ROUNDING ERROR ANALYSIS OF TRIANGULAR TRIDIAGONALIZATION

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joint work with Gil Shklarski and Sivan Toledo

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Outline

Bunch-Kaufmann factorization vs. triangular tridiagonalization

Aasen's factorization

Numerical stability

Implementation

Conclusions

Solution of a symmetric indefinite system of linear equations: direct methods

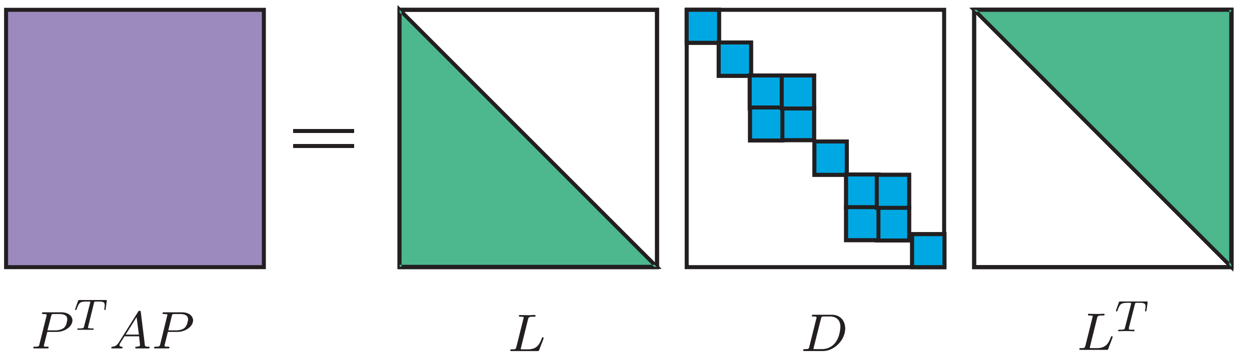
$$Ax = b$$

A is symmetric (indefinite)

$$P^T A P P^T x = P^T b$$

$$LDL^T P^T x = P^T b \qquad LTL^T P^T x = P^T b$$

Block Bunch-Kaufmann factorization



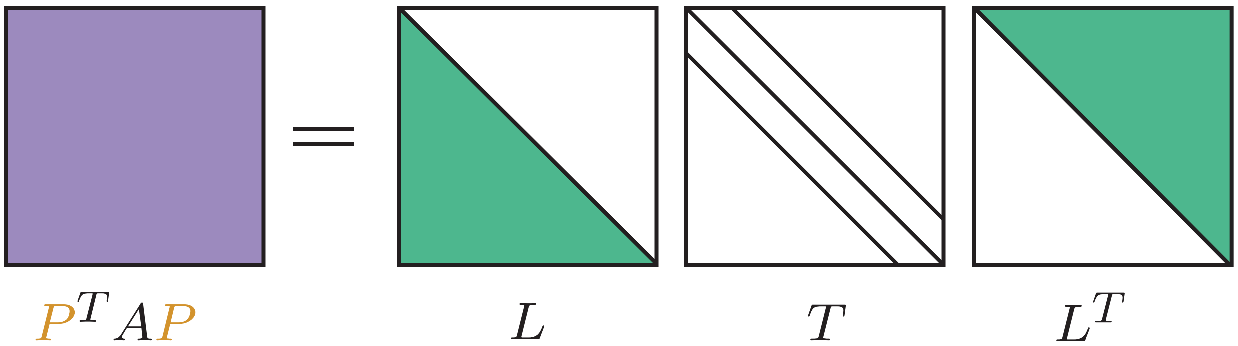
A is symmetric

L is **unit** lower triangular

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

P is a **permutation** matrix

Triangular tridiagonalization



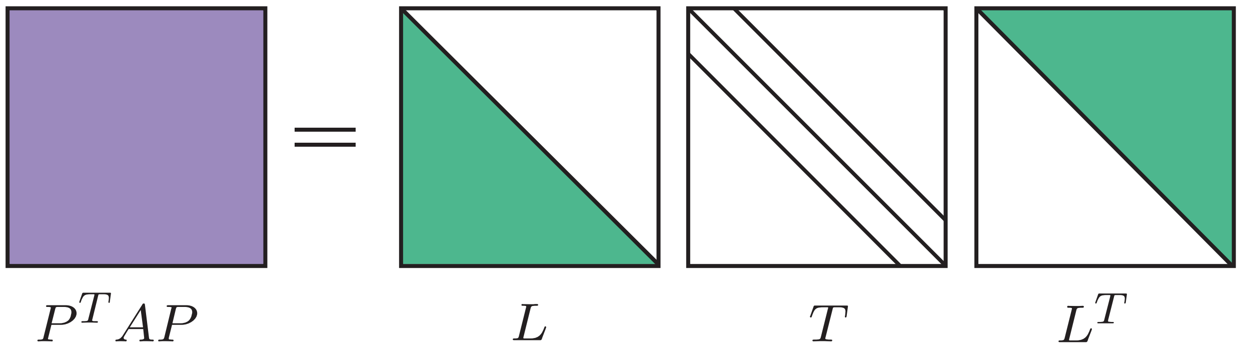
A is symmetric

L is **unit** lower triangular

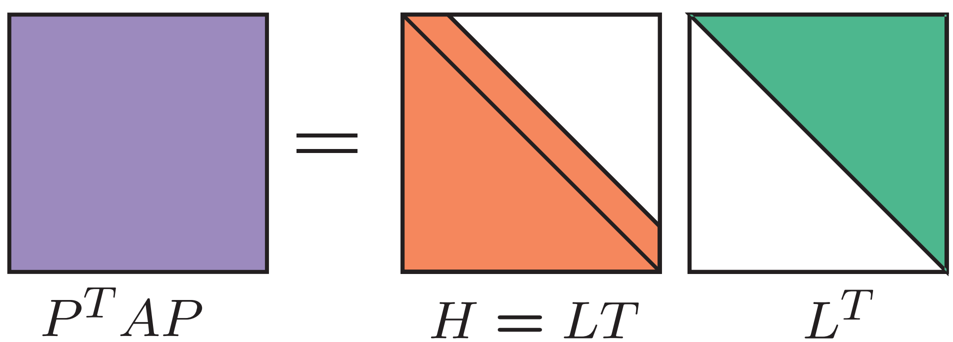
T is **symmetric** tridiagonal

P is a **permutation** matrix

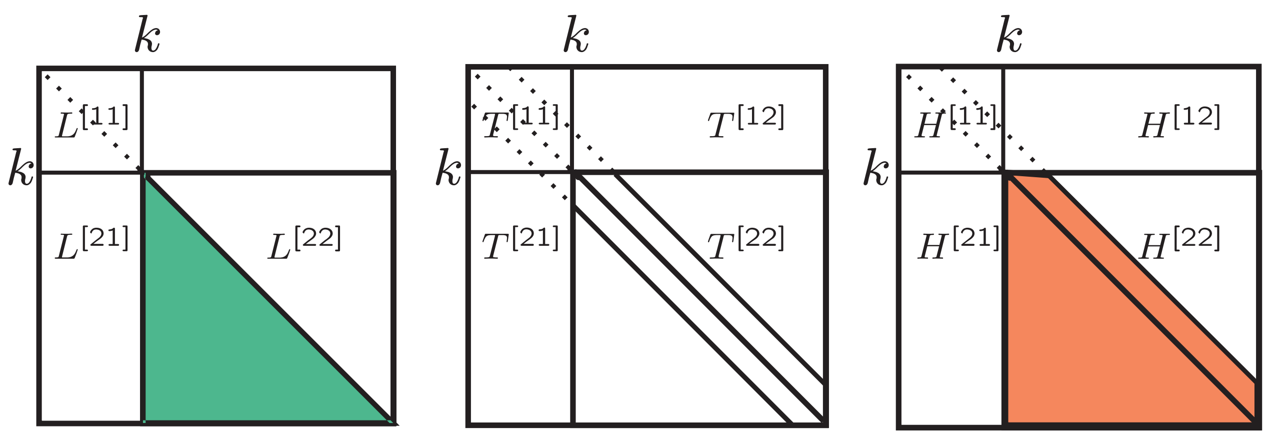
Parlett - Reid reduction



Aasen's factorization



Notation



Parlett - Reid reduction

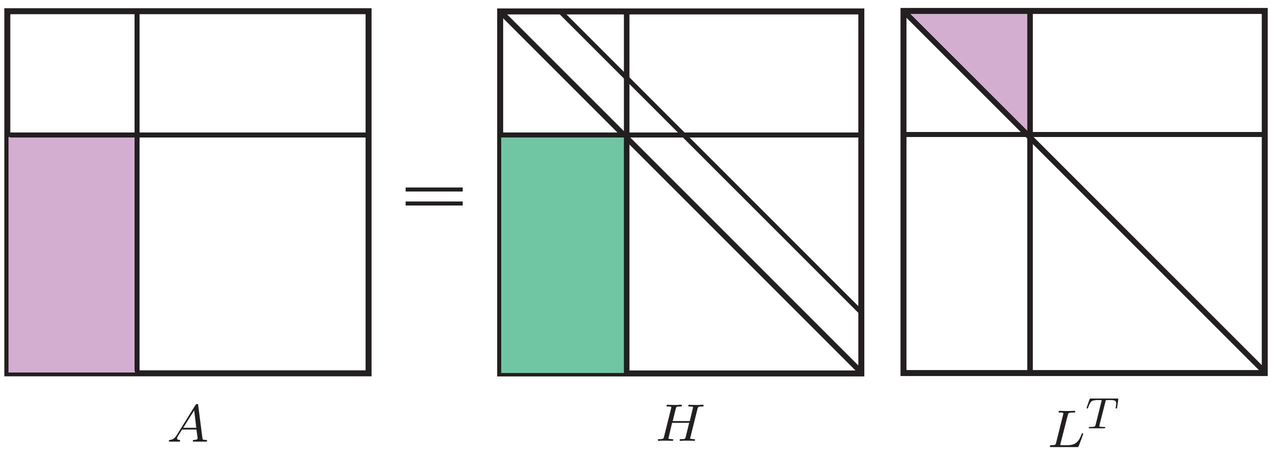
works on $L^{[22]}T^{[22]}(L^{[22]})^T$

Aasen's factorization

works on $H^{[22]}(L^{[22]})^T \neq L^{[22]}T^{[22]}(L^{[22]})^T$ for $k > 1$

1. given $L^{[11]}$, $H^{[11]}$ and $T^{[11]}$
2. compute $H^{[21]}$ and $L^{[21]}$
3. compute $(k+1)$-th column L and T
4. pivoting strategy
5. update $A^{[22]}$ to get $H^{[22]}(L^{[22]})^T$

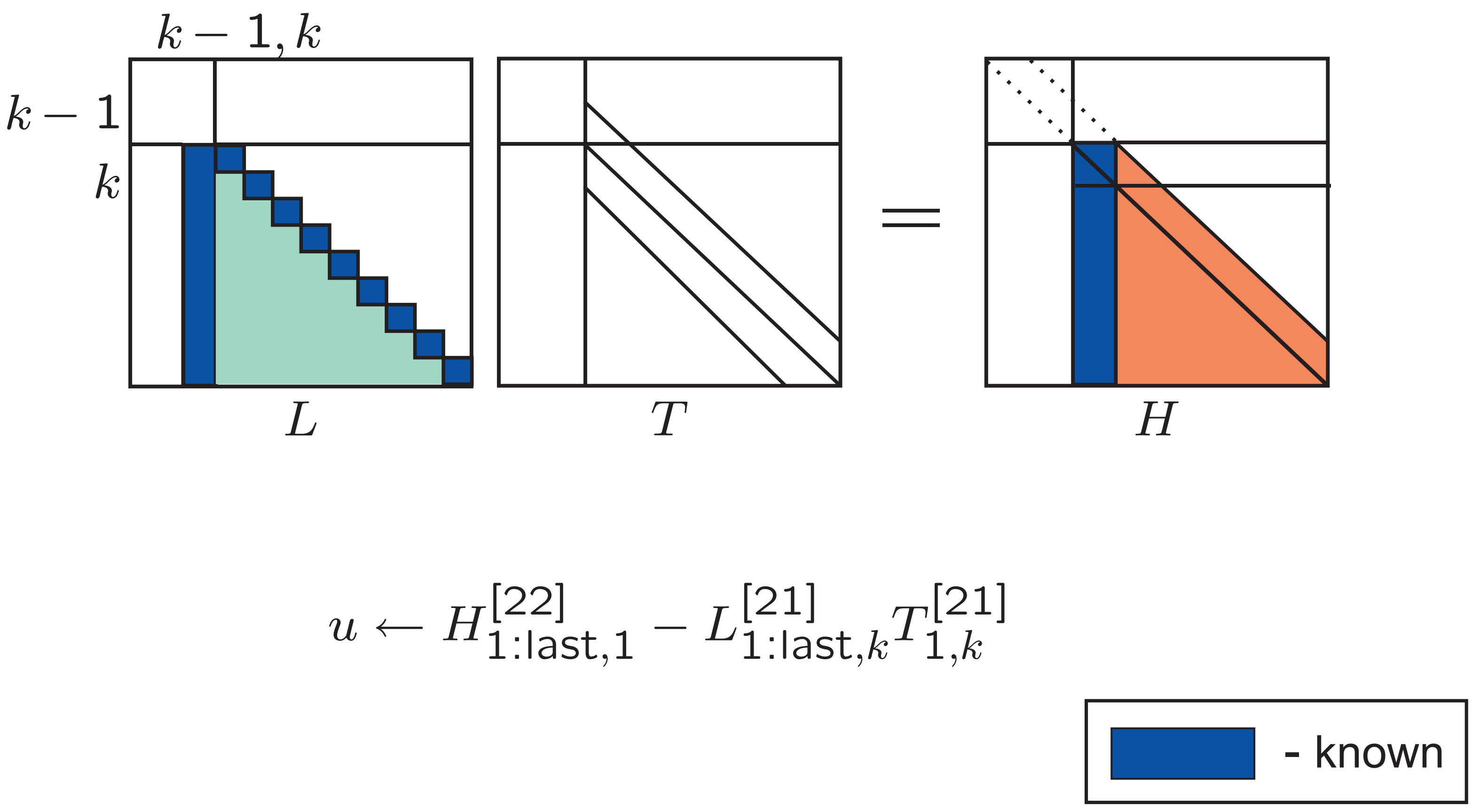
Compute $H^{[21]}$ and $L^{[21]}$



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

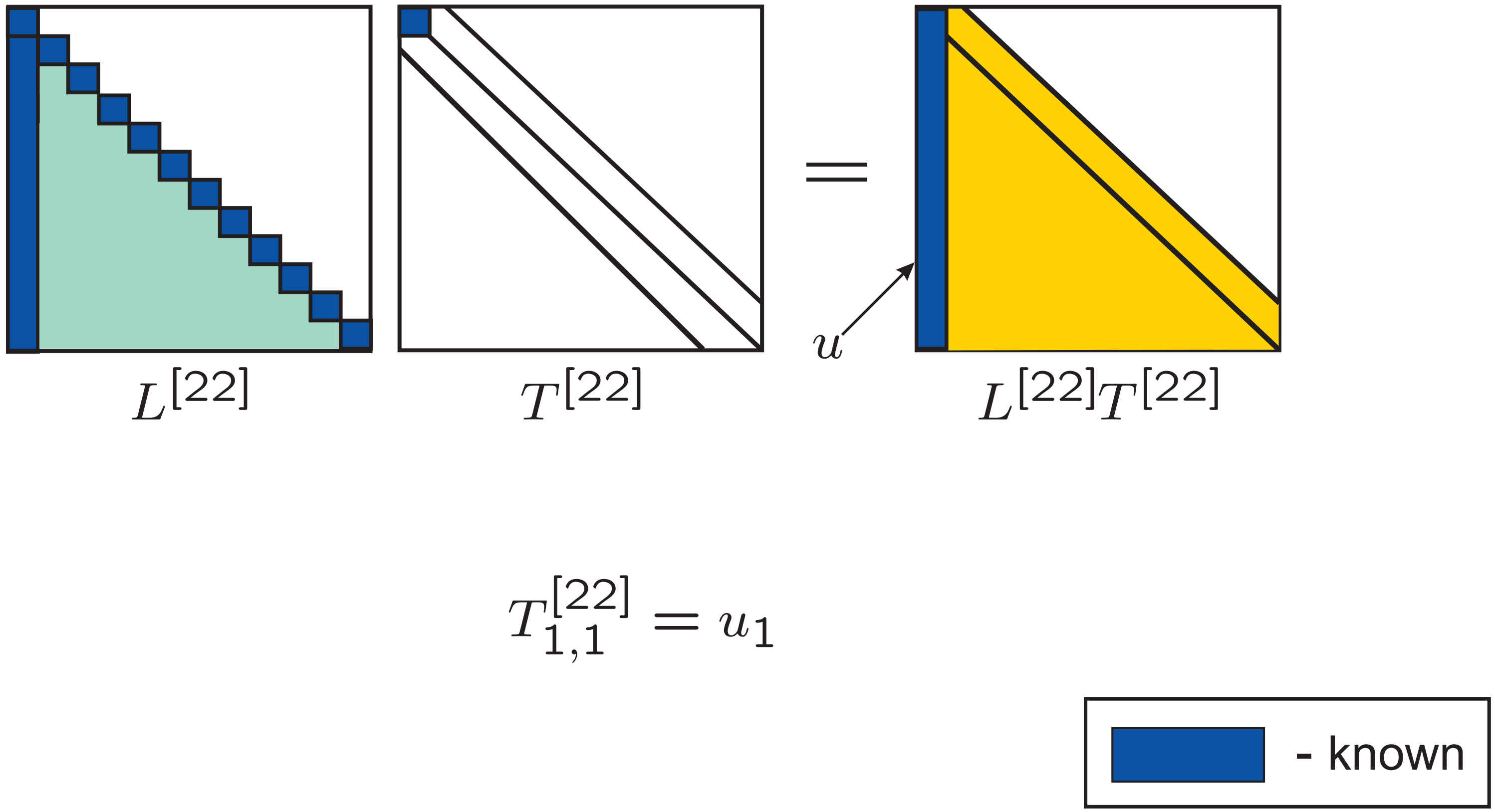
compute the i-th column of $L^{[21]}$ from i-th columns of $H^{[21]}$ and $T^{[11]}$ and previous two columns on $L^{[21]}$

Compute the first column of $L^{[22]}T^{[22]}$



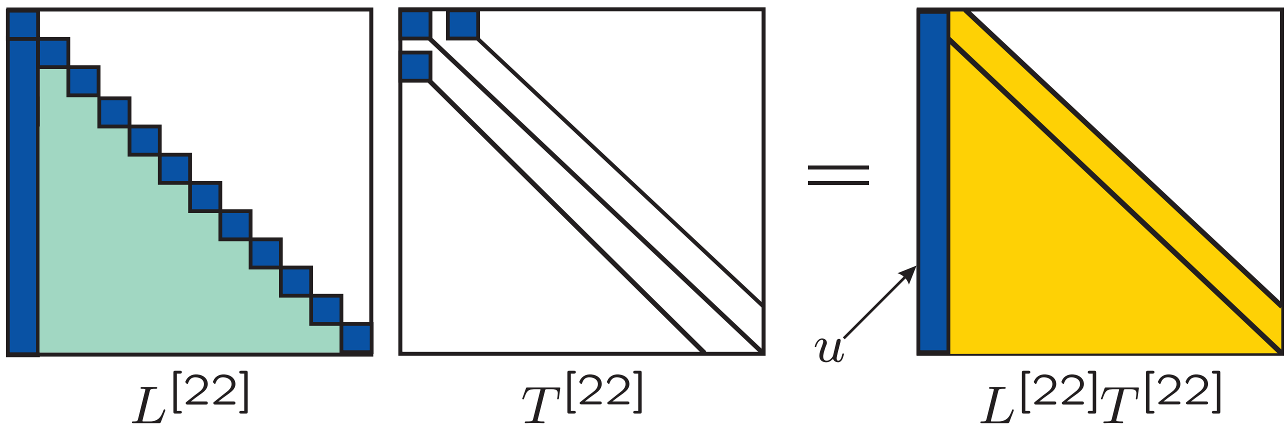
$$u \leftarrow H^{[22]}_{1:\mathrm{last},1} - L^{[21]}_{1:\mathrm{last},k} T^{[21]}_{1,k}$$

Extract $T^{[22]}_{1,1}$



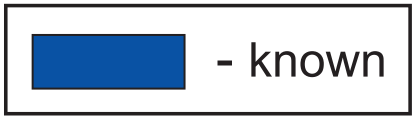
$$T^{[22]}_{1,1} = u_1$$

Extract $T^{[22]}_{1,2}$ and $L^{[22]}_{2:\text{last},2}$



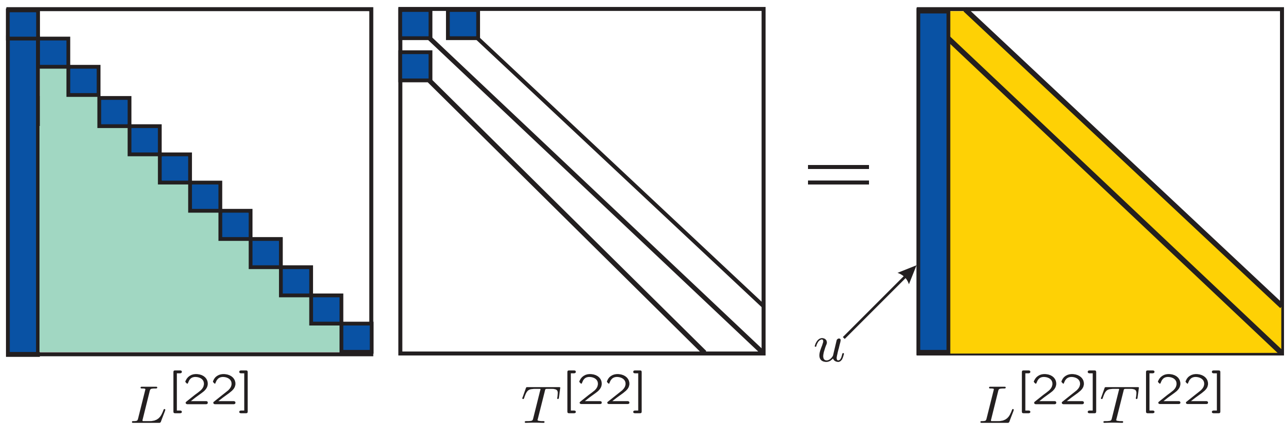
$$u_{2:\text{last}} = T^{[22]}_{1,1}\, L^{[22]}_{2:\text{last},1} + T^{[22]}_{1,2}\, L^{[22]}_{2:\text{last},2}$$

$$T^{[22]}_{1,2}\, L^{[22]}_{2:\text{last},2} = u_{2:\text{last}} - T_{1,1}\, L^{[22]}_{2:\text{last},1}$$



Pivoting strategy

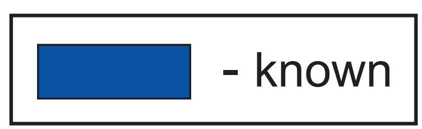
Fourth phase – extract $T^{[22]}_{1,2}$ and $L^{[22]}_{2:\text{last},2}$



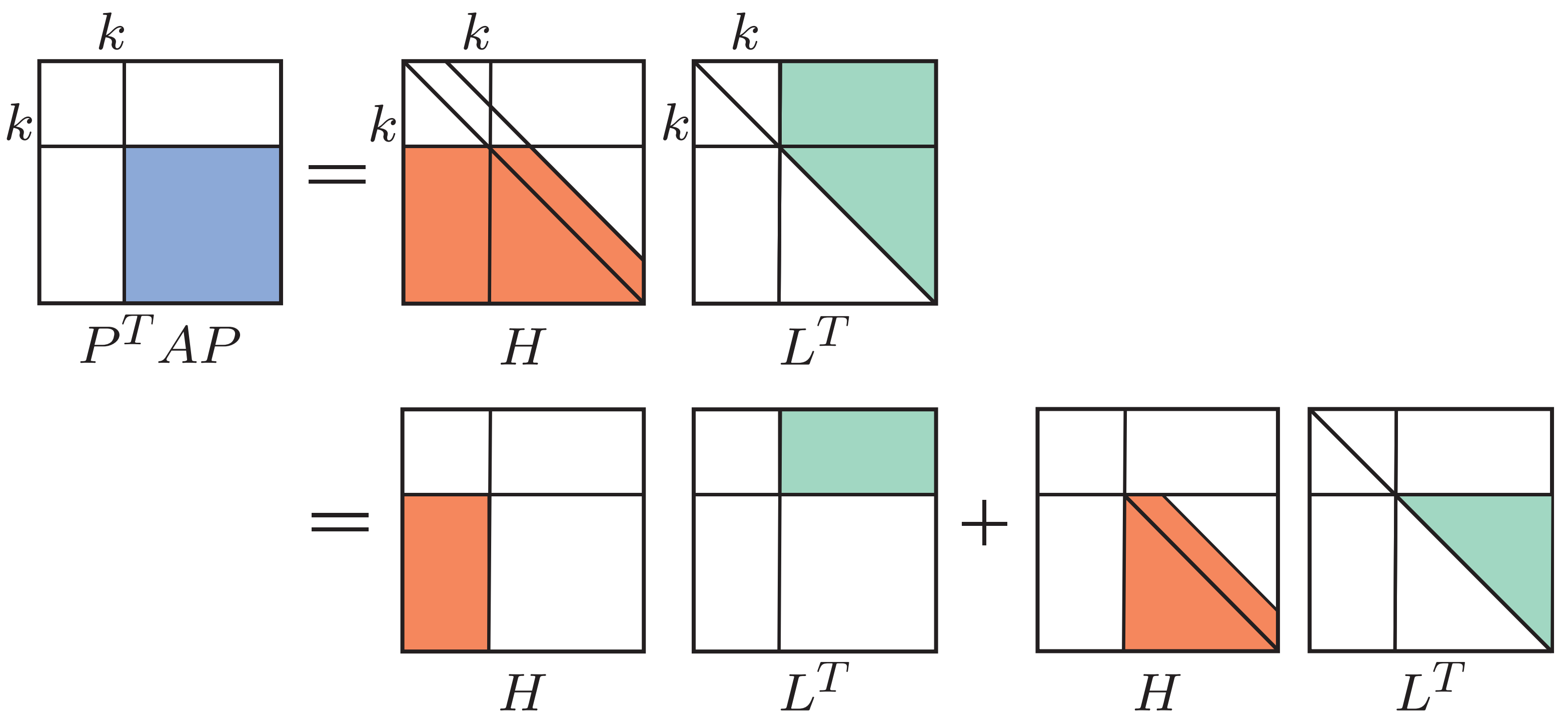
$$u_{2:\text{last}} = T^{[22]}_{1,1}\, L^{[22]}_{2:\text{last},1} + T^{[22]}_{1,2}\, L^{[22]}_{2:\text{last},2}$$

$$T^{[22]}_{1,2}\, L^{[22]}_{2:\text{last},2} = \underbrace{u_{2:\text{last}} - T_{1,1}\, L^{[22]}_{2:\text{last},1}}$$

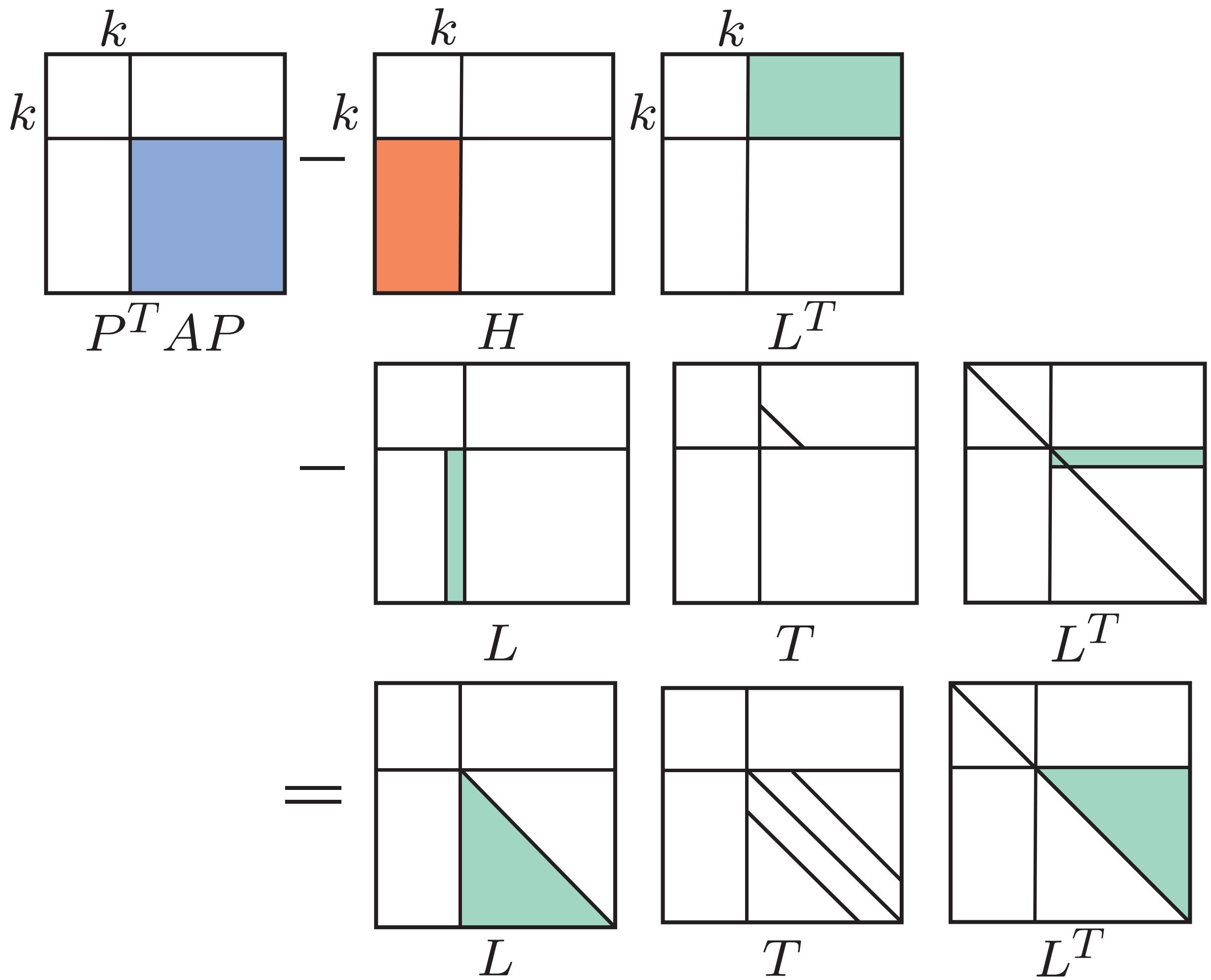
First switch variable $(i+1)$ with the largest index in



Partitioned factorization



Partitioned factorization



Partitioned Aasen's factorization: numerical stability

$$A + \Delta A = \overline{L}\,\overline{T}\,\overline{L}^T$$

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

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

Partitioned Aasen's factorization: assumptions on BLAS

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

conventional BLAS:

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

Strassen:

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

Partitioned Aasen's factorization: solution of a linear system

Assuming $c_4(n)uk_\infty\left(\overline{T}\right) < 1$

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

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

growth factor $\rho_n = \dfrac{\max_{i,j}\left|\overline{T}_{i,j}\right|}{\max_{i,j}\left|A_{i,j}\right|}$

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

Parallel implementation

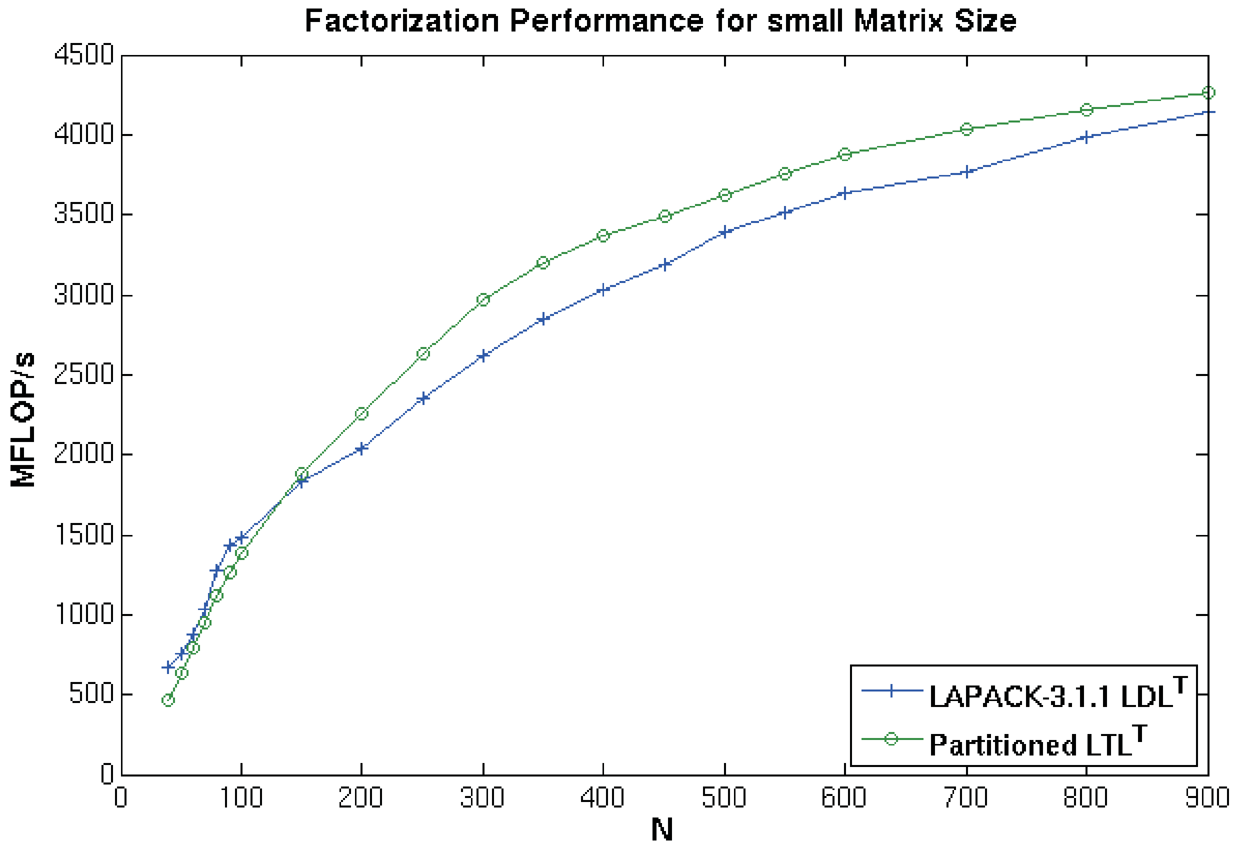
LAPACK uses blocked Bunch-Kaufmann factorization
(Dongarra, Anderson)

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

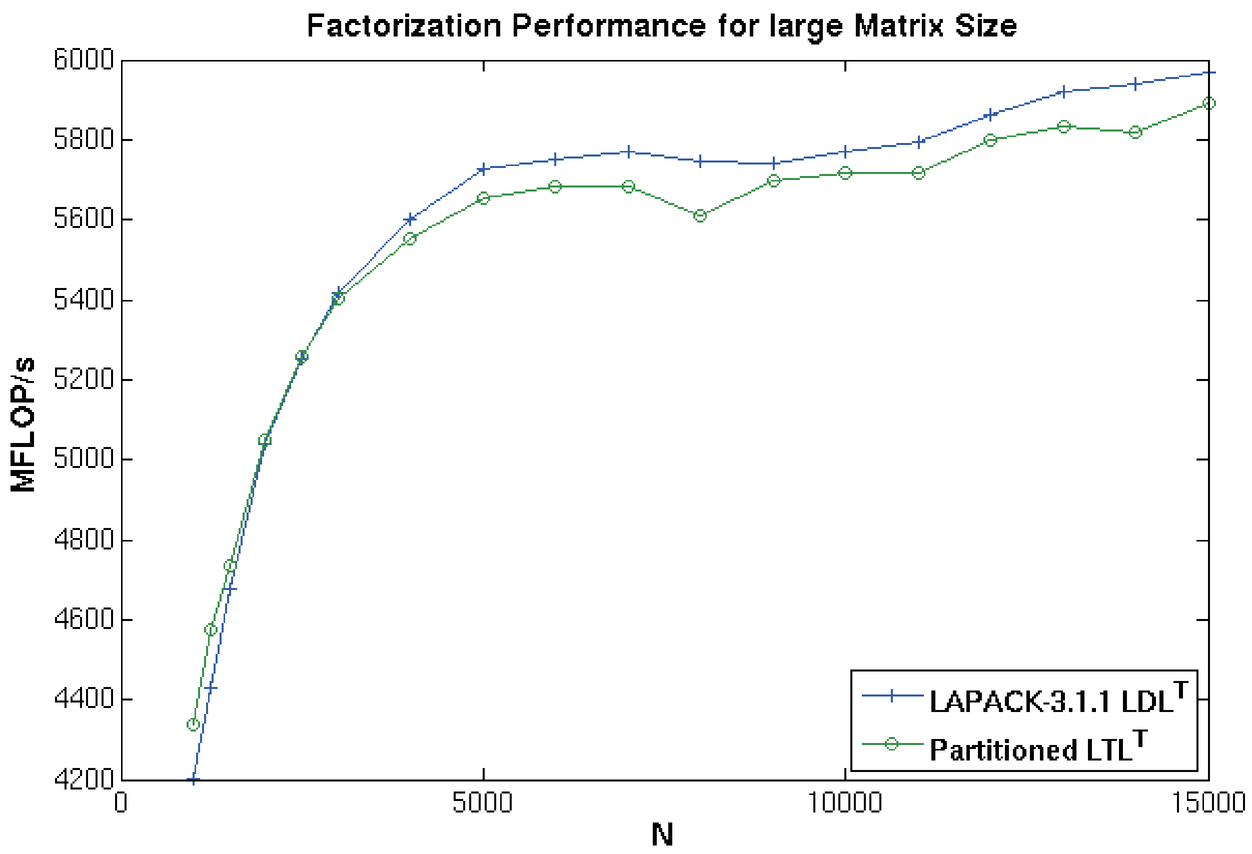
Numerical examples

- 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 $(-1, 1)$

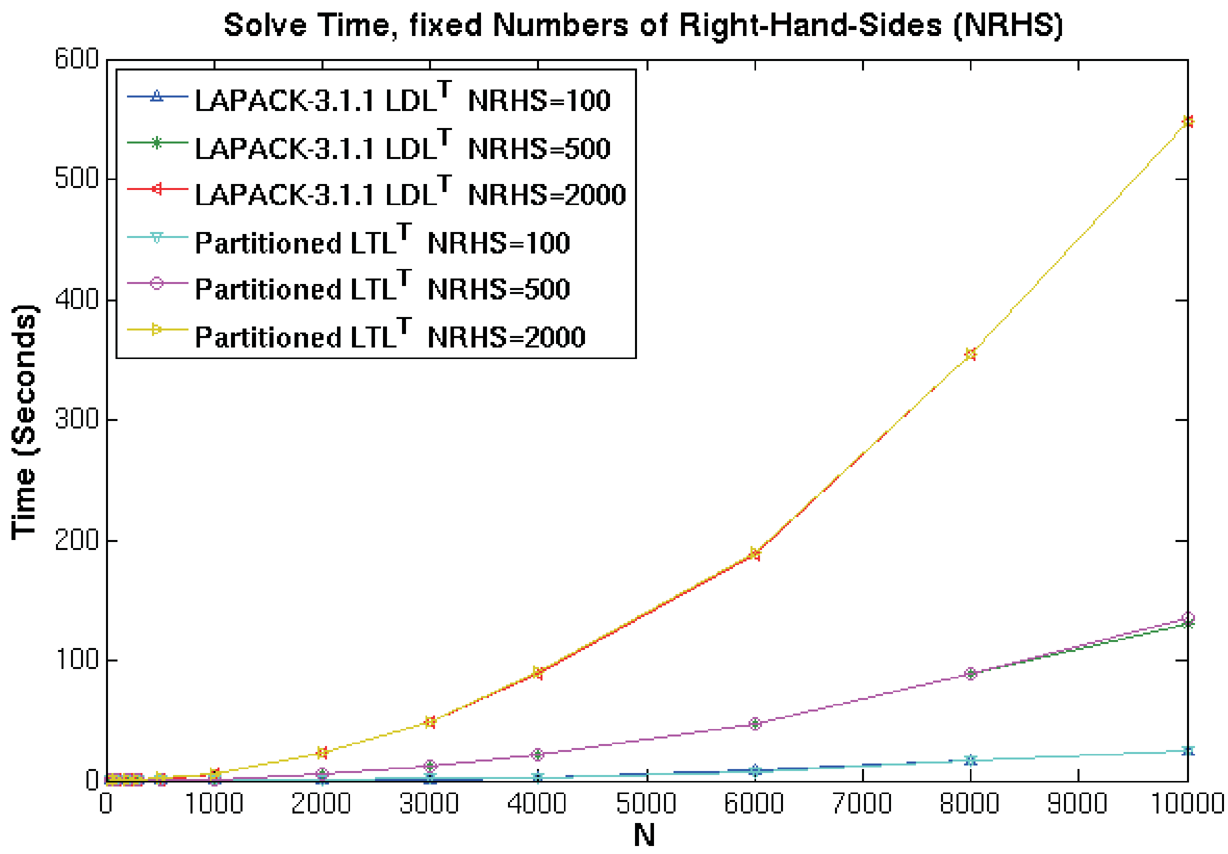
Numerical examples



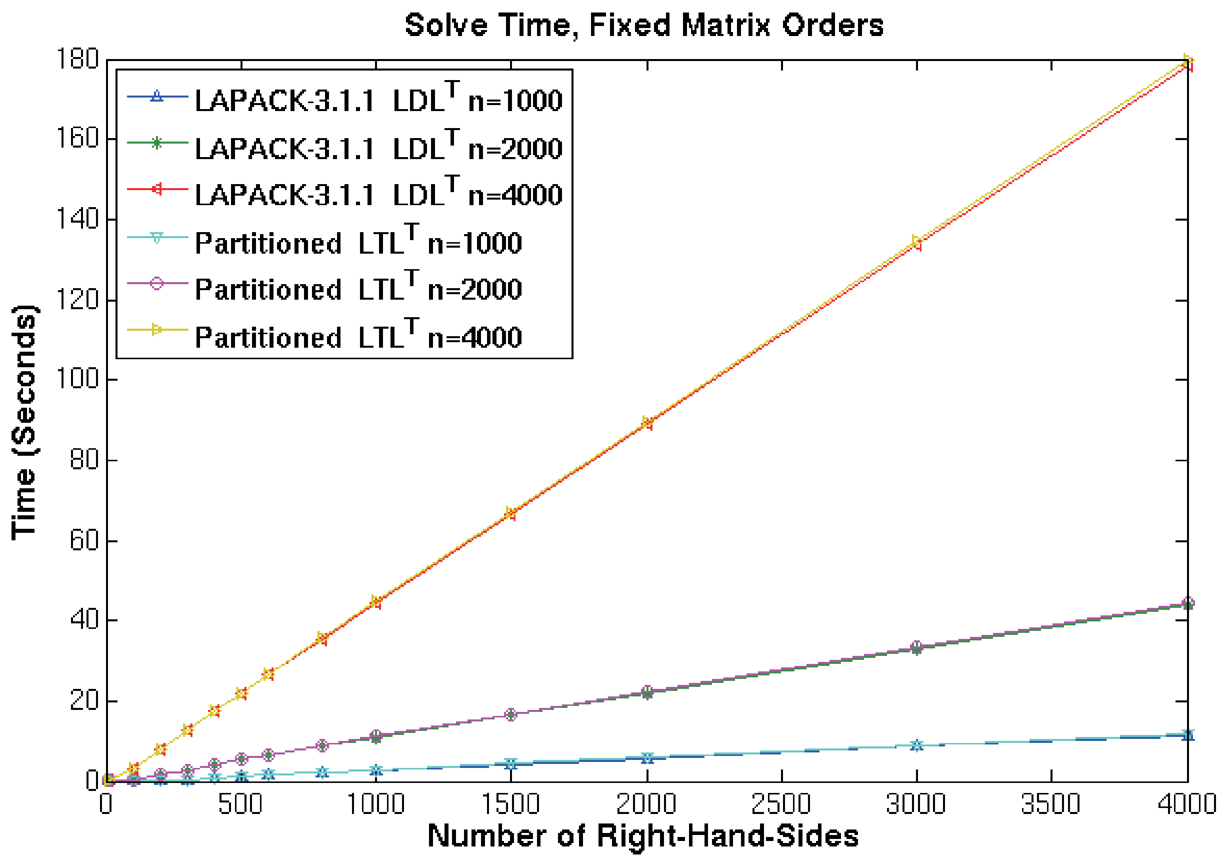
Numerical examples



Numerical examples



Numerical examples



Conclusions

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

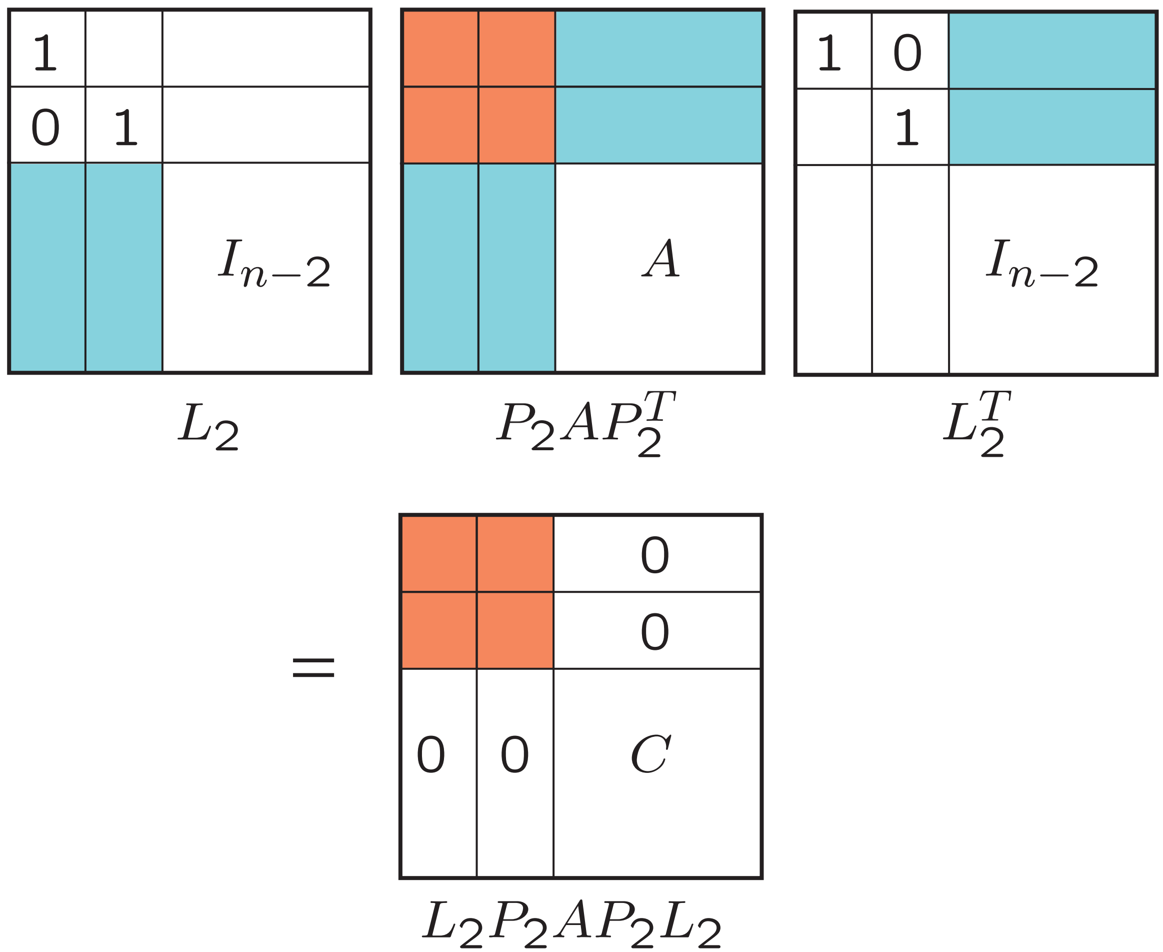
THANK YOU FOR YOUR ATTENTION

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

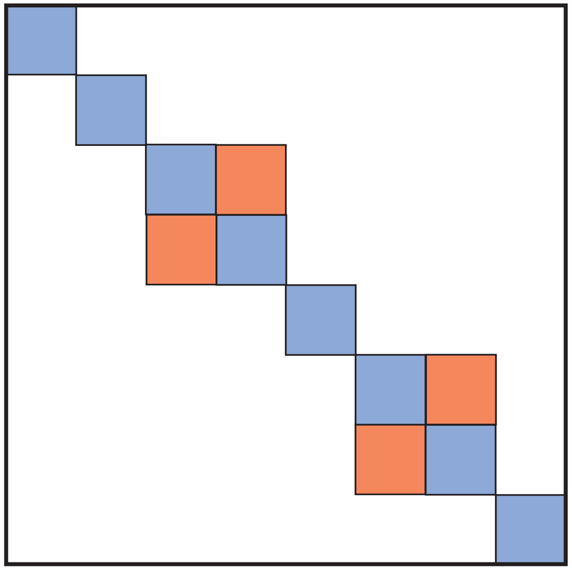
C and Matlab Codes at

`http://www.tcu.ac.il/∼stoledo/research.html`

Bunch-Kaufmann factorization



Bunch-Kaufmann factorization

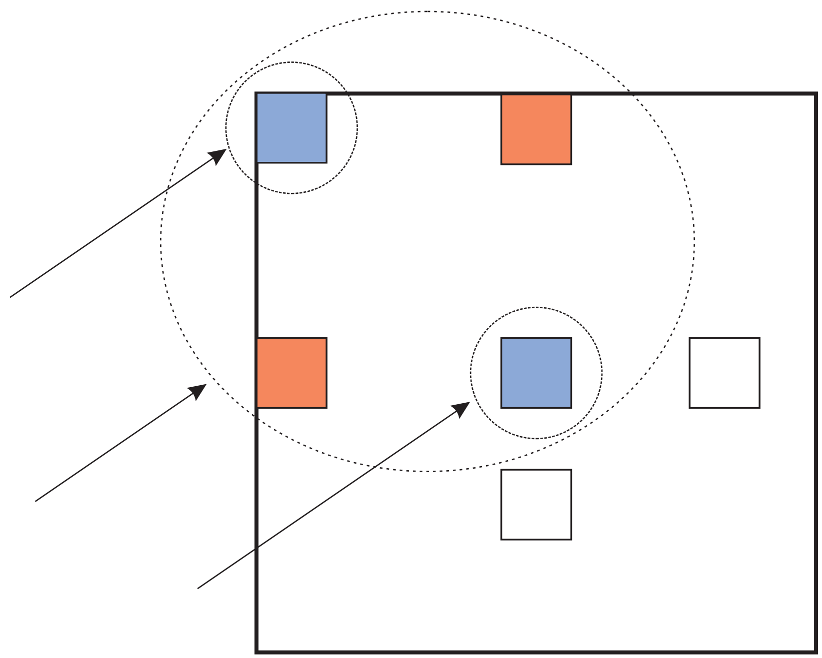


$$\underbrace{L_{n-1}P_{n-1}\ldots L_2P_2L_1P_1AP_1^TL_1^TP_2^TL_2^T\ldots P_{n-1}^TL_{n-1}^T}_{D}$$

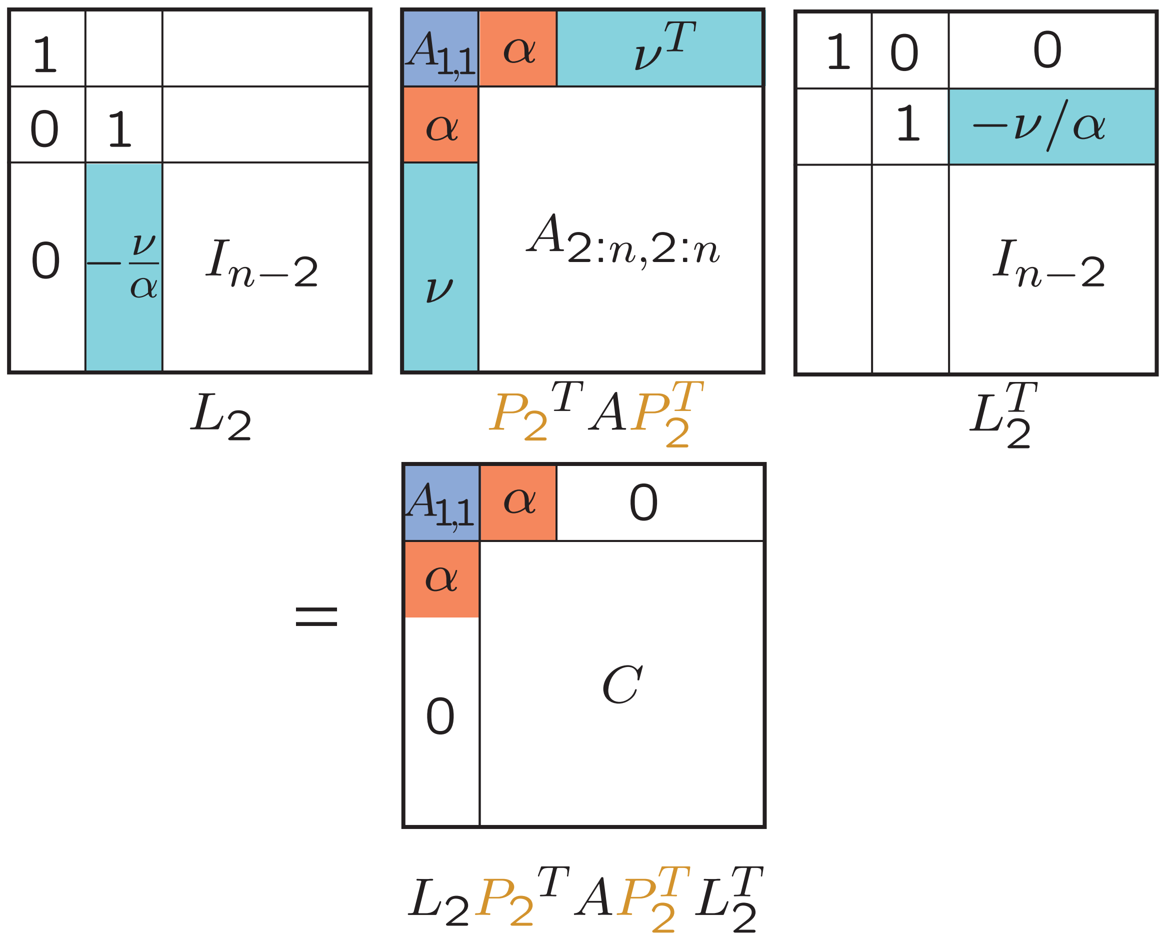
Bunch-Kaufmann pivoting strategy

- complete pivoting $O(n^3)$ comparisons Bunch, Parlett

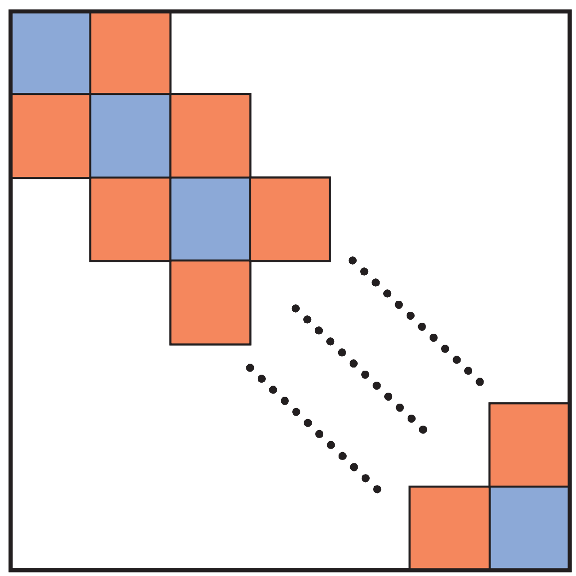
- partial pivoting $O(n^2)$ comparisons implemented in LINPACK, LAPACK



Parlett - Reid reduction



Parlett - Reid reduction



$$\underbrace{\underbrace{L_{n-1}P_{n_1}\dots L_3P_3L_2P_2}_{L^{-1}P^T}\,A\,\underbrace{P_2^TL_2^TP_3^TL_3^T\dots P_{n-1}^TL_{n-1}^T}_{PL^{-T}}}_{T}$$

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 $2/3n^3 + O(n^2)$

$\longrightarrow$ Aasen's factorization

Numerical stability – Proof 1

$$
\begin{aligned}
A^{[11]} + \Delta A^{[11]} &= \overline{L}^{[11]}\,\overline{T}^{[11]}\left(\overline{L}^{[11]}\right)^T \\
\left|\Delta A^{[11]}\right| &\leq c_3(k,1)u\left|\overline{L}^{[11]}\right|\left|\overline{T}^{[11]}\right|\left|\overline{L}^{[11]}\right|^T \\
A^{[21]} + \Delta A^{[21]} &= \overline{H}^{[21]}\left(\overline{L}^{[11]}\right)^T \\
\left|\Delta A^{[21]}\right| &\leq c_1(k)u\left|\overline{H}^{[21]}\right|\left|\overline{L}^{[11]}\right|^T \\
\overline{H}^{[21]} + \Delta H^{[21]} &= \overline{L}^{[21]}\,\overline{T}^{[11]} + \overline{L}^{[22]}_{:,1}\overline{T}^{[21]}_{1,k} \\
\left|\Delta H^{[21]}\right| &\leq c_1(3)\left(\left|\overline{L}^{[21]}\right|\left|\overline{T}^{[11]}\right| + \left|\overline{L}^{[22]}_{:,1}\right|\left|\overline{T}^{[21]}_{1,k}\right|\right)
\end{aligned}
$$

Numerical stability – Proof 2

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

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

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

$$\left|\Delta \overline{C}^{[22]}\right| \le c_3(n-k, k)\, u \left|\overline{L}^{[22]}\right| \left|\overline{T}^{[22]}\right| \left|\overline{L}^{[22]}\right|^T$$

Bunch Kaufmann factorization: numerical stability

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

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

Bunch Kaufmann factorization: Solution of a linear system

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

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

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

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

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