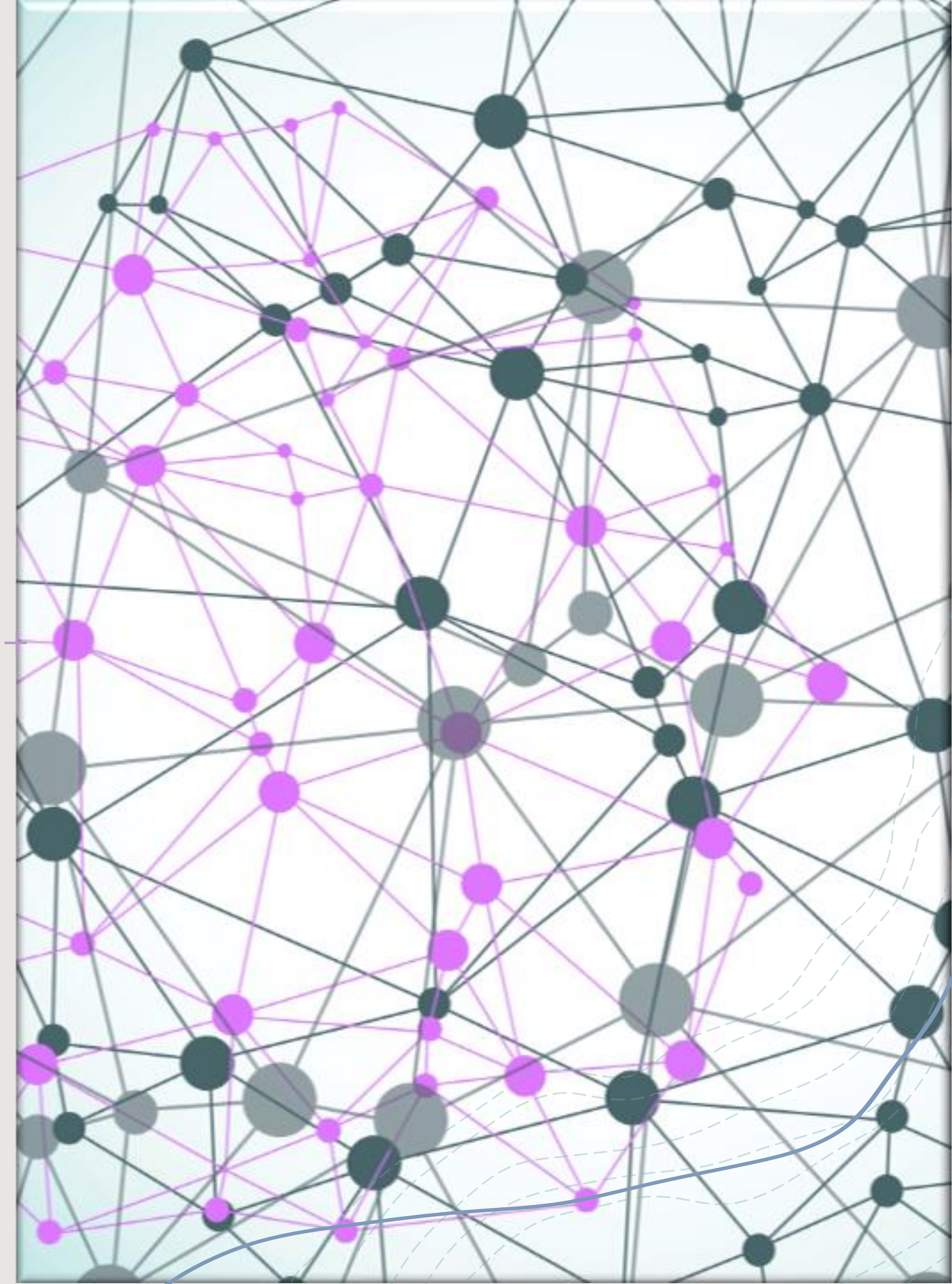
LTL^T Decomposition of a Skew-Symmetric Matrix - Derivation



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Objective

- High performance
- shared memory
- parallel implementations of a **family of algorithms**
- for the computation of the **$X = LTL^T$ decomposition**
- (with and without pivoting) of a
    - skew-symmetric X matrix factorization,
    - Unit lower triangular L,
    - tridiagonal T
- which were derived using the the FLAME methodology.
- The approach has used a number of
    - BLAS-like primitives and BLIS framework using C++
    - Gauss transform,
    - Hence, it contributes towards computing Tridiagonal decomposition of (skew)-symmetric matrix
    - For achieving high performance computing.

Introduction

Matrix Decomposition or Matrix Factorization

- factoring any matrix as a product of two or more multiplicand matrices. $A = BC$
- Cholesky, LU, QR, SVD (Singular value decomposition)
- LTL^T decomposition for skew-symmetric matrix
- A is skew-symmetric if the transpose of a matrix is equal to the negative of the matrix, ie

$$(A^T = -A \text{ or } a_{j,i} = -a_{i,j})$$

Skew-symmetric non-diagonalizable matrix X

$X = LTL^T$

where L is a unit lower-triangular matrix with first column as 0, and T is a skew-symmetric tridiagonal matrix.

$$L = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & \lambda_{2,1} & 1 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & \lambda_{n-1,1} & \lambda_{n-1,2} & \cdots & 1 \end{pmatrix},$$

$$T = \begin{pmatrix} 0 & -\tau_{1,0} & 0 & \cdots & 0 \\ \tau_{1,0} & 0 & -\tau_{2,1} & \cdots & 0 \\ 0 & \tau_{2,1} & 0 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

Pfaffian of a skew-symmetric tridiagonal matrix

$Pf(T)^2 = \det(T)$ and $\det(T) = \det(X)$

Pfaffian

Pfaffian of a skew-symmetric tridiagonal matrix

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- Pfaffian of matrix with even size:
  - $\mathbf{Pf(T) = \tau_{1,0} \times \tau_{3,2} \times \cdots \times \tau_{2n-1,2n-2}}$
- Pfaffian of matrix with odd size is **0**.

Application of Pfaffian

- Machine Learning (Markov random fields), [1]
- Physics (partition function of Ising models), [2]
- Quantum computations (electronic structure quantum Monte Carlo) [3]

1. Ziwei Liu, Xiaoxiao Li, Ping Luo, Chen Change Loy, and Xiaoou Tang. Deep Learning Markov Random Field for Semantic Segmentation, August 2017. arXiv:1606.07230 [cs].

2. Creighton K. Thomas and A. Alan Middleton. Exact Algorithm for Sampling the 2D Ising Spin Glass. Physical Review E, 80(4):046708, October 2009. arXiv:0906.5519 [cond-mat].

3. Michal Bajdich and Lubos Mitas. Electronic structure quantum Monte Carlo, August 2010. arXiv:1008.2369 [cond-mat, physics:physics].

FLAME (Formal Linear Algebra Methods Environments)

Step	Algorithm: $[X, L] := \mathrm{LTLT\_UNB\_RIGHT}(X)$
1a	$\{ X = \hat{X} \wedge (\exists L, T \mid \hat{X} = L T L^T) \}$
4	$L = I$ $X \rightarrow \begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix}, L \rightarrow \cdots, T \rightarrow \cdots$ where X_{TL} is 0×0, L_{TL} is 0×0, T_{TL} is 0×0
2	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \right\}$
3	while $m(X_{TL}) < m(X) - 1$ do
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge m(X_{TL}) < m(X) - 1 \right\}$
5a	$\begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} X_{00} & x_{01} & x_{02} & X_{03} \\ x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix}$
6	$\left\{ \begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} T_{00} & \star & \star & \star \\ \tau_{10} e_l^T & 0 & \star & \star \\ 0 & \tau_{21} \begin{pmatrix} 1 \\ l_{32} \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ l_{32} & L_{33} \end{pmatrix} \begin{pmatrix} 0 & \star \\ \tau_{32} e_f & T_{33} \end{pmatrix} \begin{pmatrix} 1 & l_{32}^T \\ 0 & L_{33}^T \end{pmatrix} \\ 0 & & \end{pmatrix} \wedge \cdots \right\}$
8	$l_{32} := x_{31} / \chi_{21}$ $x_{31} := 0$ $X_{33} := X_{33} + (l_{32} x_{32}^T - x_{32} l_{32}^T)$ (skew symmetric rank-2 update,
5b	$\begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} X_{00} & x_{01} & x_{02} & X_{03} \\ x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix}$
7	$\left\{ \begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} T_{00} & \star & \star & \star \\ \tau_{10} e_l^T & 0 & \star & \star \\ 0 & \tau_{21} & 0 & \star \\ 0 & 0 & \tau_{32} L_{33} e_f & L_{33} T_{33} L_{33}^T \end{pmatrix} \right\}$
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	endwhile
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge \neg(m(X_{TL}) < m(X) - 1) \right\}$
1b	$\{ X = T \wedge \hat{X} = L T L^T \}$

To systematically derives the algorithm

Steps: order in which assertions (in the highlighted lines) and commands are filled.

Left-Looking

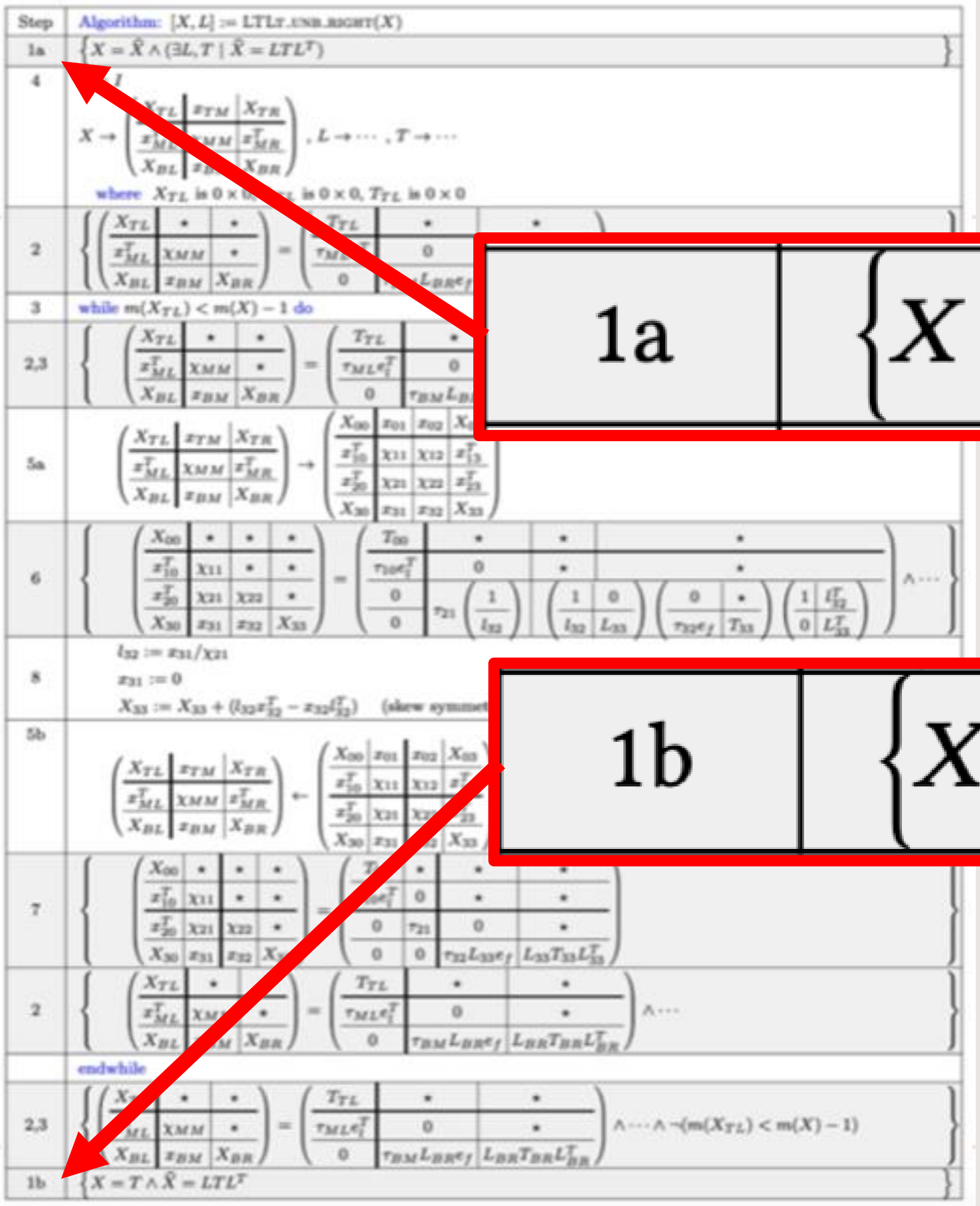
Right-Looking

Blocked

Unblocked

Pivoting

FLAME (Formal Linear Algebra Methods Environments)



Pre-Condition

1a	$\left\{ X = \widehat{X} \wedge (\exists L, T \mid \widehat{X} = LTL^T) \right.$

1b	$\left\{ X = T \wedge \widehat{X} = LTL^T \right.$

Post-Condition

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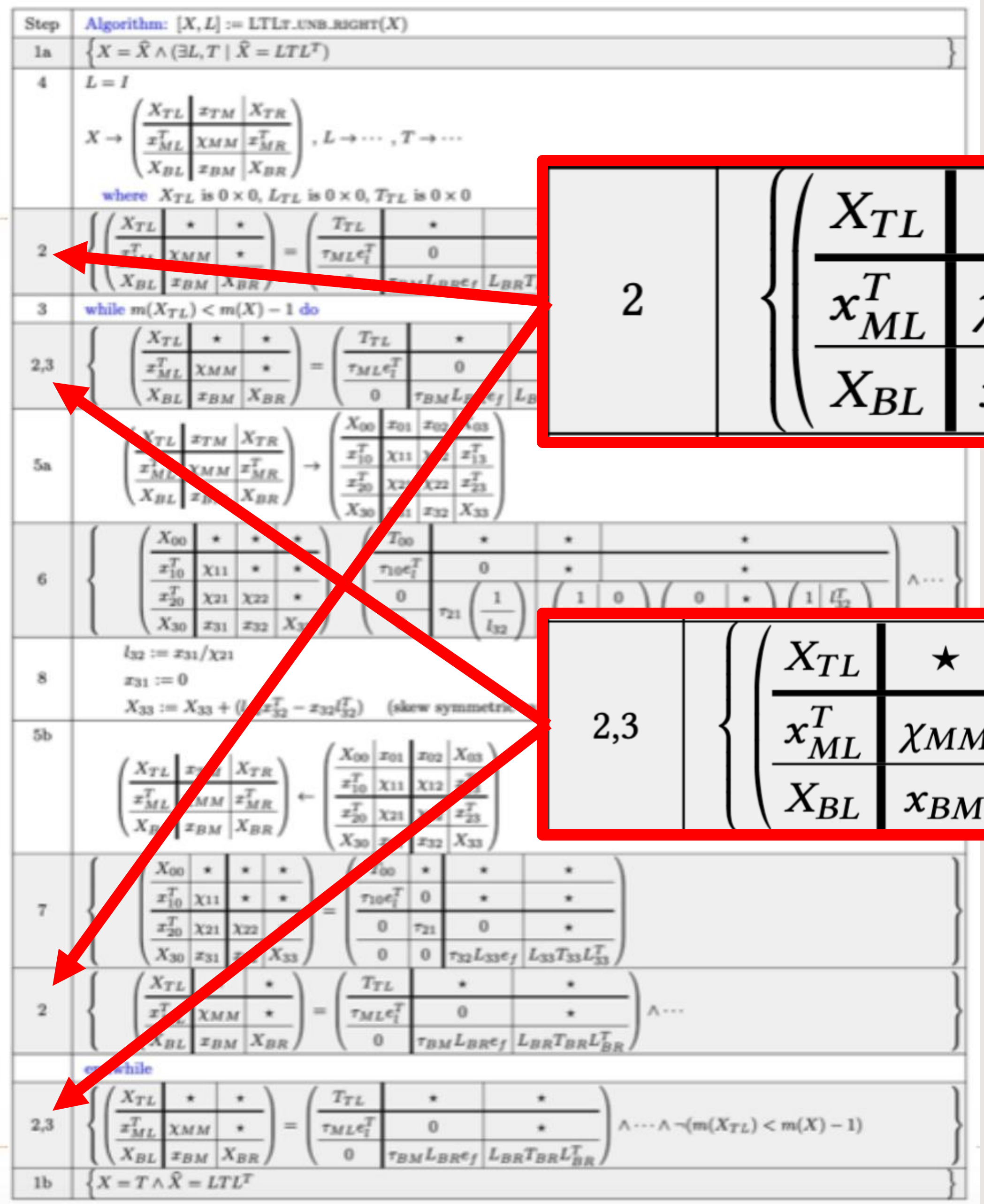
	endwhile
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge \neg(m(X_{TL}) < m(X) - 1) \right\}$
1b	$\left\{ X = T \wedge \hat{X} = LTL^T \right\}$

3	while $m(X_{TL}) < m(X) - 1$ do

Iteration

endwhile

FLAME (Formal Linear Algebra Methods Environments)



2	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \right.$

Invariant: must hold

2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge m(X_{TL}) < m(X) - 1 \right.$

Exposes a structure for the inductive proof that guides the derivation of the algorithm.

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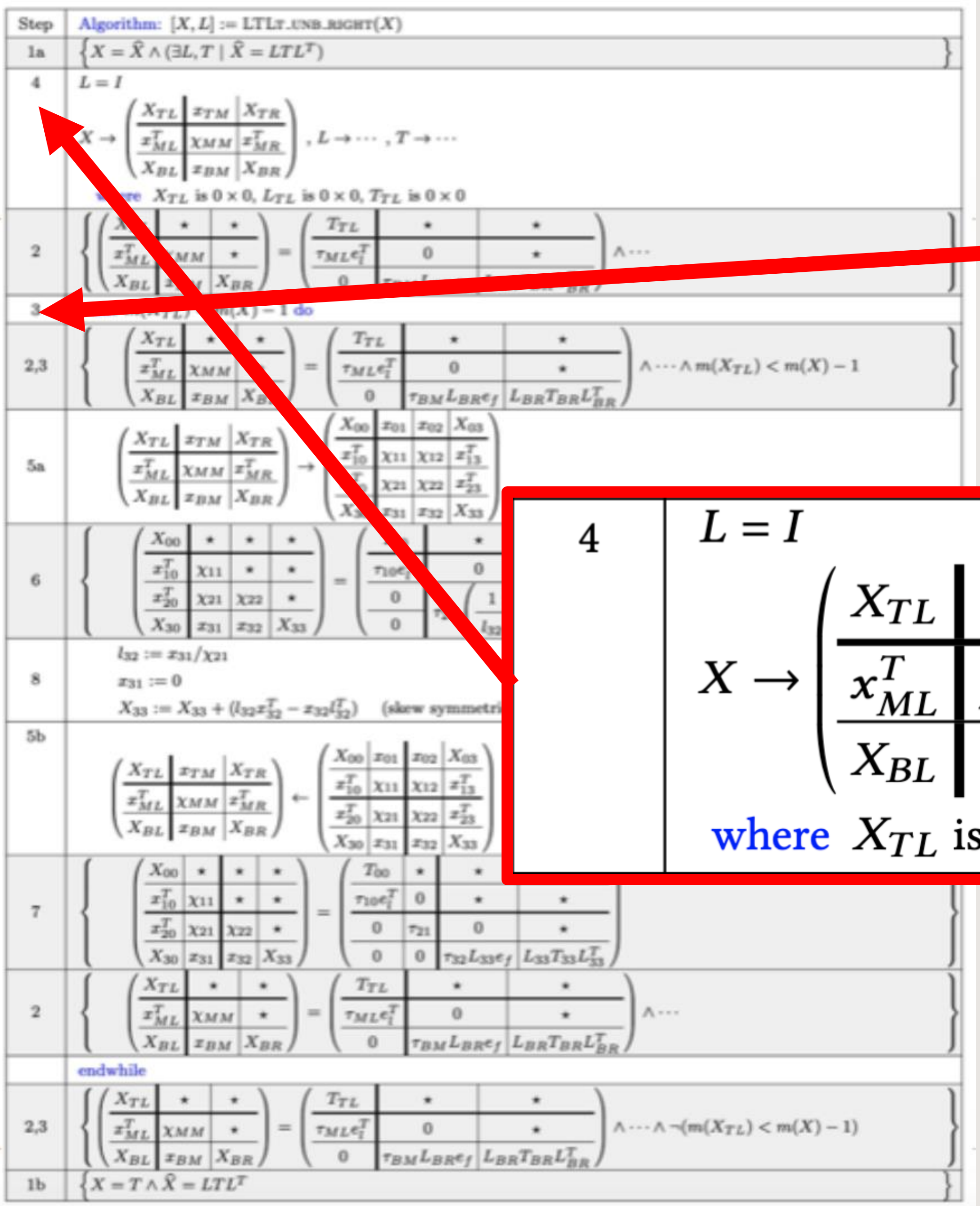

Loop Guard

3	**while** $m(X_{TL}) < m(X) - 1$ **do**

Initialization

4	$L = I$ $X \rightarrow \left(\begin{array}{c\|c\|c} X_{TL} & x_{TM} & X_{TR} \\ \hline x_{ML}^T & \chi_{MM} & x_{MR}^T \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right), L \rightarrow \left(\begin{array}{c\|c\|c} L_{TL} & l_{TM} & L_{TR} \\ \hline l_{ML}^T & \lambda_{MM} & l_{MR}^T \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right), T \rightarrow \left(\begin{array}{c\|c\|c} T_{TL} & t_{TM} & T_{TR} \\ \hline t_{ML}^T & \tau_{MM} & t_{MR}^T \\ \hline T_{BL} & t_{BM} & T_{BR} \end{array}\right)$ **where** X_{TL} is 0×0, L_{TL} is 0×0, T_{TL} is 0×0

loop invariant, the postcondition, and the precondition
-> Prescribes loop guard (Step 3) and Initialization (Step 4)

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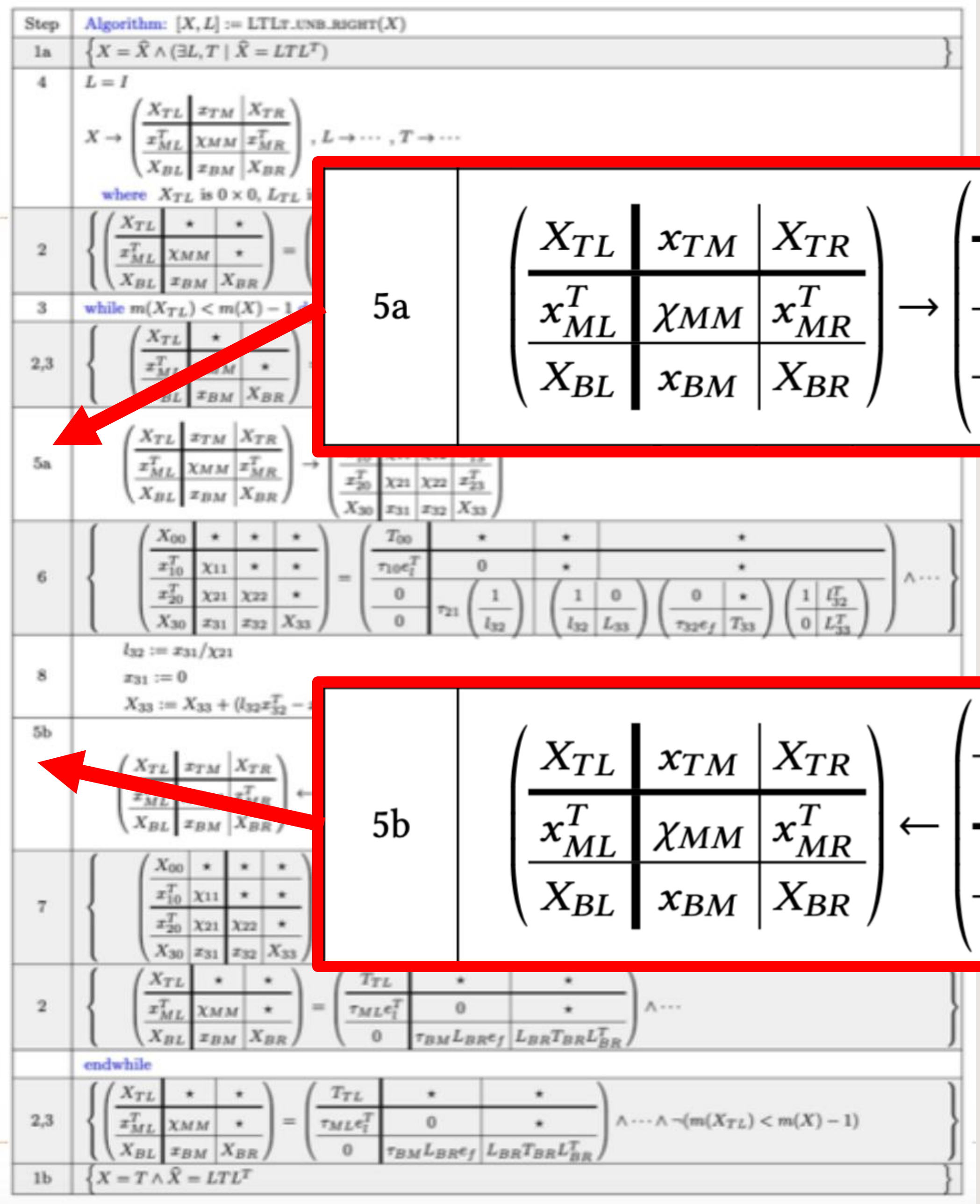
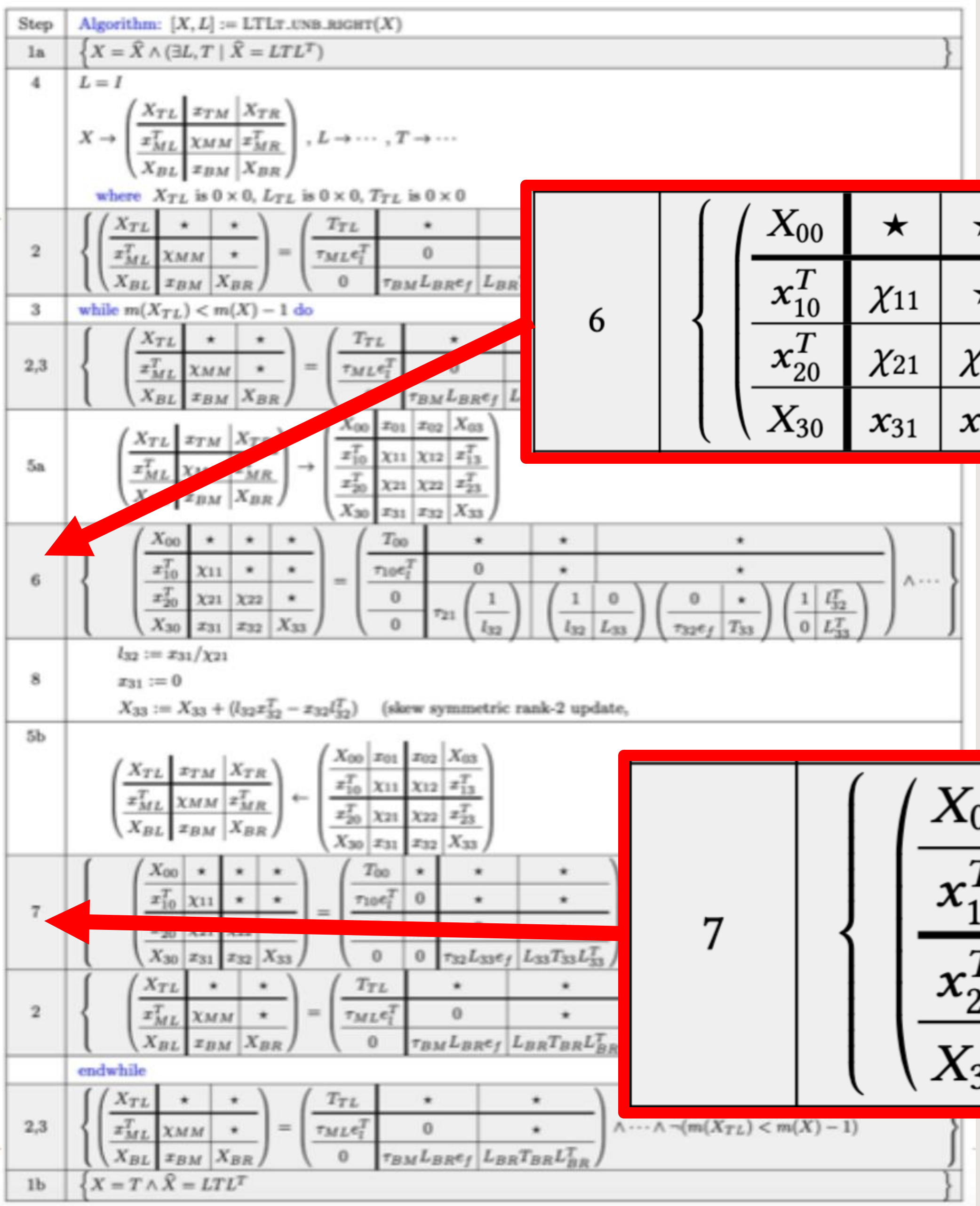


Step	
5a	$\left(\begin{array}{c\|c\|c} X_{TL} & x_{TM} & X_{TR} \\ \hline x_{ML}^T & \chi_{MM} & x_{MR}^T \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c\|c\|c\|c} X_{00} & x_{01} & x_{02} & X_{03} \\ \hline x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ \hline x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ \hline X_{30} & x_{31} & x_{32} & X_{33} \end{array}\right), \left(\begin{array}{c\|c\|c} L_{TL} & l_{TM} & L_{TR} \\ \hline l_{ML}^T & \lambda_{MM} & l_{MR}^T \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \rightarrow \cdots, \left(\begin{array}{c\|c\|c} T_{TL} & t_{TM} & T_{TR} \\ \hline t_{ML}^T & \tau_{MM} & t_{MR}^T \\ \hline T_{BL} & t_{BM} & T_{BR} \end{array}\right) \rightarrow \cdots$

Highlighted Lines Transition: to make progress

Step	
5b	$\left(\begin{array}{c\|c\|c} X_{TL} & x_{TM} & X_{TR} \\ \hline x_{ML}^T & \chi_{MM} & x_{MR}^T \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c\|c\|c\|c} X_{00} & x_{01} & x_{02} & X_{03} \\ \hline x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ \hline x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ \hline X_{30} & x_{31} & x_{32} & X_{33} \end{array}\right), \left(\begin{array}{c\|c\|c} L_{TL} & l_{TM} & L_{TR} \\ \hline l_{ML}^T & \lambda_{MM} & l_{MR}^T \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \leftarrow \cdots, \left(\begin{array}{c\|c\|c} T_{TL} & t_{TM} & T_{TR} \\ \hline t_{ML}^T & \tau_{MM} & t_{MR}^T \\ \hline T_{BL} & t_{BM} & T_{BR} \end{array}\right) \leftarrow \cdots$

FLAME (Formal Linear Algebra Methods Environments)



Content of repartitioned matrix

Step 6:

$$\left\{ \left(\begin{array}{c|c|c|c} X_{00} & \star & \star & \star \\ \hline x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{array} \right) = \left(\begin{array}{c|c|c|c} T_{00} & \star & \star & \star \\ \hline \tau_{10} e_l^T & 0 & \star & \star \\ \begin{array}{c} 0 \\ 0 \end{array} & \tau_{21} \begin{pmatrix} 1 \\ l_{32} \end{pmatrix} & \multicolumn{2}{c}{\begin{pmatrix} 1 & 0 \\ l_{32} & L_{33} \end{pmatrix} \begin{pmatrix} 0 & \star \\ \tau_{32} e_f & T_{33} \end{pmatrix} \begin{pmatrix} 1 & l_{32}^T \\ 0 & L_{33}^T \end{pmatrix}} \end{array} \right) \wedge \cdots \right.$$

Prescribes what the update to the various exposed submatrices must be.

Content after solid line shifting

Step 7:

$$\left\{ \left(\begin{array}{cc|cc} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ \hline x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{array} \right) = \left(\begin{array}{cc|cc} T_{00} & \star & \star & \star \\ \tau_{10} e_l^T & 0 & \star & \star \\ \hline 0 & \tau_{21} & 0 & \star \\ 0 & 0 & \tau_{32} L_{33} e_f & L_{33} T_{33} L_{33}^T \end{array} \right) \wedge \cdots \right.$$

FLAME (Formal Linear Algebra Methods Environments)

Step	Algorithm: $[X, L] := \text{LTLT\_UNB\_RIGHT}(X)$
1a	$\{ X = \hat{X} \wedge (\exists L, T \mid \hat{X} = LTL^T) \}$
4	$L = I$ $X \rightarrow \begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix}, L \rightarrow \cdots, T \rightarrow \cdots$ where X_{TL} is 0×0, L_{TL} is 0×0, T_{TL} is 0×0
2	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \right\}$
3	while $m(X_{TL}) < m(X) - 1$ do
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge m(X_{TL}) < m(X) - 1 \right\}$
5a	$\begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} X_{00} & x_{01} & x_{02} & X_{03} \\ x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix}$
6	$\left\{ \begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} T_{00} & \star & \star & \cdots \\ \tau_{10} e_l^T & 0 & \star & \cdots \\ 0 & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & \cdots \end{pmatrix} \right.$ [illegible]
8	$l_{32} :=$ [illegible] $x_{31} := 0$ $X_{33} := X_{33} + (l_{32} x_{32}^T - x_{32} l_{32}^T)$ (skew symmetric rank-2 [illegible]
5b	$\begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} X_{00} & x_{01} & x_{02} & X_{03} \\ x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix}$
7	$\left\{ \begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} T_{00} & \star & \star & \star \\ \tau_{10} e_l^T & 0 & \star & \star \\ 0 & \tau_{21} & 0 & \star \\ 0 & 0 & \tau_{32} L_{33} e_f & L_{33} T_{33} L_{33}^T \end{pmatrix} \right\}$
2	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \right\}$
	endwhile
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge \neg(m(X_{TL}) < m(X) - 1) \right\}$
1b	$\{ X = T \wedge \hat{X} = LTL^T \}$

Ignoring all assertions

Formal derivation using data dependency

8	$l_{32} := x_{31} / \chi_{21}$ $x_{31} := 0$ $X_{33} := X_{33} + (l_{32} x_{32}^T - x_{32} l_{32}^T)$ (skew symmetric rank-2 update)

FLAME (Formal Linear Algebra Methods Environments)

Step	Algorithm: $[X, L] := \mathrm{LTLT\_UNB\_RIGHT}(X)$
1a	$\left\{ X = \hat{X} \wedge (\exists L, T \mid \hat{X} = LTL^T) \right\}$
4	$L = I$ $X \rightarrow \begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix}$, $L \rightarrow \cdots$, $T \rightarrow \cdots$ where X_{TL} is 0×0, L_{TL} is 0×0, T_{TL} is 0×0
2	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \right\}$
3	**while** $m(X_{TL}) < m(X) - 1$ **do**
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge m(X_{TL}) < m(X) - 1 \right\}$
5a	$\begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} X_{00} & x_{01} & x_{02} & X_{03} \\ x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix}$
6	$\left\{ \begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} T_{00} & \star & \star & \star \\ \tau_{10} e_l^T & 0 & \star & \star \\ \begin{matrix} 0 \\ 0 \end{matrix} & \tau_{21} \begin{pmatrix} 1 \\ l_{32} \end{pmatrix} & \multicolumn{2}{c}{\begin{pmatrix} 1 & 0 \\ l_{32} & L_{33} \end{pmatrix} \begin{pmatrix} 0 & \star \\ \tau_{32} e_f & T_{33} \end{pmatrix} \begin{pmatrix} 1 & l_{32}^T \\ 0 & L_{33}^T \end{pmatrix}} \end{pmatrix} \wedge \cdots \right\}$
8	$l_{32} := x_{31} / \chi_{21}$ $x_{31} := 0$ $X_{33} := X_{33} + (l_{32} x_{32}^T - x_{32} l_{32}^T)$ (skew symmetric rank-2 update,
5b	$\begin{pmatrix} X_{TL} & x_{TM} & X_{TR} \\ x_{ML}^T & \chi_{MM} & x_{MR}^T \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} X_{00} & x_{01} & x_{02} & X_{03} \\ x_{10}^T & \chi_{11} & \chi_{12} & x_{13}^T \\ x_{20}^T & \chi_{21} & \chi_{22} & x_{23}^T \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix}$
7	$\left\{ \begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33} \end{pmatrix} = \begin{pmatrix} T_{00} & \star & \star & \star \\ \tau_{10} e_l^T & 0 & \star & \star \\ 0 & \tau_{21} & 0 & \star \\ 0 & 0 & \tau_{32} L_{33} e_f & L_{33} T_{33} L_{33}^T \end{pmatrix} \right\}$
2	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \right\}$
	endwhile
2,3	$\left\{ \begin{pmatrix} X_{TL} & \star & \star \\ x_{ML}^T & \chi_{MM} & \star \\ X_{BL} & x_{BM} & X_{BR} \end{pmatrix} = \begin{pmatrix} T_{TL} & \star & \star \\ \tau_{ML} e_l^T & 0 & \star \\ 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{pmatrix} \wedge \cdots \wedge \neg(m(X_{TL}) < m(X) - 1) \right\}$
1b	$\left\{ X = T \wedge \hat{X} = LTL^T \right\}$

Left-Looking

Right-Looking

Blocked

Unblocked

Pivoting

Background

Parlett-Reid algorithm

- Unblocked Right-looking algorithm
- Modification of LU factorization
- Iteratively applies Gauss transforms and pivoting on both side of equation.
- Uses skew-symmetric rank-2 updates (SKR2),

$$A := A + (wy^T - yw^T)$$

- Approximate cost for LU is $2m^3/3$ floating point operations (flops) when matrix is $m \times m$

Beresford N. Parlett and William T. Reid. On the solution of a system of linear equations whose matrix is symmetric but not definite. BIT, 10:386–397, 1970.

Wimmer's two-step algorithm

- Right-looking algorithm
- Unblocked algorithm for skew-LTL^T
- Performs single skew-symmetric rank-2 (SKR2) update for every other iteration
- SKR2 is skew-symmetric rank 2 update:
  - $(A := A + (wy^T - yw^T))$
- Wimmer's algorithm for skew-LTL^T can be blocked if all rank-2 updates can be aggregated and computation performed as skew-symmetric rank-2k updates (SKR2K): $A := A + (W Y^T - Y W^T)$, where W and Y are matrices with k columns
- Approximate cost is $m^3/3$ floating point operations (flops) when matrix is $m \times m$. ie fewer flops than Parlett-Reid.

M. Wimmer. Efficient numerical computation of the Pfaffian for dense and banded skew-symmetric matrices. ACM Transactions on Mathematical Software, 38(4):1–17, August 2012. arXiv:1102.3440 [cond-mat, physics:physics].

Aasen's algorithm

- Left-looking algorithm
- Unblocked algorithm for skew-LTL^T
- Performs GEMV per iteration
- GEMV is matrix vector operations
- Approximate cost is $m^3/3$ floating point operations (flops) when matrix is $m \times m$.

Jan Ole Aasen. On the reduction of a symmetric matrix to tridiagonal form. BIT Numerical Mathematics, 11(3):233–242, September 1971.

Miroslav et al.

- Proposed a blocked right-looking algorithm for LTL^T
- Uses BLAS-like operations- GEMMT
- GEMMT routines compute a scalar-matrix-matrix product and add the result to the upper or lower part of a scalar-matrix product.
- Uses Hessenberg TL^T matrix
- Approximate cost is $m^3/3$ floating point operations (flops) when matrix is $m \times m$.

Miroslav Rozložník, Gil Shklarski, and Sivan Toledo. Partitioned Triangular Tridiagonalization. ACM Trans. Math. Softw., 37(4):38:1–38:16, February 2011.

Comparison

SN	Parlett-Reid	Aasen's	Miroslav	Wimmer's two-step
Year	1970	1971	2011	2012
Blocked/ Unblocked	Unblocked	Unblocked	Blocked	Unblocked/ Blocked
Left-Looking/ Right-Looking	Right Looking	Left Looking	Right Looking	Right Looking
Factorization	LU	Skew-LTL^T	LTL^T	Skew-LTL^T
BLAS Operation	SKR2	GEMV	GEMMT	SKR2-UB SKR2K-Blk
Cost (In FLOPS)	$2m^3/3$	$m^3/3$	$m^3/3$	$m^3/3$

Formal Derivation of LTL^T

Introduction

- Precondition:

$$X = \hat{X} \wedge (\exists L, T \mid \hat{X} = LTL^T)$$

- Postcondition

$$X = T, L \wedge \widehat{X} = LTL^T$$

- where initially $\hat{X}$ equals the original contents of X.
- X - skew-symmetric matrix
- L - unit lower triangular matrix
- T - tri-diagonal matrix

$\hat{X}$ – Original Matrix
X – Current matrix/ changes after each loop.

Deriving the Partitioned Matrix Expression

- A PME is a recursive definition of the operation to be computed, by partitioning the matrices and substituting the partitioned matrices into the postcondition.
- Obtained from partitioning the post-condition.
- Why PME – To identify Data dependencies - Which helps us in identifying the type of dependencies we have.

$$X = T, L \wedge \widehat{X} = LTL^T$$

$$\left(\begin{array}{c|c|c} X_{TL} & \star & \star \\ \hline x_{ML}^T & \chi_{MM} & \star \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right) = \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \wedge \left(\begin{array}{c|c|c} \widehat{X}_{TL} & -\widehat{x}_{ML} & -\widehat{X}_{BL} \\ \hline -\widehat{x}_{ML}^T & 0 & -\widehat{x}_{BM}^T \\ \hline \widehat{X}_{BL} & \widehat{x}_{BM} & \widehat{X}_{BR} \end{array}\right)$$

$$= \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \left(\begin{array}{c|c|c} T_{TL} & -\tau_{ML} e_l & 0 \\ \hline \tau_{ML} e_l^T & 0 & -\tau_{BM} e_f^T \\ \hline 0 & \tau_{BM} e_f & T_{BR} \end{array}\right) \left(\begin{array}{cc|c} L_{TL}^T & l_{ML} & L_{BL}^T \\ \hline 0 & 1 & l_{BM}^T \\ \hline 0 & 0 & L_{BR}^T \end{array}\right)$$

Loop invariants

Loop Invariants: are certain logical conditions that remain same/ true before and after each iterations

For each loop/iteration :

- Iterate the process of partitioning the matrices in sub-matrices and
- Shifting the highlighted line indicating the progress of computation of matrices
- Making sure of how the pre-conditions and post-conditions are met

1. Iterate the process of partitioning the matrices in sub-matrices

$$\left(\begin{array}{c|c|c} X_{TL} & \star & \star \\ \hline x_{ML}^T & \chi_{MM} & \star \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right) = \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \wedge \left(\begin{array}{c|c|c} \widehat{X}_{TL} & -\widehat{x}_{ML} & -\widehat{x}_{BL}^T \\ \hline \widehat{x}_{ML}^T & 0 & -\widehat{x}_{BM}^T \\ \hline \widehat{X}_{BL} & \widehat{x}_{BM} & \widehat{X}_{BR} \end{array}\right)$$

$$= \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \left(\begin{array}{c|c|c} T_{TL} & -\tau_{ML} e_l & 0 \\ \hline \tau_{ML} e_l^T & 0 & -\tau_{BM} e_f^T \\ \hline 0 & \tau_{BM} e_f & T_{BR} \end{array}\right) \left(\begin{array}{c|c|c} L_{TL}^T & l_{ML} & L_{BL}^T \\ \hline 0 & 1 & l_{BM}^T \\ \hline 0 & 0 & L_{BR}^T \end{array}\right).$$

$$\left(\begin{array}{c|c|c|c} X_{00} & \star & \star & \star \\ \hline x_{10}^T & \chi_{11} & \star & \star \\ \hline x_{20}^T & \chi_{21} & \chi_{22} & \star \\ \hline X_{30} & x_{31} & x_{32} & X_{33} \end{array}\right) = \left(\begin{array}{c|c|c|c} L_{00} & \star & \star & \star \\ \hline l_{10}^T & 1 & \star & \star \\ \hline l_{20}^T & \lambda_{21} & 1 & \star \\ \hline L_{30} & l_{31} & l_{32} & L_{33} \end{array}\right) \wedge \left(\begin{array}{c|c|c|c} \widehat{X}_{00} & -\widehat{x}_{10} & -\widehat{x}_{20} & -\widehat{X}_{30}^T \\ \hline \widehat{x}_{10}^T & 0 & -\widehat{\chi}_{21}^T & -\widehat{x}_{31}^T \\ \hline \widehat{x}_{20}^T & \widehat{\chi}_{21} & 0 & -\widehat{x}_{32}^T \\ \hline \widehat{X}_{30} & \widehat{x}_{31} & \widehat{x}_{32} & \widehat{X}_{33} \end{array}\right)$$

$$= \left(\begin{array}{c|c|c|c} L_{00} & 0 & 0 & 0 \\ \hline l_{10}^T & 1 & 0 & 0 \\ \hline l_{20}^T & \lambda_{21} & 1 & 0 \\ \hline L_{30} & l_{31} & l_{32} & L_{33} \end{array}\right) \left(\begin{array}{c|c|c|c} T_{00} & -\tau_{10} e_l & 0 & 0 \\ \hline \tau_{10} e_l^T & 0 & -\tau_{21} & 0 \\ \hline 0 & \tau_{21} & 0 & -\tau_{32} e_f^T \\ \hline 0 & 0 & \tau_{32} e_f & T_{33} \end{array}\right) \left(\begin{array}{c|c|c|c} L_{00}^T & l_{10} & l_{20} & L_{30}^T \\ \hline 0 & 1 & \lambda_{21} & l_{31}^T \\ \hline 0 & 0 & 1 & l_{32}^T \\ \hline 0 & 0 & 0 & L_{33}^T \end{array}\right)$$

2. Shifting the highlighted line indicating the progress of computation of matrices

$$\begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33}\end{pmatrix} = \begin{pmatrix} L_{00} & \star & \star & \star \\ l_{10}^T & 1 & \star & \star \\ l_{20}^T & \lambda_{21} & 1 & \star \\ L_{30} & l_{31} & l_{32} & L_{33}\end{pmatrix} \wedge \begin{pmatrix}\widehat{X}_{00} & -\widehat{x}_{10} & -\widehat{x}_{20} & -\widehat{X}_{30}^T \\ \widehat{x}_{10}^T & 0 & -\widehat{\chi}_{21} & -\widehat{x}_{31}^T \\ \widehat{x}_{20}^T & \widehat{\chi}_{21} & 0 & -\widehat{x}_{32}^T \\ \widehat{X}_{30} & \widehat{x}_{31} & \widehat{x}_{32} & \widehat{X}_{33}\end{pmatrix}$$

$$= \begin{pmatrix} L_{00} & 0 & 0 & 0 \\ l_{10}^T & 1 & 0 & 0 \\ l_{20}^T & \lambda_{21} & 1 & 0 \\ L_{30} & l_{31} & l_{32} & L_{33}\end{pmatrix} \begin{pmatrix} T_{00} & -\tau_{10}e_l & 0 & 0 \\ \tau_{10}e_l^T & 0 & -\tau_{21} & 0 \\ 0 & \tau_{21} & 0 & -\tau_{32}e_f^T \\ 0 & 0 & \tau_{32}e_f & T_{33}\end{pmatrix} \begin{pmatrix} L_{00}^T & l_{10} & l_{20} & L_{30}^T \\ 0 & 1 & \lambda_{21} & l_{31}^T \\ 0 & 0 & 1 & l_{32}^T \\ 0 & 0 & 0 & L_{33}^T\end{pmatrix}$$

$$\begin{pmatrix} X_{00} & \star & \star & \star \\ x_{10}^T & \chi_{11} & \star & \star \\ x_{20}^T & \chi_{21} & \chi_{22} & \star \\ X_{30} & x_{31} & x_{32} & X_{33}\end{pmatrix} = \begin{pmatrix} L_{00} & \star & \star & \star \\ l_{10}^T & 1 & \star & \star \\ l_{20}^T & \lambda_{21} & 1 & \star \\ L_{30} & l_{31} & l_{32} & L_{33}\end{pmatrix} \wedge \begin{pmatrix}\widehat{X}_{00} & -\widehat{x}_{10} & -\widehat{x}_{20} & -\widehat{X}_{30}^T \\ \widehat{x}_{10}^T & 0 & -\widehat{\chi}_{21} & -\widehat{x}_{31}^T \\ \widehat{x}_{20}^T & \widehat{\chi}_{21} & 0 & -\widehat{x}_{32}^T \\ \widehat{X}_{30} & \widehat{x}_{31} & \widehat{x}_{32} & \widehat{X}_{33}\end{pmatrix}$$

$$= \begin{pmatrix} L_{00} & 0 & 0 & 0 \\ l_{10}^T & 1 & 0 & 0 \\ l_{20}^T & \lambda_{21} & 1 & 0 \\ L_{30} & l_{31} & l_{32} & L_{33}\end{pmatrix} \begin{pmatrix} T_{00} & -\tau_{10}e_l & 0 & 0 \\ \tau_{10}e_l^T & 0 & -\tau_{21} & 0 \\ 0 & \tau_{21} & 0 & -\tau_{32}e_f^T \\ 0 & 0 & \tau_{32}e_f & T_{33}\end{pmatrix} \begin{pmatrix} L_{00}^T & l_{10} & l_{20} & L_{30}^T \\ 0 & 1 & \lambda_{21} & l_{31}^T \\ 0 & 0 & 1 & l_{32}^T \\ 0 & 0 & 0 & L_{33}^T\end{pmatrix}.$$

Left-Looking / Right-looking

On comparing the before and after matrices of each iteration, we determine

- the contents of X, T and L after the matrix is re-partitioned and
- the contents of the exposed submatrices so that the invariant holds at the bottom of the loop.
- the the dependency graph of known and unknown from PME and invariants helps to identify the sequence in which the unknowns can be solved.

These logical conditions helps in identifying the Algorithmic Variants (Actual algorithms):

- Variant2 or Left-Looking
- Variant3 or Right-looking

Right-looking Invariant

$$\left(\begin{array}{c|c|c} X_{TL} & \star & \star \\ \hline x_{ML}^T & \chi_{MM} & \star \\ \hline X_{BL} & x_{BM} & X_{BR}\end{array}\right) = \left(\begin{array}{c|c|c} T_{TL} & \star & \star \\ \hline \tau_{ML} e_l^T & 0 & \star \\ \hline 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{array}\right) \wedge \left(\begin{array}{c|c|c} \widehat{X}_{TL} & -\widehat{x}_{ML} & -\widehat{X}_{BL}^T \\ \hline \widehat{x}_{ML}^T & 0 & -\widehat{x}_{BM}^T \\ \hline \widehat{X}_{BL} & \widehat{x}_{BM} & \widehat{X}_{BR}\end{array}\right)$$

$$= \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & I\end{array}\right) \left(\begin{array}{c|c|c} T_{TL} & -\tau_{ML} e_l & 0 \\ \hline \tau_{ML} e_l^T & 0 & -\tau_{BM} (L_{BR} e_f)^T \\ \hline 0 & \tau_{BM} L_{BR} e_f & L_{BR} T_{BR} L_{BR}^T \end{array}\right) \left(\begin{array}{c|c|c} L_{TL}^T & l_{ML} & L_{BL}^T \\ \hline 0 & 1 & l_{BM}^T \\ \hline 0 & 0 & I\end{array}\right).$$

$$\left(\begin{array}{c|c|c} X_{TL} & \star & \star \\ \hline x_{ML}^T & \chi_{MM} & \star \\ \hline X_{BL} & x_{BM} & X_{BR}\end{array}\right) = \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & L_{BR}\end{array}\right) \wedge \left(\begin{array}{c|c|c} \widehat{X}_{TL} & -\widehat{x}_{ML} & -\widehat{x}_{BL}^T \\ \hline \widehat{x}_{ML}^T & 0 & -\widehat{x}_{BM}^T \\ \hline \widehat{X}_{BL} & \widehat{x}_{BM} & \widehat{X}_{BR}\end{array}\right)$$

$$= \left(\begin{array}{c|c|c} L_{TL} & 0 & 0 \\ \hline l_{ML}^T & 1 & 0 \\ \hline L_{BL} & l_{BM} & L_{BR}\end{array}\right) \left(\begin{array}{c|c|c} T_{TL} & -\tau_{ML} e_l & 0 \\ \hline \tau_{ML} e_l^T & 0 & -\tau_{BM} e_f^T \\ \hline 0 & \tau_{BM} e_f & T_{BR} \end{array}\right) \left(\begin{array}{c|c|c} L_{TL}^T & l_{ML} & L_{BL}^T \\ \hline 0 & 1 & l_{BM}^T \\ \hline 0 & 0 & L_{BR}^T\end{array}\right).$$

Left-looking Invariant

Pivoting

- As seen previously, the update of l_{32} by dividing the vector x with scalar χ, the magnitude can be either >1 or <1.
- Hence, to improve this numerical instability: $l_{32} := x_{31}^{+}/\tau_{21}$
  - introduce a pivot term to makes sure: (value of chi χ or tau $\boldsymbol{\tau}$) >= (vector x), that is, l_{32} is always less than 1
  - Obtain **IAMAX(x)** as index of vector x with maximum magnitude
  - Calculate the Permutation matrix **P(π)**, by swapping the top element, χ_0, with the element indexed by a non-negative integer π

$$P(\pi) = \begin{cases} I & \textit{if } \pi = 0 \\ \left(\begin{array}{c|c|c|c} 0 & 0 & 1 & 0 \\ \hline 0 & I_{\pi-1} & 0 & 0 \\ \hline 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & I_{m-\pi-1}. \end{array}\right) & \textit{otherwise}, \end{cases}$$

Families of skew-symmetric LTL^T Algorithm

The unblocked algorithms

Algorithm: $[X, L] := \text{LTLT\_UNB\_RIGHT/LEFT}(X)$

$L = I$

$$X \rightarrow \left(\begin{array}{c|c|c} X_{TL} & x_{TM} & X_{TR} \\ \hline x_{ML}^T & \chi_{MM} & x_{MR}^T \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right), L \rightarrow \left(\begin{array}{c|c|c} L_{TL} & l_{TM} & L_{TR} \\ \hline l_{ML}^T & \lambda_{MM} & l_{MR}^T \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right)$$

where X_{TL} and L_{TL} are 0×0

while $m(X_{TL}) < m(X) - 1$ **do**

$$\left(\begin{array}{c|c|c} X_{TL} & x_{TM} & X_{TR} \\ \hline x_{ML}^T & \chi_{MM} & x_{MR}^T \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c|c} X_{00} & x_{01} & x_{02} & X_{03} \\ \hline x_{10}^T & \chi_{11} & \chi_{12}^T & x_{13}^T \\ \hline x_{20}^T & \chi_{21} & \chi_{22}^T & x_{23}^T \\ \hline X_{30} & x_{31} & x_{32} & X_{33} \end{array}\right), \left(\begin{array}{c|c|c} L_{TL} & l_{TM} & L_{TR} \\ \hline l_{ML}^T & \lambda_{MM} & l_{MR}^T \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \rightarrow \cdots$$

Right-looking

$l_{32} := x_{31} / \chi_{21}$

$x_{31} := 0$

$X_{33} := X_{33} + (l_{32} x_{32}^T - x_{32} l_{32}^T)$

Left-looking

$$\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right) := \left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right) - \left(\begin{array}{c|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right) \left(\begin{array}{c|c} X_{00} & -x_{10} \\ \hline x_{10}^T & 0 \end{array}\right) \left(\begin{array}{c} l_{10} \\ \hline 1 \end{array}\right)$$

$l_{32} := x_{31} / \chi_{21}$

$x_{31} := 0$

$$\left(\begin{array}{c|c|c} X_{TL} & x_{TM} & X_{TR} \\ \hline x_{ML}^T & \chi_{MM} & x_{ML}^T \\ \hline X_{BL} & x_{BM} & X_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c|c} X_{00} & x_{01} & x_{02} & X_{03} \\ \hline x_{10}^T & \chi_{11} & \chi_{12}^T & x_{13}^T \\ \hline x_{20}^T & \chi_{21} & \chi_{22}^T & x_{23}^T \\ \hline X_{30} & x_{31} & x_{32} & X_{33} \end{array}\right), \left(\begin{array}{c|c|c} L_{TL} & l_{TM} & L_{TR} \\ \hline l_{ML}^T & \lambda_{MM} & l_{ML}^T \\ \hline L_{BL} & l_{BM} & L_{BR} \end{array}\right) \leftarrow \cdots$$

endwhile

WITHOUT PIVOTING: UNBLOCKED ALGORITHMS

Unblocked	
Left-looking **GEMV**	**Right-looking** **SKR2**
$\left(\frac{\chi_{21}}{x_{31}}\right) := \left(\frac{\chi_{21}}{x_{31}}\right) - \left(\begin{array}{c\|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right) \left(\begin{array}{c\|c} X_{00} & -x_{10}^T \\ \hline x_{10} & 0 \end{array}\right) \left(\frac{l_{10}}{1}\right)$ $l_{32} := x_{31}/\tau_{21}$	$l_{32} := x_{31}/\tau_{21}$ $X_{33} := X_{33} + (l_{32}x_{32}^T - x_{32}l_{32}^T)$

WITHOUT PIVOTING: UNBLOCKED 2-STEP WIMMER'S RL

$$\left(\begin{array}{c|c|c|c|c} X_{00} & \star & \star & \star & \star \\ \hline x_{10}^T & \chi_{11} & \star & \star & \star \\ \hline x_{20}^T & \chi_{21} & \chi_{22} & \star & \star \\ \hline x_{30}^T & \chi_{31} & \chi_{32} & \chi_{33} & \star \\ \hline X_{40} & x_{41} & x_{42} & x_{43} & X_{44} \end{array}\right) = \left(\begin{array}{c|c} T_{00} & \star \quad \star \quad \star \quad \star \\ \hline \tau_{10} e_l^T & 0 \quad \star \quad \star \quad \star \\ \hline \begin{array}{c} 0 \\ 0 \\ 0 \end{array} & \tau_{21}\left(\begin{array}{c} 1 \\ \hline \lambda_{32} \\ \hline l_{42} \end{array}\right)\left(\begin{array}{c|c|c} 1 & 0 & 0 \\ \hline \lambda_{32} & 1 & 0 \\ \hline l_{42} & l_{43} & L_{44} \end{array}\right)\left(\begin{array}{c|c|c} 0 & -\tau_{32} & 0 \\ \hline \tau_{32} & 0 & -\tau_{43} e_f^T \\ \hline 0 & \tau_{43} e_f & T_{44} \end{array}\right)\left(\begin{array}{c|c|c} 1 & \lambda_{32} & l_{42}^T \\ \hline 0 & 1 & l_{43}^T \\ \hline 0 & 0 & L_{44}^T \end{array}\right) \end{array}\right)$$

$$\left(\begin{array}{c|c|c|c|c} X_{00}^{+} & \star & \star & \star & \star \\ \hline x_{10}^{+T} & 0 & \star & \star & \star \\ \hline x_{20}^{+T} & \chi_{21}^{+} & 0 & \star & \star \\ \hline x_{30}^{+T} & \chi_{31}^{+} & \chi_{32}^{+} & 0 & \star \\ \hline X_{40}^{+} & x_{41}^{+} & x_{42}^{+} & x_{43}^{+} & X_{44}^{+} \end{array}\right) = \left(\begin{array}{c|c|c|c|c} T_{00} & \star & \star & \star & \star \\ \hline \tau_{10} e_l^T & 0 & \star & \star & \star \\ \hline 0 & \tau_{21} & 0 & \star & \star \\ \hline 0 & 0 & \tau_{32} & 0 & \star \\ \hline 0 & 0 & 0 & \tau_{43} L_{44} e_f & L_{44} T_{44} L_{44}^T \end{array}\right).$$

2-step Wimmer's Unblocked Right-looking **SKR2**

$$\left(\begin{array}{c} \lambda_{32} \\ \hline l_{42} \end{array}\right) := \left(\begin{array}{c} \chi_{31} \\ \hline x_{41} \end{array}\right) / \tau_{21}$$

$$l_{43} := x_{42} / \tau_{32}$$

$$x_{43} := x_{43} + \tau_{32} l_{42} - \tau_{32} \lambda_{32} l_{43}$$

$$X_{44} := X_{44} + l_{43}(x_{43} - \tau_{32} l_{42})^T - (x_{43} - \tau_{32} l_{42}) l_{43}^T$$

WITHOUT PIVOTING: BLOCKED ALGORITHMS

Blocked

Right-looking **GEMMT, SKR2**

$$\left[\left(\begin{array}{c|c}\chi_{11} & \star \\ \hline x_{21} & X_{22} \\ \hline \chi_{31} & x_{32}^T \\ \hline x_{41} & X_{42}\end{array}\right), \left(\begin{array}{c|c} L_{22} & 0 \\ \hline l_{32}^T & 1 \\ \hline L_{42} & l_{43}\end{array}\right)\right] := \mathrm{LTLT\_UNB\_0}\left(\left(\begin{array}{c|c}\chi_{11} & \star \\ \hline x_{21} & X_{22} \\ \hline \chi_{31} & x_{32}^T \\ \hline x_{41} & X_{42}\end{array}\right)\right)$$

$$\left(\begin{array}{c|c}\chi_{33} & \star \\ \hline x_{43} & X_{44}\end{array}\right) := \left(\begin{array}{c|c}\chi_{33} & \star \\ \hline x_{43} & X_{44}\end{array}\right) - \left(\begin{array}{c|c} l_{32}^T & 1 \\ \hline L_{42} & l_{43}\end{array}\right)\left(\begin{array}{c|c} X_{22} & \star \\ \hline x_{32}^T & 0\end{array}\right)\left(\begin{array}{c|c} l_{32} & L_{42}^T \\ \hline 1 & l_{43}^T\end{array}\right)$$

$$X_{44} := X_{44} + (l_{43}x_{43}^T - x_{43}l_{43}^T)$$

Left-looking **GEMM**

$$\left(\begin{array}{c|c} x_{21} & X_{22} \\ \hline \chi_{31} & x_{32}^T \\ \hline x_{41} & X_{42}\end{array}\right) := \left(\begin{array}{c|c} x_{21} & X_{22} \\ \hline \chi_{31} & x_{32}^T \\ \hline x_{41} & X_{42}\end{array}\right) - \left(\begin{array}{c|c} L_{20} & l_{21} \\ \hline l_{30}^T & \lambda_{31} \\ \hline L_{40} & l_{41}\end{array}\right)\left(\begin{array}{c|c} X_{00} & \star \\ \hline x_{10}^T & 0\end{array}\right)\left(\begin{array}{c|c} l_{10} & L_{20}^T \\ \hline 1 & l_{21}^T\end{array}\right)$$

$$\left[\left(\begin{array}{c|c}\chi_{11} & \star \\ \hline x_{21} & X_{22} \\ \hline \chi_{31} & x_{32}^T \\ \hline x_{41} & X_{42}\end{array}\right), \left(\begin{array}{c|c} L_{22} & 0 \\ \hline l_{32}^T & 1 \\ \hline L_{42} & l_{43}\end{array}\right)\right] := \mathrm{LTLT\_UNB}\left(\left(\begin{array}{c|c}\chi_{11} & \star \\ \hline x_{21} & X_{22} \\ \hline \chi_{31} & x_{32}^T \\ \hline x_{41} & X_{42}\end{array}\right)\right)$$

PIVOTING: BLOCKED AND UNBLOCKED ALGORITHMS

<table>
<tr><th>Blocked</th><th colspan="2">Unblocked</th></tr>
<tr><th>Right-looking uses UNB-LL</th><th>Right-looking</th><th>Left-looking</th></tr>
<tr>
<td>

$$\left[\left(\begin{array}{c|c||c|c} \chi_{11} & \star & \star & \star \\ \hline x_{21} & X_{22} & \star & \star \\ \hline \chi_{31} & x_{32}^T & \chi_{33} & \star \\ \hline x_{41} & X_{42} & x_{43} & X_{44} \end{array}\right), \left(\begin{array}{c|c} L_{22} & 0 \\ \hline l_{32}^T & 1 \\ \hline L_{42} & l_{43} \end{array}\right), \left(\begin{array}{c} p_2 \\ \hline \pi_3 \end{array}\right)\right]$$

$$:= \text{LTLT\_UNB\_0}\left(\left(\begin{array}{c|c||c|c} \chi_{11} & \star & \star & \star \\ \hline x_{21} & X_{22} & \star & \star \\ \hline \chi_{31} & x_{32}^T & \chi_{33} & \star \\ \hline x_{41} & X_{42} & x_{43} & X_{44} \end{array}\right)\right)$$

$$\left(\begin{array}{c|c} L_{20} & l_{21} \\ \hline l_{30}^T & \lambda_{31} \\ \hline L_{40} & l_{41} \end{array}\right) := p\left(\left(\begin{array}{c} p_2 \\ \hline \pi_3 \end{array}\right)\right)\left(\begin{array}{c|c} L_{20} & l_{21} \\ \hline l_{30}^T & \lambda_{31} \\ \hline L_{40} & l_{41} \end{array}\right)$$

$$\left(\begin{array}{c|c} \chi_{33} & \star \\ \hline x_{43} & X_{44} \end{array}\right) := \left(\begin{array}{c|c} \chi_{33} & \star \\ \hline x_{43} & X_{44} \end{array}\right) - \left(\begin{array}{c|c} l_{32}^T & 1 \\ \hline L_{42} & l_{43} \end{array}\right)\left(\begin{array}{c|c} X_{22} & \star \\ \hline x_{32}^T & 0 \end{array}\right)\left(\begin{array}{c|c} l_{32} & L_{42}^T \\ \hline 1 & l_{34}^T \end{array}\right)$$

$$X_{44} := X_{44} + (l_{43}x_{43}^T - x_{43}l_{43}^T)$$

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$$\pi_2 = \text{IAMAX}\left(\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right)\right)$$

$$\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right) := P(\pi_2)\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right)$$

$$l_{32} := x_{31}/\tau_{21}$$

$$\left(\begin{array}{c|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right) := P(\pi_2)\left(\begin{array}{c|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right)$$

$$\left(\begin{array}{c|c} \chi_{22} & \star \\ \hline x_{32} & X_{33} \end{array}\right) := P(\pi_2)\left(\begin{array}{c|c} \chi_{22} & \star \\ \hline x_{32} & X_{33} \end{array}\right)P(\pi_2)$$

$$X_{33} := X_{33} + (l_{32}x_{32}^T - x_{32}l_{32}^T)$$

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$$\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right) := \left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right) - \left(\begin{array}{c|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right)\left(\begin{array}{c|c} X_{00} & -x_{10}^T \\ \hline x_{10} & 0 \end{array}\right)\left(\begin{array}{c} l_{10} \\ \hline 1 \end{array}\right)$$

$$\pi_2 = \text{IAMAX}\left(\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right)\right)$$

$$\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right) := P(\pi_2)\left(\begin{array}{c} \chi_{21} \\ \hline x_{31} \end{array}\right)$$

$$l_{32} := x_{31}/\tau_{21}$$

$$\left(\begin{array}{c|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right) := P(\pi_2)\left(\begin{array}{c|c} l_{20}^T & \lambda_{21} \\ \hline L_{30} & l_{31} \end{array}\right)$$

$$\left(\begin{array}{c|c} \chi_{22} & \star \\ \hline x_{32} & X_{33} \end{array}\right) := P(\pi_2)\left(\begin{array}{c|c} \chi_{22} & \star \\ \hline x_{32} & X_{33} \end{array}\right)P(\pi_2)$$

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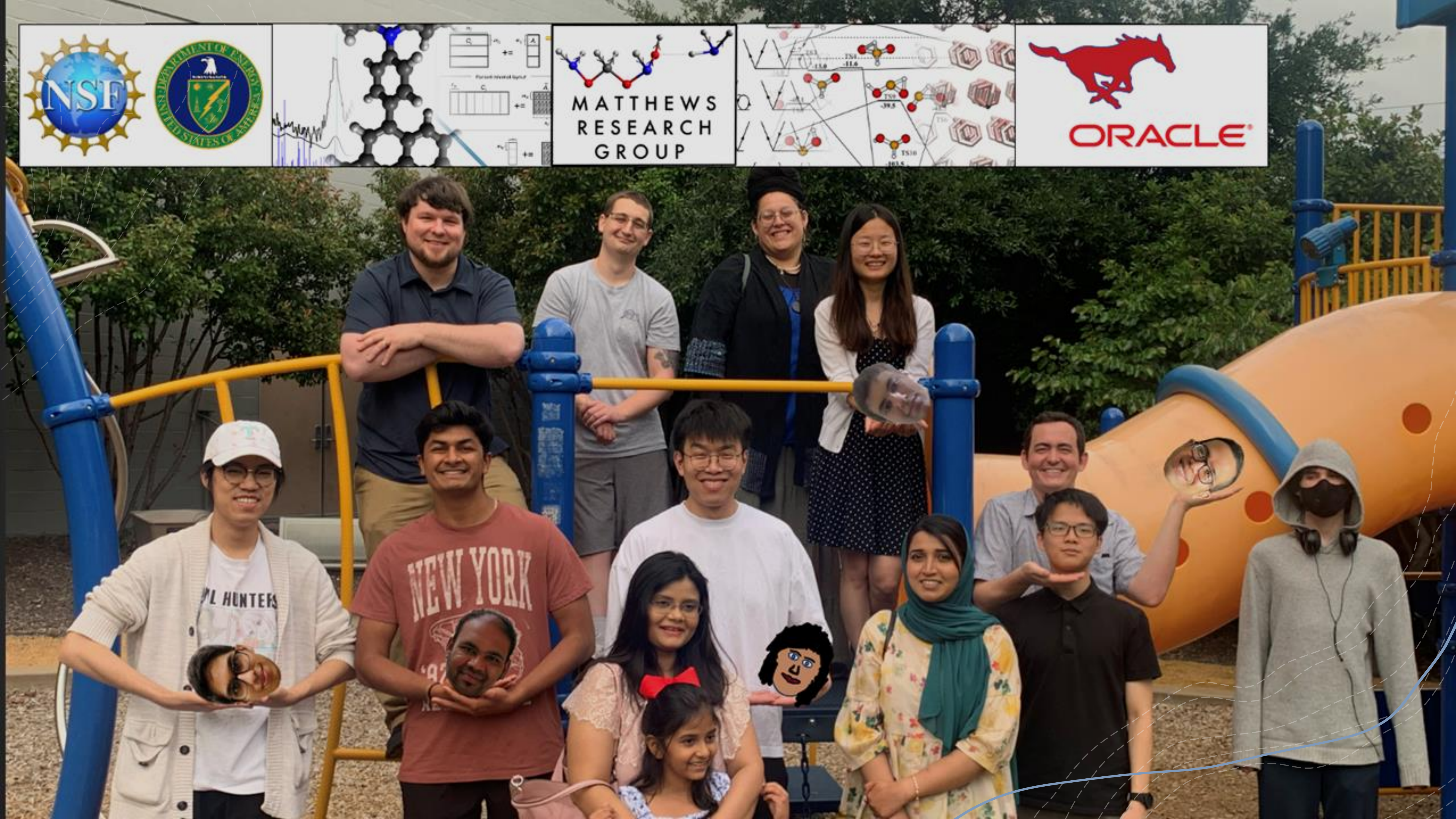
</table>

To Be Continued … (By Chao)

- Discuss additional functions to BLIS and BLAS.
- Brief discussion of FLOP counts of the family of algorithm.
- Results of testing and profiling over range of sizes.
- Optimization on the family of algorithm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