



Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Automation in Dense Linear Algebra

Paper by Paolo Bientinesi and Robert van de Geijn

Presented by Sämy Zehnder

Content

Motivation

Building a new algorithm

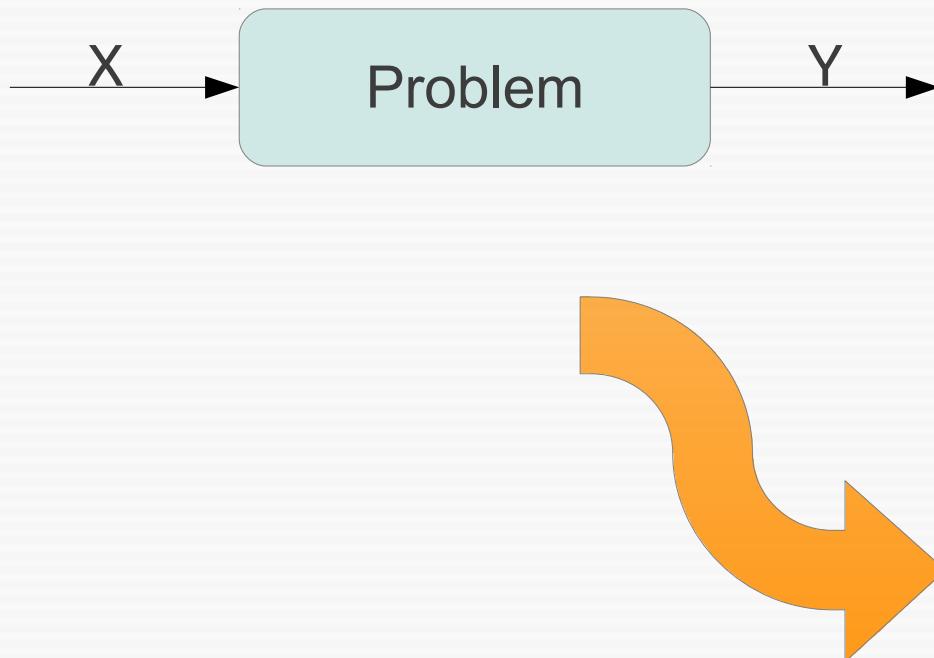
Prototype

Conclusion

Motivation

- Best algorithm for a dense linear algebra problem?
 - LU
 - Cholesky
 - Eigenvalues
 - SVD
 - ...
- Highly used for:
 - Interpolation of functions
 - Solving systems of equations
 - Optimization

Idea: Automatically build it!



```
function [A] = choleskyLi( A , nb )

[ ATL, ATR, ...
ABL, ABR ] = FLA_Part_2x2( A,0,0,'FLA_TL');

%% Loop Invariant
%% ATL=choleskyL[ATL]
%% ABL'=0
%% ABL=ABL
%% ABR=ABR

while( size(ATL,1) ~= size(A,1) | size(ATL,2) ~= size(A,2) )
b = min( nb, min( size(ABR,1), size(ABR,2) ));

[ A00, A01, A02, ...
A10, A11, A12, ...
A20, A21, A22 ] = FLA_Repart_2x2_to_3x3(ATL, ATR, ...
                                              ABL, ABR, ...
                                              b, b, 'FLA_BR');

%* ****
A10 = A10 . inv(A00)';
A11 = choleskyL(A11 - A10 . A10');
%* ****
[ ATL, ATR, ...
ABL, ABR ] = FLA_Cont_with_3x3_to_2x2(A00, A01, A02, ...
                                         A10, A11, A12, ...
                                         A20, A21, A22, ...
                                         'FLA_TL');

end;
A = ATL;
return;
```

Content

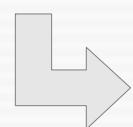
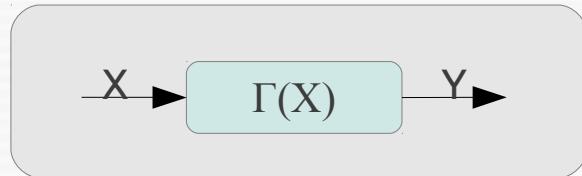
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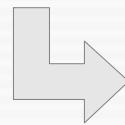
Prototype

Conclusion

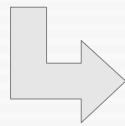
Steps needed



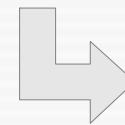
PME



Loop-invariant



Loop



Code

Layout of the algorithm

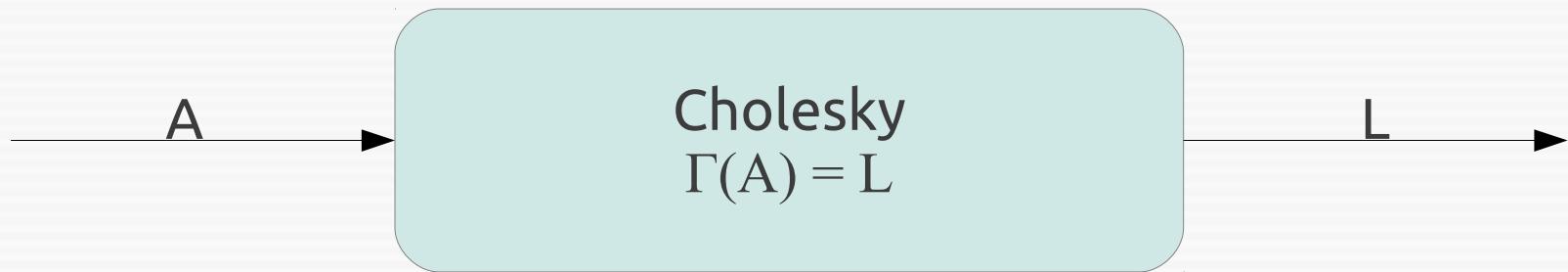
```
function  $\Gamma(A, B, \dots)$ 
    // Some arrangements of the input

    while  $G$  do
        // Stepwise computation of  $\Gamma$ 
    end while

end function
```



Example: Cholesky factorization



- How do we compute L , so that $A = LL^\top$?

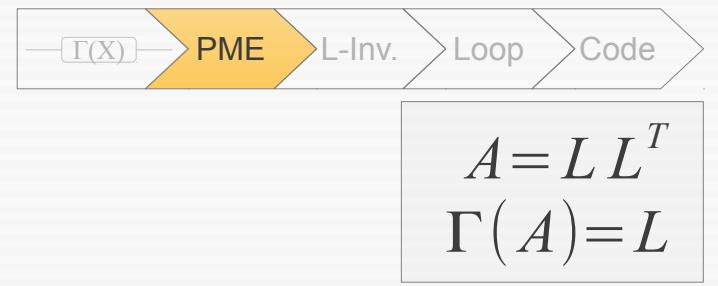


Problem to PME

$$A = LL^T$$

$$\Gamma(A) = L$$

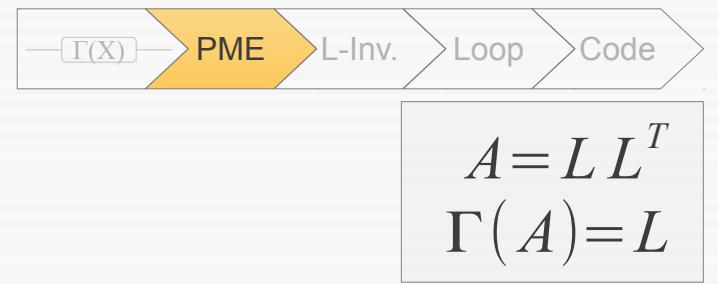
$$\begin{aligned}
 \underbrace{\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)}_A &= \underbrace{\left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right)}_L \underbrace{\left(\begin{array}{c|c} L_{TL}^T & L_{BL}^T \\ \hline 0 & L_{BR}^T \end{array} \right)}_{L^T} \\
 &= \left(\begin{array}{c|c} L_{TL}L_{TL}^T & L_{TL}L_{BL}^T \\ \hline L_{BL}L_{TL}^T & L_{BL}L_{BL}^T + L_{BR}L_{BR}^T \end{array} \right)
 \end{aligned}$$



Problem to PME

$$\begin{aligned}
 \underbrace{\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)}_A &= \underbrace{\left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right)}_L \underbrace{\left(\begin{array}{c|c} L_{TL}^T & L_{BL}^T \\ \hline 0 & L_{BR}^T \end{array} \right)}_{L^T} \\
 &= \left(\begin{array}{c|c} L_{TL}L_{TL}^T & L_{TL}L_{BL}^T \\ \hline L_{BL}L_{TL}^T & L_{BL}L_{BL}^T + L_{BR}L_{BR}^T \end{array} \right)
 \end{aligned}$$

$$A_{TL} = L_{TL}L_{TL}^T \Rightarrow L_{TL} = \Gamma(A_{TL})$$



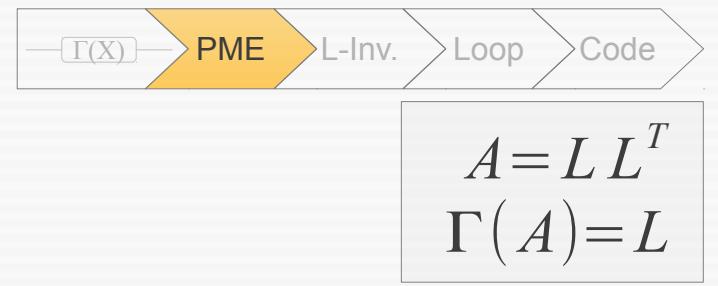
Problem to PME

$$\underbrace{\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)}_A = \underbrace{\left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right)}_L \underbrace{\left(\begin{array}{c|c} L_{TL}^T & L_{BL}^T \\ \hline 0 & L_{BR}^T \end{array} \right)}_{L^T}$$

$$= \left(\begin{array}{c|c} L_{TL}L_{TL}^T & L_{TL}L_{BL}^T \\ \hline L_{BL}L_{TL}^T & L_{BL}L_{BL}^T + L_{BR}L_{BR}^T \end{array} \right)$$

$$A_{TL} = L_{TL}L_{TL}^T \Rightarrow L_{TL} = \Gamma(A_{TL})$$

$$A_{BL} = L_{BL}L_{TL}^T \Rightarrow L_{BL} = A_{BL}L_{TL}^{-T}$$



Problem to PME

$$\begin{aligned}
 \underbrace{\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)}_A &= \underbrace{\left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right)}_L \underbrace{\left(\begin{array}{c|c} L_{TL}^T & L_{BL}^T \\ \hline 0 & L_{BR}^T \end{array} \right)}_{L^T} \\
 &= \left(\begin{array}{c|c} L_{TL}L_{TL}^T & L_{TL}L_{BL}^T \\ \hline L_{BL}L_{TL}^T & L_{BL}L_{BL}^T + L_{BR}L_{BR}^T \end{array} \right)
 \end{aligned}$$

$$A_{TL} = L_{TL}L_{TL}^T \Rightarrow L_{TL} = \Gamma(A_{TL})$$

$$A_{BL} = L_{BL}L_{TL}^T \Rightarrow L_{BL} = A_{BL}L_{TL}^{-T}$$

$$A_{BR} - L_{BL}L_{BL}^T = L_{BR}L_{BR}^T \Rightarrow L_{BR} = \Gamma(A_{BR} - L_{BL}L_{BL}^T)$$



Problem to PME

$$A_{TL} = L_{TL}L_{TL}^T \Rightarrow L_{TL} = \Gamma(A_{TL})$$

$$A_{BL} = L_{BL}L_{TL}^T \Rightarrow L_{BL} = A_{BL}L_{TL}^{-T}$$

$$A_{BR} - L_{BL}L_{BL}^T = L_{BR}L_{BR}^T \Rightarrow L_{BR} = \Gamma(A_{BR} - L_{BL}L_{BL}^T)$$

PME: $\left\{ \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right) = \left(\begin{array}{c|c} \Gamma(A_{TL}) & 0 \\ \hline A_{BL}L_{TL}^{-T} & \Gamma(A_{BR} - L_{BL}L_{BL}^T) \end{array} \right) \right\}$



Loop-invariant

- Holds before, at the begin and after the loop

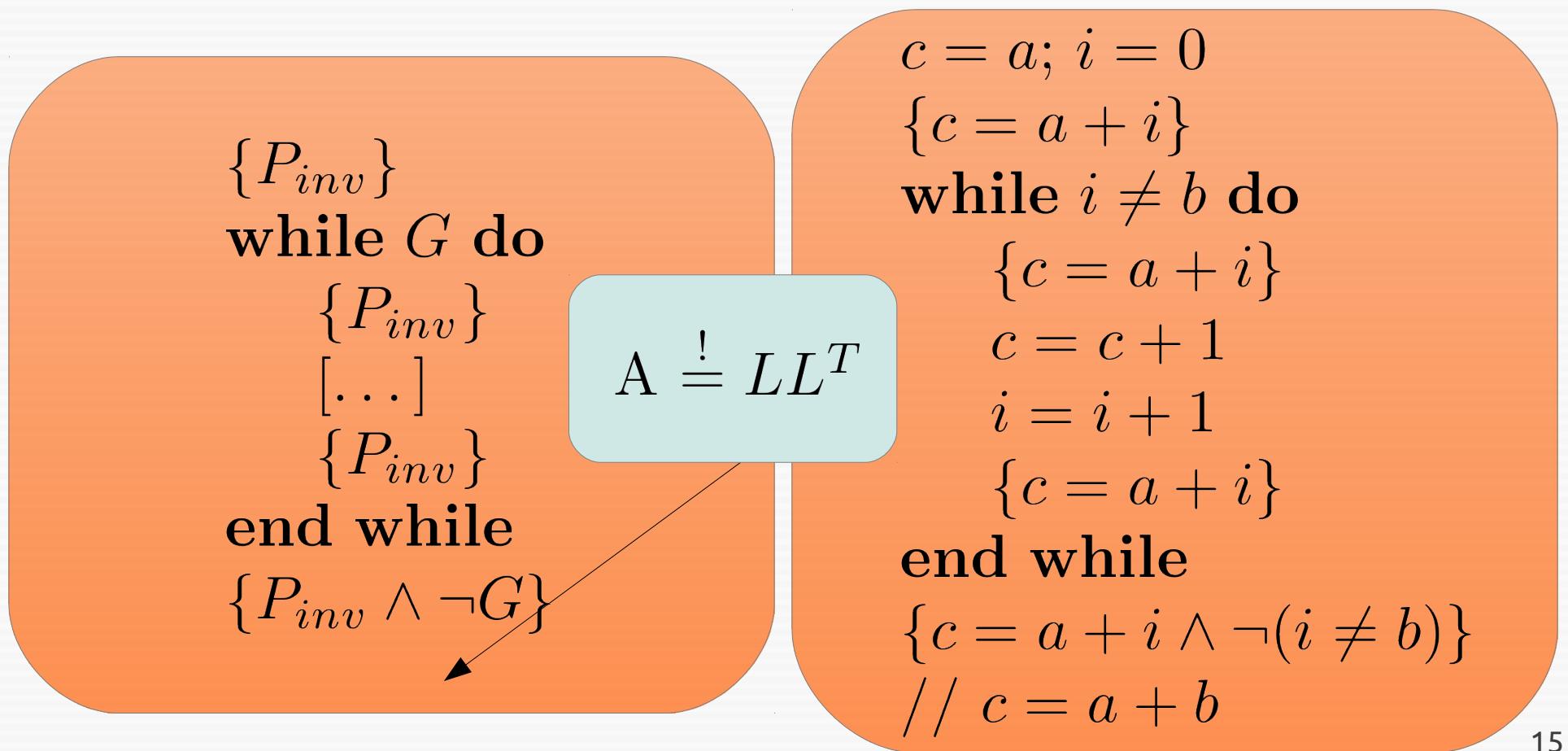
$\{P_{inv}\}$
while G **do**
 $\{P_{inv}\}$
 \dots
 $\{P_{inv}\}$
end while
 $\{P_{inv} \wedge \neg G\}$

$c = a; i = 0$
 $\{c = a + i\}$
while $i \neq b$ **do**
 $\{c = a + i\}$
 $c = c + 1$
 $i = i + 1$
 $\{c = a + i\}$
end while
 $\{c = a + i \wedge \neg(i \neq b)\}$
 $// c = a + b$



Loop-invariant

- Holds before, at the begin and after the loop





Choosing a Loop-invariant

$$\text{PME: } \left\{ \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right) = \left(\begin{array}{c|c} \Gamma(A_{TL}) & 0 \\ \hline A_{BL}L_{TL}^{-T} & \Gamma(A_{BR} - L_{BL}L_{BL}^T) \end{array} \right) \right\}$$

- Any subset of the PME
- Some blocks can be 0x0-matrices
- Has to respect the dependencies

#	Loop-invariants for Cholesky Factorization
1	$\left(\begin{array}{c c} L_{TL} = \Gamma(A_{TL}) & * \\ \hline L_{BL} = 0 & L_{BR} = 0 \end{array} \right)$
2	$\left(\begin{array}{c c} L_{TL} = \Gamma(A_{TL}) & * \\ \hline L_{BL} = A_{BL}L_{TL}^{-T} & L_{BR} = 0 \end{array} \right)$
3	$\left(\begin{array}{c c} L_{TL} = \Gamma(A_{TL}) & * \\ \hline L_{BL} = A_{BL}L_{TL}^{-T} & L_{BR} = A_{BR} - L_{BL}L_{BL}^T \end{array} \right)$

4	$\left(\begin{array}{c c} L_{TL} = 0 & * \\ \hline L_{BL} = A_{BL}L_{TL}^{-T} & L_{BR} = 0 \end{array} \right)$
---	--



Choosing a Loop-invariant

$$\{P_{inv}\}: \left\{ \left(\begin{array}{c|c} \frac{L_{TL} = \Gamma(A_{TL})}{L_{BL} = 0} & \frac{L_{TR} = 0}{L_{BR} = 0} \end{array} \right) \right\}$$



Choosing a Loop-invariant

$$\{P_{inv}\}: \left\{ \left(\begin{array}{c|c} \frac{L_{TL} = \Gamma(A_{TL})}{L_{BL} = 0} & \frac{L_{TR} = 0}{L_{BR} = 0} \end{array} \right) \right\}$$

- At the beginning:

$$\{P_{inv}\}: \left\{ \left(\begin{array}{c|c} \frac{L_{TL} = 0 \times 0}{ } & \frac{}{L_{BR} = L = 0} \end{array} \right) \right\}$$



Choosing a Loop-invariant

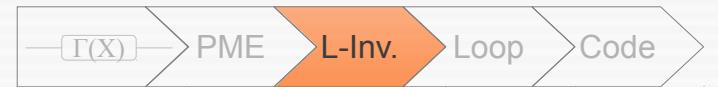
$$\{P_{inv}\}: \left\{ \left(\frac{L_{TL} = \Gamma(A_{TL})}{L_{BL} = 0} \middle| \frac{L_{TR} = 0}{L_{BR} = 0} \right) \right\}$$

- At the beginning:

$$\{P_{inv}\}: \left\{ \left(\frac{L_{TL} = 0 \times 0}{L_{BR} = L = 0} \right) \right\}$$

- At the end:

$$\{P_{inv}\}: \left\{ \left(\frac{L_{TL} = \Gamma(A_{TL}) \Rightarrow L = \Gamma(A)}{L_{BR} = 0 \times 0} \right) \right\}$$



Ensuring progress

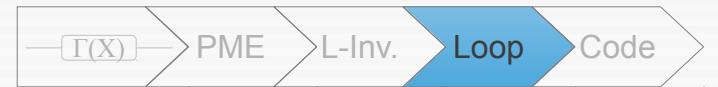
$$\left(\begin{array}{c|c} A_{TL} & * \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|cc} A_{00} & * & * \\ \hline A_{10} & A_{11} & * \\ A_{20} & A_{21} & A_{22} \end{array} \right)$$

$$\left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|cc} L_{00} & 0 & 0 \\ \hline L_{10} & L_{11} & 0 \\ L_{20} & L_{21} & L_{22} \end{array} \right)$$



$$\left(\begin{array}{cc|c} A_{00} & * & * \\ A_{10} & A_{11} & * \\ \hline A_{20} & A_{21} & A_{22} \end{array} \right) \rightarrow \left(\begin{array}{c|c} A_{TL} & * \\ \hline A_{BL} & A_{BR} \end{array} \right)$$

$$\left(\begin{array}{cc|c} L_{00} & 0 & 0 \\ L_{10} & L_{11} & 0 \\ \hline L_{20} & L_{21} & L_{22} \end{array} \right) \rightarrow \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right)$$



Construction of the loop

$\{P_{inv}\}$

while $\neg \text{SAMESIZE}(L, L_{TL})$ **do**

$\{P_{inv}\}$

// Repartition of A and L

$$\left\{ \left(\begin{array}{c|cc} L_{00} = \Gamma(A_{00}) & L_{01} = 0 & L_{02} = 0 \\ \hline L_{10} = 0 & L_{11} = 0 & L_{12} = 0 \\ L_{20} = 0 & L_{21} = 0 & L_{22} = 0 \end{array} \right) \right\}$$

$$L_{10} = A_{10}L_{00}^{-T}$$

$$L_{11} = \text{CHOLESKY}(A_{11} - L_{10}L_{10}^T)$$

$$\left\{ \left(\begin{array}{c|c} L_{TL} = \Gamma(A_{TL}) & L_{TR} = 0 \\ \hline L_{BL} = 0 & L_{BR} = 0 \end{array} \right) \right\}$$

$$\left(\begin{array}{c|c} A_{TL} & * \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|cc} A_{00} & * & * \\ \hline A_{10} & A_{11} & * \\ A_{20} & A_{21} & A_{22} \end{array} \right)$$

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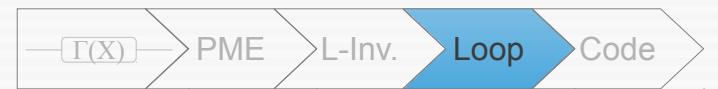
$$\left\{ \left(\begin{array}{ccc|cc} L_{00} = \Gamma(A_{00}) & L_{01} = 0 & L_{02} = 0 & & \\ \hline L_{10} = A_{10}L_{00}^{-T} & L_{11} = \Gamma(A_{11} - L_{10}L_{10}^T) & L_{12} = 0 & L_{20} = 0 & \\ L_{20} = 0 & L_{21} = 0 & L_{22} = 0 & & \end{array} \right) \right\}$$

// Recombination of A and L

$\{P_{inv}\}$

end while

$\{P_{inv} \wedge \text{SAMESIZE}(L, L_{TL})\}$



Construction of the loop

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while $\neg \text{SAMESIZE}(L, L_{TL})$ **do**

$\{P_{inv}\}$

// Repartition of A and L

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$$L_{10} = A_{10}L_{00}^{-T}$$

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$$\left\{ \left(\begin{array}{c|c} L_{TL} = \Gamma(A_{TL}) & L_{TR} = 0 \\ \hline L_{BL} = 0 & L_{BR} = 0 \end{array} \right) \right\}$$

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$$\left(\begin{array}{cc|c} L_{00} & 0 & 0 \\ L_{10} & L_{11} & 0 \\ \hline L_{20} & L_{21} & L_{22} \end{array} \right) \rightarrow \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right)$$

$$\left\{ \left(\begin{array}{ccc|c} L_{00} = \Gamma(A_{00}) & L_{01} = 0 & L_{02} = 0 & \\ \hline L_{10} = A_{10}L_{00}^{-T} & L_{11} = \Gamma(A_{11} - L_{10}L_{10}^T) & L_{12} = 0 & \\ L_{20} = 0 & L_{21} = 0 & L_{22} = 0 & \end{array} \right) \right\}$$

// Recombination of A and L

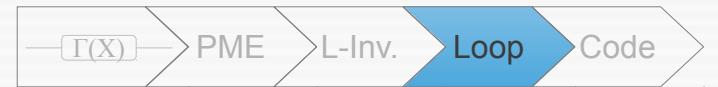
$\{P_{inv}\}$

end while

$\{P_{inv} \wedge \text{SAMESIZE}(L, L_{TL})\}$

PME:

$$\left\{ \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right) = \left(\begin{array}{c|c} \Gamma(A_{TL}) & 0 \\ \hline A_{BL}L_{TL}^{-T} & \Gamma(A_{BR} - L_{BL}L_{BL}^T) \end{array} \right) \right\}$$



Construction of the loop

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while $\neg \text{SAMESIZE}(L, L_{TL})$ **do**

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$$\left\{ \left(\begin{array}{c|c} L_{TL} = \Gamma(A_{TL}) & L_{TR} = 0 \\ \hline L_{BL} = 0 & L_{BR} = 0 \end{array} \right) \right\}$$

$$\begin{aligned} \left(\begin{array}{cc|c} A_{00} & * & * \\ A_{10} & A_{11} & * \\ \hline A_{20} & A_{21} & A_{22} \end{array} \right) &\rightarrow \left(\begin{array}{c|c} A_{TL} & * \\ \hline A_{BL} & A_{BR} \end{array} \right) \\ \left(\begin{array}{cc|c} L_{00} & 0 & 0 \\ L_{10} & L_{11} & 0 \\ \hline L_{20} & L_{21} & L_{22} \end{array} \right) &\rightarrow \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right) \end{aligned}$$

$$\left\{ \left(\begin{array}{ccc|c} L_{00} = \Gamma(A_{00}) & L_{01} = 0 & L_{02} = 0 & \\ \hline L_{10} = A_{10}L_{00}^{-T} & L_{11} = \Gamma(A_{11} - L_{10}L_{10}^T) & L_{12} = 0 & \\ L_{20} = 0 & L_{21} = 0 & L_{22} = 0 & \end{array} \right) \right\}$$

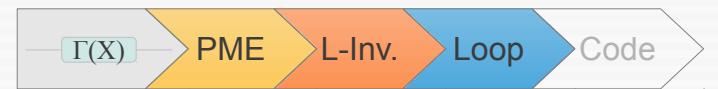
// Recombination of A and L

$\{P_{inv}\}$

end while

$\{P_{inv} \wedge \text{SAMESIZE}(L, L_{TL})\}$

$$\left\{ \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array} \right) = \left(\begin{array}{c|c} \Gamma(A_{TL}) & 0 \\ \hline A_{BL}L_{TL}^{-T} & \Gamma(A_{BR} - L_{BL}L_{BL}^T) \end{array} \right) \right\}$$



Recap

1. Building the PME
2. Choosing the Loop-Invariant
3. Construction of the loop
 - Repartitioning
 - Computation of one step



Recap

1. Building the PME
2. Choosing the Loop-Invariant
3. Construction of the loop
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Recap

1. Building the PME



2. Choosing the Loop-Invariant



3. Construction of the loop

- Repartitioning
- Computation of one step



Recap

1. Building the PME
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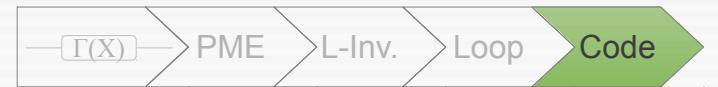
Content

Motivation

Building a new algorithm

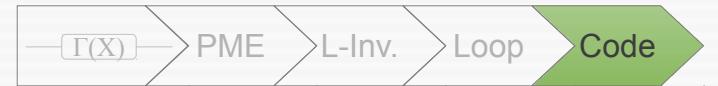
Prototype

Conclusion



Prototype system

- Takes loop-invariant, returns loop-algorithm
- Generates worksheet, Matlab- or C-code
- More than 300 algorithms for the Level-3 BLAS library
- Found 50 algorithms for the triangular coupled Sylvester equation (3 previously known)



Prototype system

```

function [A] = choleskyL1( A , nb )

[ ATL, ATR, ...
ABL, ABR ] = FLA_Part_2x2( A,0,0,'FLA_TL');

%> Loop Invariant
%> ATL=choleskyL[ATL]
%> ABL'=0
%> ABL=ABL
%> ABR=ABR

while( size(ATL,1) ~= size(A,1) | size(ATL,2) ~= size(A,2) )
    b = min( nb, min( size(ABR,1), size(ABR,2) ) );
    [ A00, A01, A02, ...
      A10, A11, A12, ...
      A20, A21, A22 ] = FLA_Repart_2x2_to_3x3(ATL, ATR, ...
                                                    ABL, ABR, ...
                                                    b, b, 'FLA_BR');

%> *****
A10 = A10 . inv(A00)';
A11 = choleskyL(A11 - A10 . A10');

%> *****

[ ATL, ATR, ...
ABL, ABR ] = FLA_Cont_with_3x3_to_2x2(A00, A01, A02, ...
                                         A10, A11, A12, ...
                                         A20, A21, A22, 'FLA_TL');

end;
return ATL;

```

Content

Motivation

Building a new algorithm

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Conclusion

Conclusion

- + Problem description ($A = LL^T$) sufficient for automatic algorithm generation
- + Possible to generate proof of correctness side by side with generation of algorithm
- + Performance: Family of algorithms => autotune these
- Numerical stability is not ensured.
Proof for every algorithm needed.



Thank you!

Are there any questions?