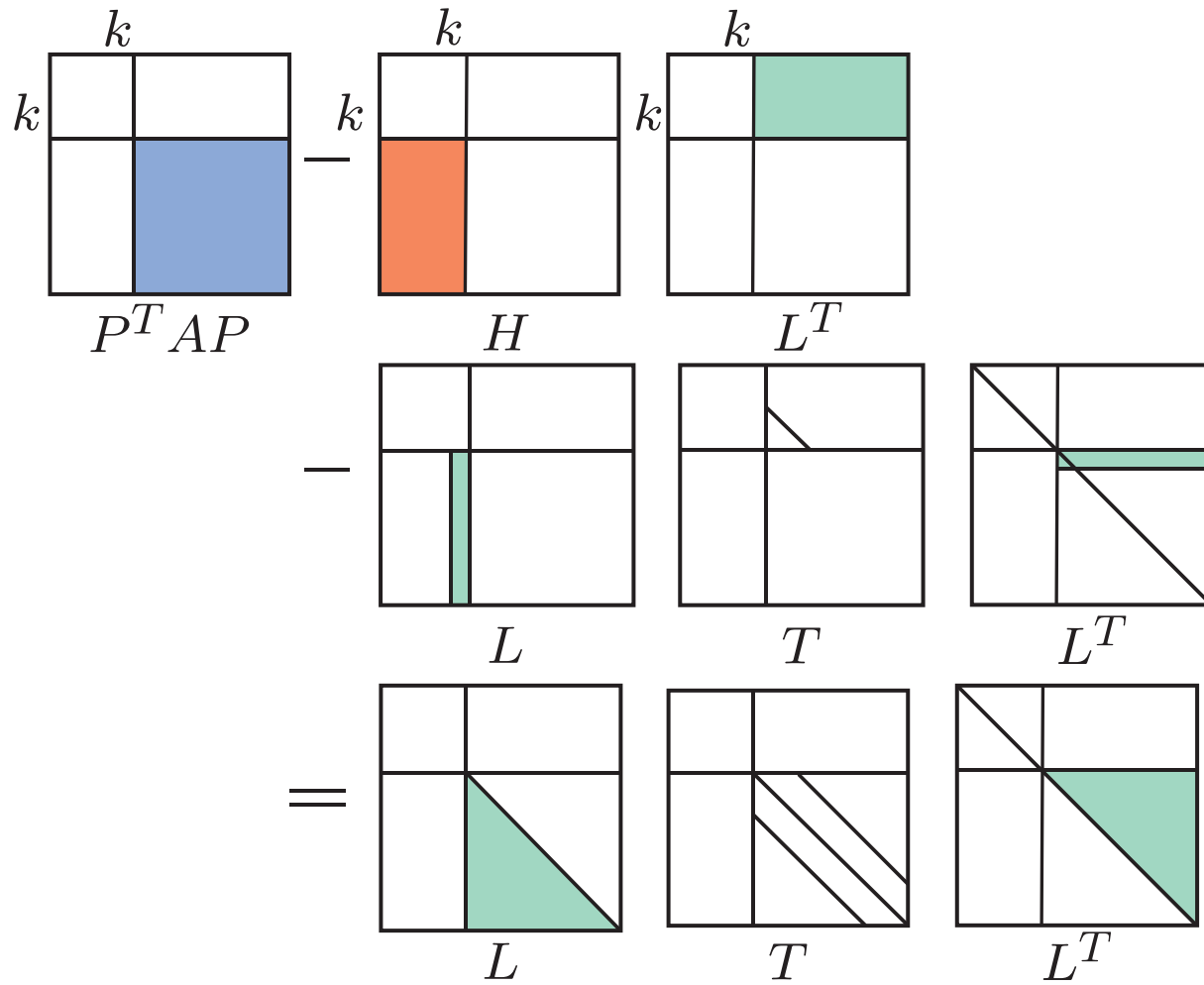
First switch variable $(i + 1)$
with the largest index in



Partitioned factorization

Diagram illustrating the LU decomposition of a matrix $P^T A P$. The matrix is partitioned into four quadrants, each of size k by k . The bottom-right quadrant is shaded blue. The matrix is equal to the product of three matrices: H , L^T , and another matrix. The matrix H is the product of the first two matrices, and the matrix L^T is the product of the last two matrices. The matrix H is shown as the product of a matrix with a shaded bottom-left quadrant and a matrix with a shaded bottom-right quadrant. The matrix L^T is shown as the product of a matrix with a shaded top-right quadrant and a matrix with a shaded bottom-right quadrant.

Partitioned factorization



Numerical stability – main result

$$A + \Delta A = \bar{L} \bar{T} \bar{L}^T$$

$$|\Delta A| \leq c_3(n, k) u |\bar{L}| |\bar{T}| |\bar{L}|^T$$

$$c_3(n, k) = c_1 \left(n + \left\lfloor \frac{n}{k} \right\rfloor + 2 \right), \quad c_3(n, 1) = c_1(n+3)$$

Basic assumptions on BLAS

$$X \in \mathbb{R}^{m,k}, \quad Y \in \mathbb{R}^{k,n}, \quad Z = XY \in \mathbb{R}^{m,n}, \quad \bar{Z} = fl(XY)$$

conventional BLAS:

$$|\bar{Z} - Z| \leq c_1(k)u|X||Y| \quad c_1(k) = \frac{k}{1 - ku}$$

Strassen:

$$\|\bar{Z} - Z\| \leq c_3(m, n, k, p)u\|X\| \|Y\|$$

Numerical stability – Proof 1

$$A^{[11]} + \Delta A^{[11]} = \bar{L}^{[11]} \bar{T}^{[11]} \left(\bar{L}^{[11]} \right)^T$$

$$\left| \Delta A^{[11]} \right| \leq c_3(k, 1) u \left| \bar{L}^{[11]} \right| \left| \bar{T}^{[11]} \right| \left| \bar{L}^{[11]} \right|^T$$

$$A^{[21]} + \Delta A^{[21]} = \bar{H}^{[21]} \left(\bar{L}^{[11]} \right)^T$$

$$\left| \Delta A^{[21]} \right| \leq c_1(k) u \left| \bar{H}^{[21]} \right| \left| \bar{L}^{[11]} \right|^T$$

$$\bar{H}^{[21]} + \Delta H^{[21]} = \bar{L}^{[21]} \bar{T}^{[11]} + \bar{L}_{:,1}^{[22]} \bar{T}_{1,k}^{[21]}$$

$$\left| \Delta H^{[21]} \right| \leq c_1(3) \left(\left| \bar{L}^{[21]} \right| \left| \bar{T}^{[11]} \right| + \left| \bar{L}_{:,1}^{[22]} \right| \left| \bar{T}_{1,k}^{[21]} \right| \right)$$

Numerical stability – Proof 2

$$\bar{C}^{[22]} + \Delta C^{[22]} = A^{[22]} - \bar{H}^{[21]} \left(\bar{L}^{[21]} \right)^T - \bar{L}_{:,k}^{[21]} \bar{T}_{1,k}^{[21]} \left(\bar{L}_{:,1}^{[22]} \right)^T$$

$$|\Delta C^{[22]}| \leq c_1(k+1) u \left(|\bar{H}^{[21]}| |\bar{L}^{[21]}|^T + |\bar{L}_{:,k}^{[21]}| |\bar{T}_{1,k}^{[21]}| |\bar{L}_{:,1}^{[22]}|^T \right)$$

$$\bar{C}^{[22]} + \Delta \bar{C}^{[22]} = \bar{L}^{[22]} \bar{T}^{[22]} \left(\bar{L}^{[22]} \right)^T$$

$$|\Delta \bar{C}^{[22]}| \leq c_3(n-k, k) u |\bar{L}^{[22]}| |\bar{T}^{[22]}| |\bar{L}^{[22]}|^T$$

Solution of a linear system

Assuming $c_4(n)uk_\infty(\bar{T}) < 1$

$$(A + \widehat{\Delta A}) \bar{x} = b + \widehat{\Delta b}$$

$$\|\widehat{\Delta A}\|_\infty \leq c_5(n, k)u \|\bar{T}\|_\infty, \|\widehat{\Delta b}\|_\infty \leq c_5(n, k)u \|\bar{T}\|_\infty \|\bar{x}\|_\infty$$

$$\text{growth factor} \quad \rho_n = \frac{\max_{i,j} |\bar{T}_{i,j}|}{\max_{i,j} |A_{i,j}|}$$

$$\max \left\{ \frac{\|\widehat{\Delta A}\|_\infty}{\|A\|_\infty}, \frac{\|\widehat{\Delta b}\|_\infty}{\|A\|_\infty \|\bar{x}\|_\infty} \right\} \leq c_5(n, k)nu\rho_n$$

Bunch Kaufmann factorization – numerical stability

$$P(A + \Delta A)P^T = \bar{L} \bar{D} \bar{L}^T$$

$$|\Delta A| \leq c_6(n)u \left(|A| + \underbrace{|\bar{L}|}_{\nearrow} |\bar{D}| \underbrace{|\bar{L}^T|}_{\nearrow} \right)$$

Solution of a linear systems

Assuming that $c_7(n)uk \left(\overline{D} \right) < 1$

$$\left(A + \widehat{\Delta A} \right) \overline{x} = b$$

$$\left| \widehat{\Delta A} \right| \leq c_6(n)u \left(|A| + |\overline{L}| \left| \overline{D} \right| \left| \overline{L} \right|^T \right)$$

growth factor $\rho_n = \frac{\max_{i,j,k} |\overline{a}_{ij}^{(k)}|}{\max_{i,j} |a_{ij}|}$

$$\frac{\left\| \widehat{\Delta A} \right\|_{\infty}}{\left\| A \right\|_{\infty}} \leq c_6(n)nu\rho_n$$

Parallel implementation

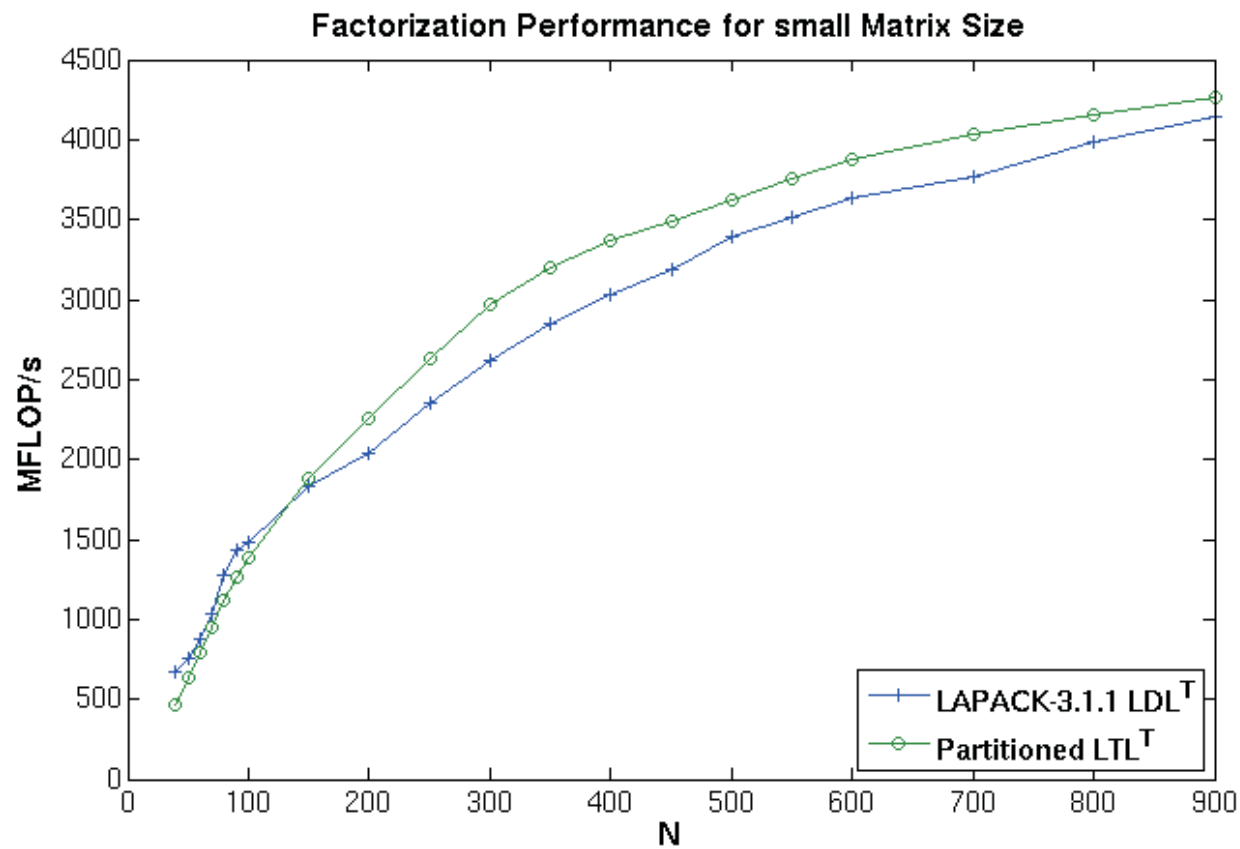
LAPACK uses blocked Bunch-Kaufmann factorization
(Dongarra, Anderson)

Cache-efficient partitioned triangular tridiagonalization
(Shklarski, Toledo – submitted to ACM TOMS)

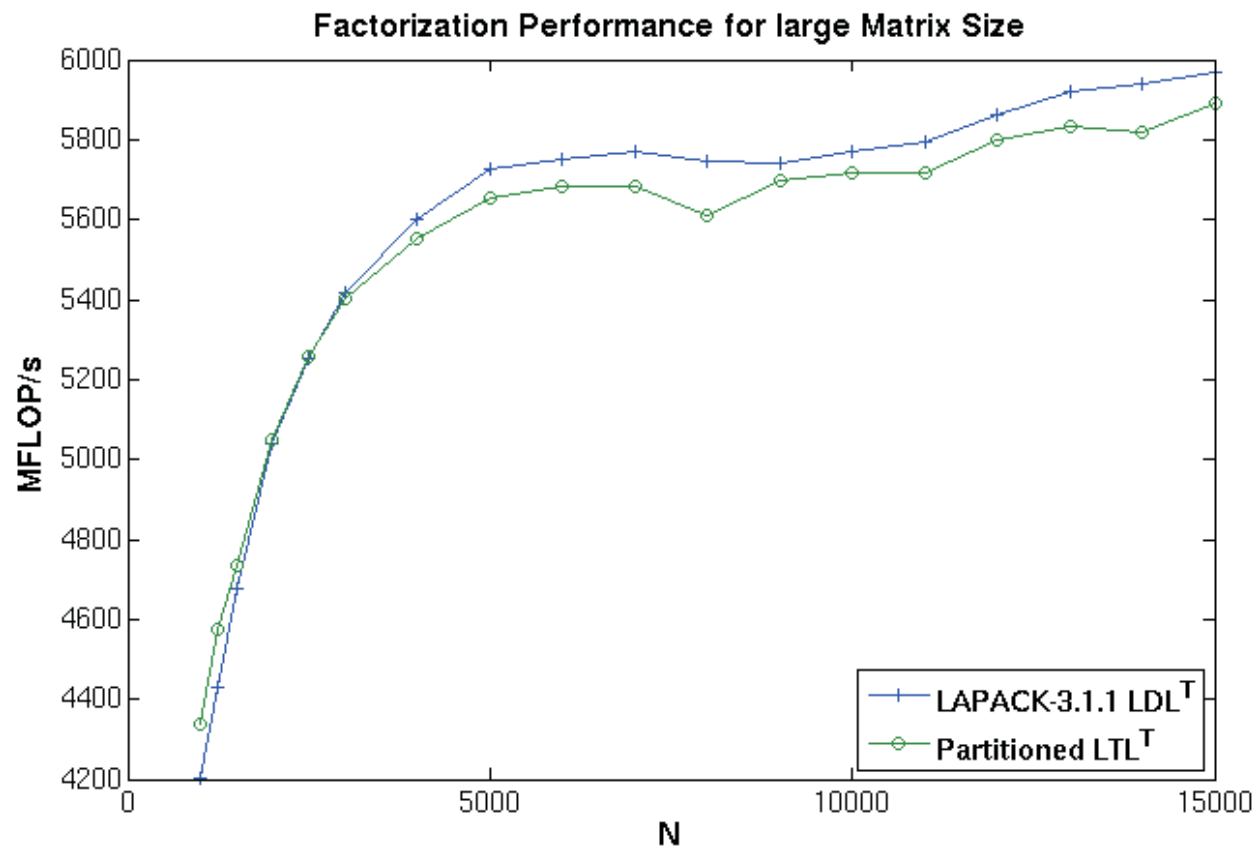
Numerical examples

- ✧ Machine
 - ✧ Core 2 Duo 6400, 2.13Ghz, 4GB of main memory
 - ✧ Linux x86_64
- ✧ Partitioned LTL^T
 - ✧ C implementation, GCC
 - ✧ Batch size = 64
 - ✧ Fused LTL^T factor and QR of T
- ✧ Partitioned LDL^T
 - ✧ LAPACK 3.1.1 (Bunch-Kaufman)
 - ✧ Block size = 64
- ✧ BLAS: GOTO BLAS 1.12, confined to a single core
- ✧ Matrices:
 - ✧ Symmetric matrices, elements uniformly distributed in $(-1, 1)$

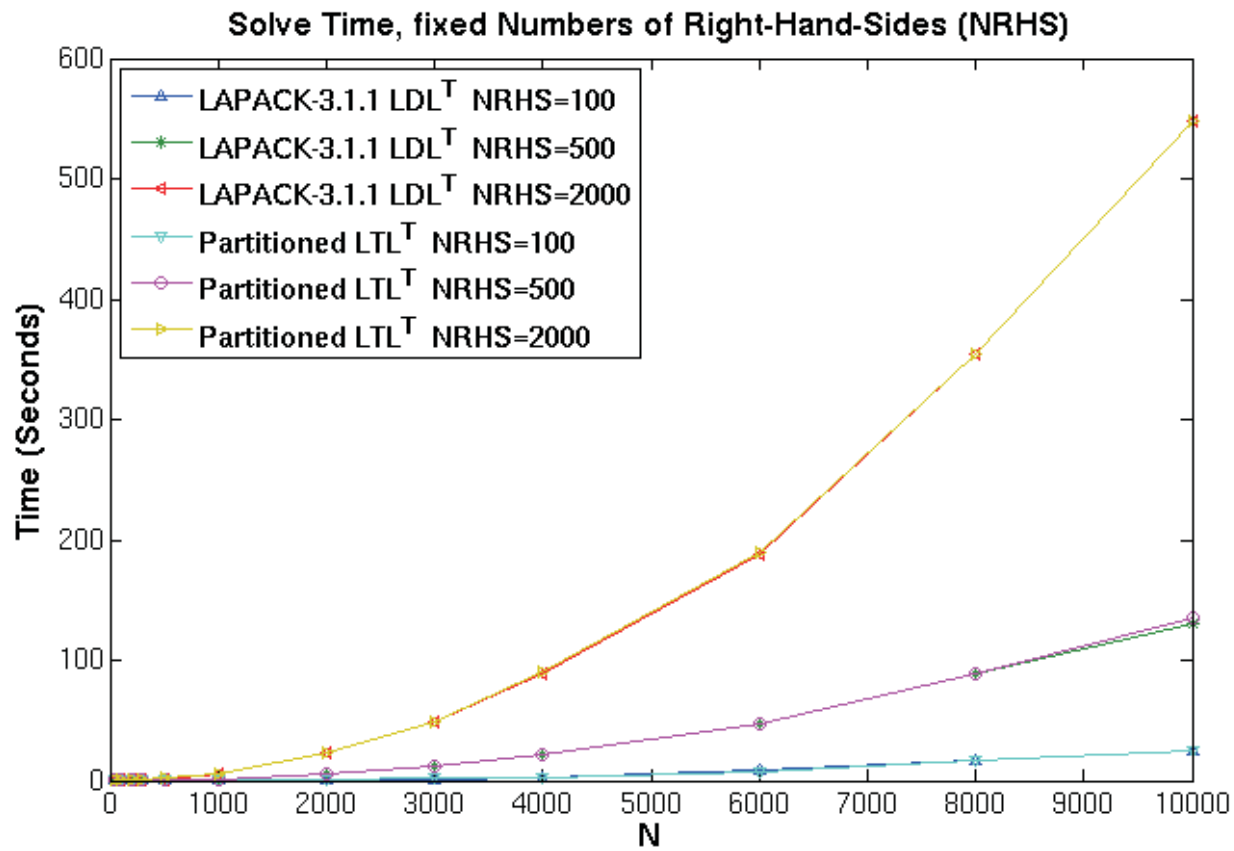
Numerical examples



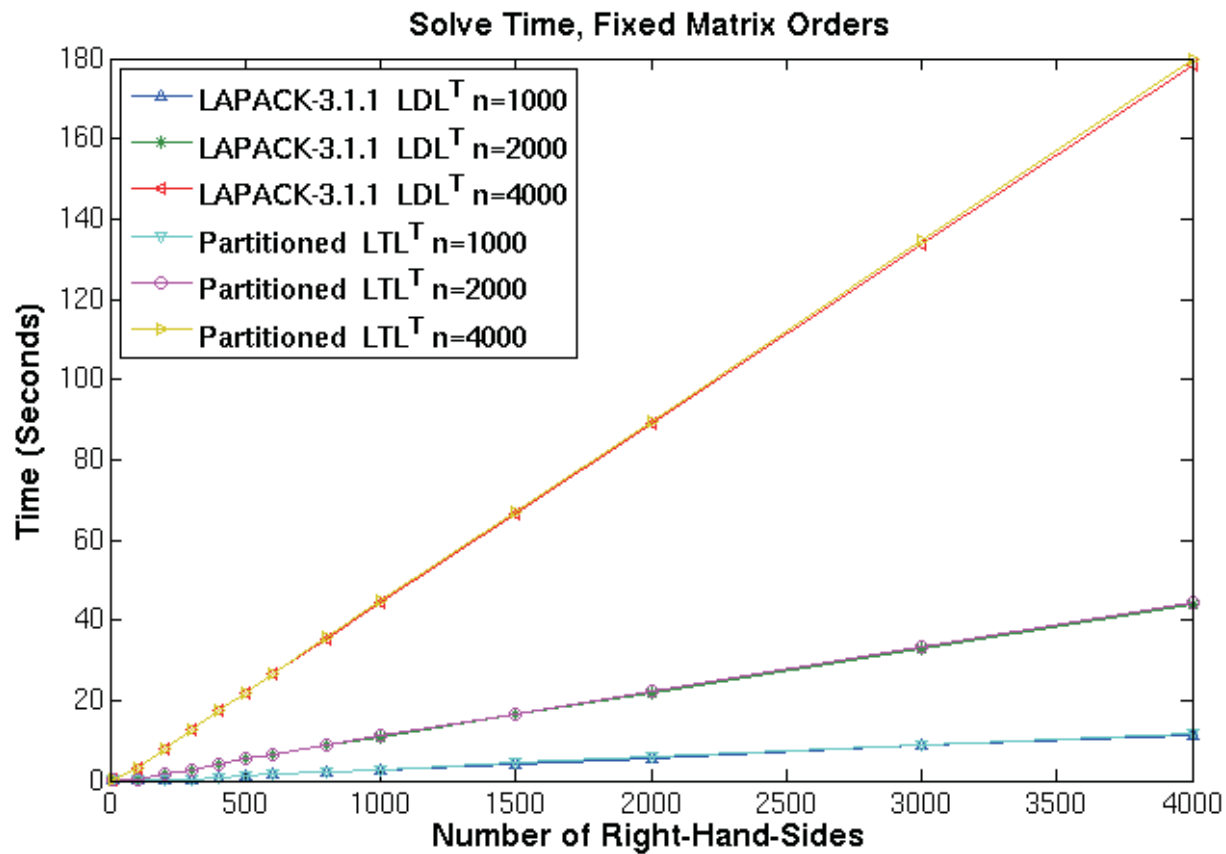
Numerical examples



Numerical examples



Numerical examples



Conclusions

LDL^T	LTL^T
✧ Reveals inertia ✧ Easy to solve with D ✧ Bunch Kauffman Pivoting ✧ $L_{i,j}$ can grow ✧ Bounded D	✧ Does not reveal inertia ✧ Slightly harder to solve with T ✧ Simple Pivoting ✧ Bounded $L_{i,j}$ ✧ T can grow

THANK YOU FOR YOUR ATTENTION

R, G. Shklarski, S. Toledo: Partitioned triangular tridiagonalization, submitted to ACM Transactions on Mathematical Software

C and Matlab Codes at

<http://www.tcu.ac.il/~stoledo/research.html>