Parallel Numerical Algorithms

Need for standardization

- With the advent of parallel (high performance) computers came the disillusion of bad performance
- The peak rates advertised with the introduction of new machines were mostly not attainable for real life applications
- A need arose to standardize primitives of computations
- This effort also was based on already developed numerical software libraries: LINPACK, EISPACK, FISHPACK, Harwell

Basic Linear Algebra Subroutines (BLAS)

Three levels

– BLAS 1: vector/vector operations

SAXPY	$y \leftarrow y + \alpha.x$	$x, y =$ vector, $\alpha =$ scalar
DOTPR	$\alpha \leftarrow (x, y)$	
SUM	$y \leftarrow y + x$	

– BLAS 2: matrix/vector operations

$$y \leftarrow By + \alpha Ax$$
$$y \leftarrow A^T x$$
$$(\alpha = \text{scalar},\ A = \text{matrix},\ x = \text{vector})$$

– BLAS 3: matrix/matrix operations

$$C \leftarrow \beta.B + \alpha.A.B$$
$$C \leftarrow C + A.B.$$

Input/Output Data Reuse

BLAS 1 Example: Dotproduct (x, y)

Input Size: $2n$

Operation Count: $2n-1$

Output Size: 1

➔ 1 operation per input element and 2n per output element

BLAS 2 Example: $y = Ax$

Input Size: n^2+n

Operation Count: $2n^2-n$

Output Size: n

➔ 2 operations per input element and 2n per output element

BLAS 3 Example: $C=A.B$

Input Size: $2n^2$

Operation Count: $2n^3-n^2$

Output Size: n^2

➔ n operations per input element and 2n per output element

More data reuse leads to

- Better Cache/Register Utilization
- Less Communication Overhead
- More effective input, output, or intermediate data decomposition

Example Dotproduct (BLAS 1)

```
DO I = 1, N
    C = C + A(I) * B(I)
ENDDO
```

Straightforward parallel execution on P processors:

```
DOALL II = 1,N, N/P
    DO I = II, II+N/P – 1
        C(II) = C(II) + A(I) * B(I)
    ENDDO
    C = C + C(II)
ENDDOALL
```

However, communication costs are involved!!!!!!!

```
DOALL II = 1, N, N/P          # N/P is the stride, so II = 1, 1+N/P, 1+2*N/P, …
      RECEIVE (A(II:II+N/P-1), B(II:II+N/P-1))
      DO I = II, II+N/P – 1
            C(II) = C(II) + A(I) * B(I)
      ENDDO
      C = C + C(II)       ←synchronization, i.e. SEND C(J) TO MASTER PROCESS
ENDDOALL
```

So, on a total of 2N-1 computations: 2N continuous data transmissions and P separate communications are needed. With t_s+mt_w (t_s startup time, t_w per word transmission time) communication costs for m words, this gives:

$$P.(t_s+(2N/P)t_w)+P.(t_s+t_w) =$$

$$(P+P).t_s+(2N+P)t_w = 2Pt_s + (2N+P)t_w$$

communication costs, which is significant! For instance if t_s is comparable to the cost of a computational step, then the communication overhead is greater than the computational costs (2P+1).

➔ BLAS 1 routines were mainly used for VECTOR computing (pipelining)

vadd, vdotpr, vmultadd, etc.

Example MatVec (BLAS 2)

```
DO I = 1, N
    DO J = 1, N
        C(I) = C(I) + A(I,J) * B(J)
    ENDDO
ENDDO
```

Parallel execution on P processors:

```
DO I = 1, N
    DOALL JJ = 1, N, N/P
        DO J = JJ, JJ+N/P – 1
            C(JJ) = C(JJ) + A(I,J) * B(J)
        ENDDO
        C(I) = C(I) + C(JJ)
    ENDDOALL
ENDDO
```

This is essentially is a repetition of BLAS 1 (dotproduct) operations!!!!! NOTHING GAINED. HOWEVER…

MatVec can also be computed as:

```
DO J =1, N
    DOALL II = 1, N, N/P
        DO I= II, II+N/P-1
            C(I) = C(I)+A(I,J)*B(J)
        ENDDO
    ENDDOALL
ENDDO
```

In this computation the basic (inner) loop does not execute a dotproduct, but a BLAS 1 SAXPY operation: $y = y + a.x$

More importantly, the vector C(II:II+N/P-1) can be stored in registers in each processor, and reused N times

Also the fan-in computations for each C(I) are not needed anymore!! So only initial distribution costs are paid for. So, overhead is reduced to

$$Pt_s+(2N)t_w$$

Example MatMat (BLAS 3)

```
DO I = 1, N
    DO J = 1, N
        DO K = 1, N
            C(I,K) = C(I,K) + A(I,J) * B(J,K)
        ENDO
    ENDDO
ENDDO
```

Then because of the multi dimensionality we have different ways of executing this loop in parallel.

Middle product form (K-loop outer loop):

```
DO K = 1, N
      DOALL II = 1,N, N/√P
            DOALL JJ = 1,N, N/√P
                  DO I = II, II+N/√P-1
                        DO J = JJ, JJ+N/√P-1
                              C(I,K) = C(I,K) + A(I,J) * B(J,K)
                        ENDO
                  ENDDO
            ENDDOALL
      ENDOALL
ENDDO
```

In this implementation the inner loop is a BLAS 2 MatVec routine.

Inner product form (I-loop outer loop):

```
DO I = 1, N
    DO J = 1, N
        DOALL KK = 1, N, N/P
            DO K = KK, KK+N/P-1
                C(I,K) = C(I,K) + A(I,J) * B(J,K)
            ENDO
        ENDDOALL
    ENDDO
ENDDO
```

➔ In this implementation the inner loop is a BLAS 1 SAXPY routine.

The inner product form has a second variant:

```
DO K = 1, N
    DO I = 1, N
        DOALL JJ = 1,N, N/P
            DO J = JJ, JJ+N/P-1
                C(I,K) = C(I,K) + A(I,J) * B(J,K)
            ENDO
        ENDDOALL
    ENDDO
ENDDO
```

In this implementation the inner loop executes a BLAS 1 DOTPRODUCT

Outer product form (J-loop outer loop):

```
DO J = 1, N
    DO K = 1, N
        DOALL II = 1, N, N/P
            DO I = II, II+N/P-1
                C(I,K) = C(I,K) + A(I,J) * B(J,K)
            ENDO
        ENDDOALL
    ENDDO
ENDDO
```

Another look at MatMat

The original loop can be written as follows:

```
DO II = 1, N, M1
    DO JJ = 1 ,N, M2
        DO KK = 1, N, M3
            DO I = II, II + M1 - 1
                DO J = JJ, JJ + M2 - 1
                    DO K = KK, KK + M3 - 1
                        C(I,K) = C(I,K) + A(I,J) * B(J,K)
                    ENDO
                ENDDO
            ENDDO
        ENDDO
    ENDDO
ENDDO
```

- ➔ Any of these loops can be executed in parallel!!
- ➔ These loops can be permuted in any order as long as II becomes before I, etc.
- ➔ So many different implementations possible
- ➔ M1, M2, and M3 can be used to control the degree of parallelism but also the size of cache usage.

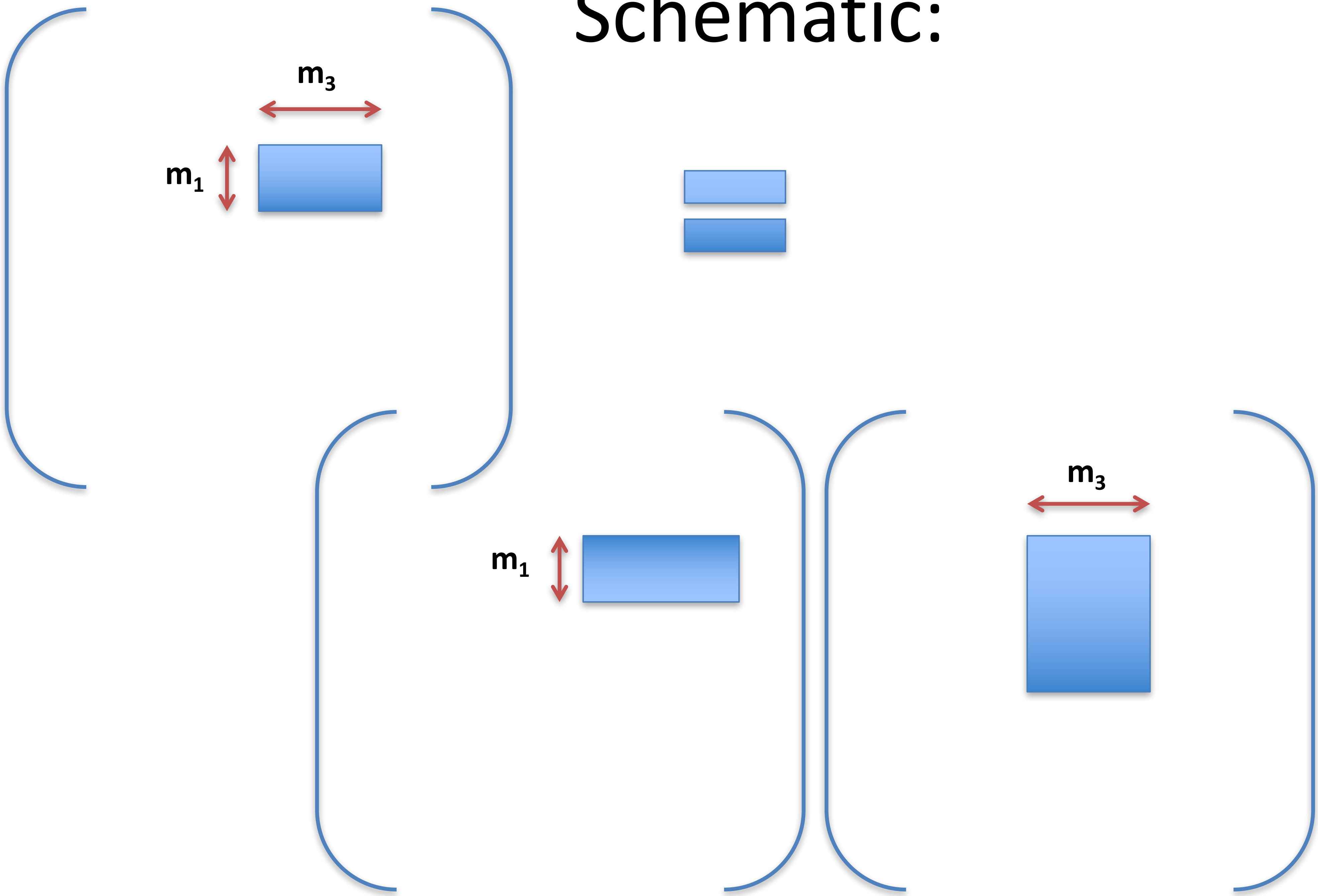
In fact

```
DO I = II, II + M1 - 1
    DO J = JJ, JJ + M2 - 1
        DO K = KK, KK + M3 - 1
            C(I,K) = C(I,K) + A(I,J) * B(J,K)
        ENDO
    ENDDO
ENDDO
```

Corresponds to a sub matrix multiply of size M1xM2 times M2xM3

By choosing M1, M2 and M3 carefully, this triple nested loop can each time run out of cache

Schematic:



Embeddings of BLAS routines

Many scientific computations involve the solution of a system of linear equations

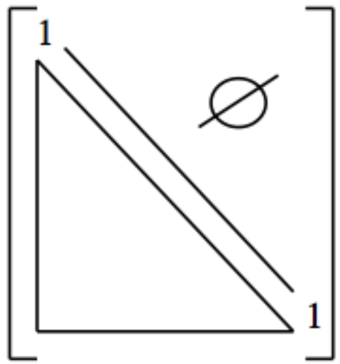
$$\begin{array}{ccccccccc} a_{0,0}x_0 & + & a_{0,1}x_1 & + & \cdots & + & a_{0,n-1}x_{n-1} & = & b_0, \\ a_{1,0}x_0 & + & a_{1,1}x_1 & + & \cdots & + & a_{1,n-1}x_{n-1} & = & b_1, \\ \vdots & & \vdots & & & & \vdots & & \vdots \\ a_{n-1,0}x_0 & + & a_{n-1,1}x_1 & + & \cdots & + & a_{n-1,n-1}x_{n-1} & = & b_{n-1}. \end{array}$$

This is written as Ax = b where A is an n x n matrix with A[i, j] = a_{ij}, b is an n x 1 vector [b_0, b_1, … , b_n]$^{\mathrm{T}}$, and x is the solution.

LU Factorization

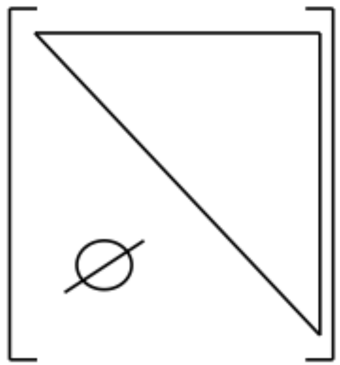
Find

L =



and

U =



Such that A = L.U

Then solving Ax = b corresponds to solving

$$L\,(U\,x) = b$$

This can be done in 2 steps, triangular solves:

$$L\,c = b \text{ (forward substitution)}$$

$$U\,x = c \text{ (backward substitution)}$$

Backward substitution U x = y

$$\begin{array}{rcrcrcccrcl}
x_0 & + & u_{0,1}x_1 & + & u_{0,2}x_2 & + & \cdots & + & u_{0,n-1}x_{n-1} & = & y_0, \\
 & & x_1 & + & u_{1,2}x_2 & + & \cdots & + & u_{1,n-1}x_{n-1} & = & y_1, \\
 & & & & & & & & \vdots & & \vdots \\
 & & & & & & & & x_{n-1} & = & y_{n-1}.
\end{array}$$

The factors L and U can be obtained through Gaussian Elimination

$$\begin{cases} 2x_1 & + & 3x_2 & + & x_3 & = 1 \\ x_1 & + & x_2 & + & 3x_3 & = 2 \\ 3x_1 & + & 2x_2 & + & x_3 & = 3 \end{cases}$$

$$A = \begin{pmatrix} 2 & 3 & 1 \\ 1 & 1 & 3 \\ 3 & 2 & 1 \end{pmatrix}, B = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

```
DO I = 1, N
    PIVOT = A(I, I)
    DO J = I+1, N
        MULT = A(J, I)/PIVOT
        A(J, I) = MULT
        DO K = I+1, N
            A(J, K) = A(J, K) - MULT * A(I, K)
        ENDDO
    ENDDO
ENDDO
```

This yields:

$$\tilde{A} = \begin{pmatrix} 2 & 3 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 2\frac{1}{2} \\ 1\frac{1}{2} & 5 & -13 \end{pmatrix}. \text{ So, } L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 1\frac{1}{2} & 5 & 1 \end{bmatrix} \text{ and } U = \begin{pmatrix} 2 & 3 & 1 \\ 0 & -\frac{1}{2} & 2\frac{1}{2} \\ 0 & 0 & -13 \end{pmatrix}.$$

After L and U are computed the system is solved by:

forward substitution:

```
DO I = 1, N
   C(I) = B(I)
   DO J = 1, I-1
      C(I) = C(I) - A(I, J) * C(J)
   ENDDO
ENDDO
```

back substitution:

```
DO I = N, 1
   X(I) = C(I)
   DO J = I+1, N
      X(I) = X(I) - A(I, J) * X(J)
   ENDDO
   X(I) = X(I)/A(I, I)
ENDDO
```

Block LU decomposition

Write A as follows

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ 0 & B \end{pmatrix}$$

To be stored as:

$$\begin{bmatrix} A_{11}^{-1} & A_{12} \\ L_{21} & B \end{bmatrix}$$

So

$$A = \begin{pmatrix} A_{11} & A_{12} \\ L_{21}A_{11} & L_{21}A_{12} + B \end{pmatrix}$$

Let k be the dimension of A_{11} and N-k the dimension of A_{22}
Then the algorithm becomes:

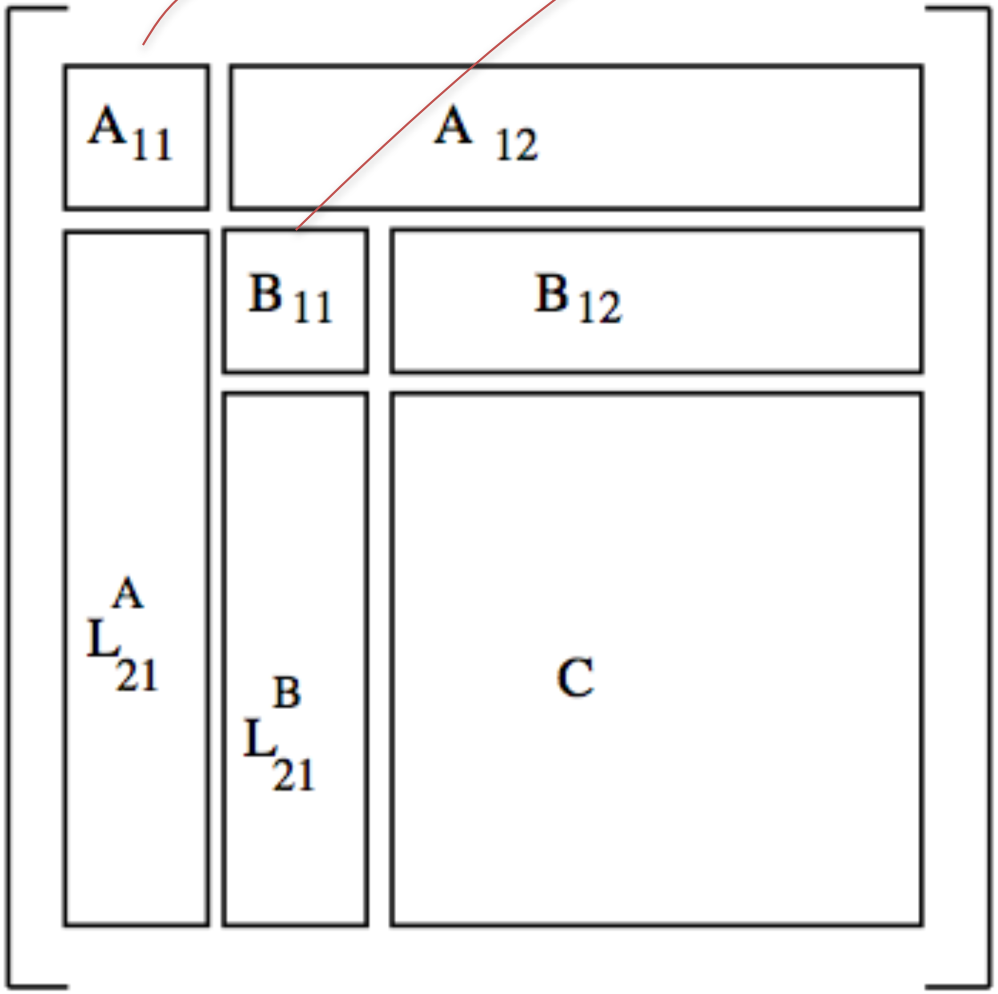
$$\left[\begin{array}{l} A_{11} \leftarrow A_{11}^{-1} \\ A_{21} \leftarrow L_{21} = A_{21}A_{11} \\ A_{22} \leftarrow B = A_{22} - L_{21}A_{12} \end{array}\right.$$

$(A_{21}A_{11}^{-1})A_{11}=A_{21}$

And proceed recursively on B

In a picture

In fact A_{11}^{-1}, B_{11}^{-1}, etc are stored in these positions



Note that the
I diagonal blocks
do not need to
be kept.

As a results

➔ This algorithm only has only to compute the inverse of A_{11}, otherwise **only matrix multiplies** are performed

The only complication is that back substitution is a bit more tedious.

Backward Substitution

$$
\left[\begin{array}{cccc}
U_1 & \multicolumn{3}{c}{\tilde{U}_1} \\
 & U_2 & \multicolumn{2}{c}{\tilde{U}_2} \\
 & & U_3 & \tilde{U}_3 \\
\emptyset & & & U_4
\end{array}\right]
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}
=
\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}
$$

Note that $U_4 x_4 = c_4$ can be solved directly by $x_4 = A_{44}^{-1} c_4$ etc

1. Solve $U_4 x_4 = c_4$
2. $c_3 = c_3 - \tilde{U}_3 \cdot x_4$
3. Solve $U_3 x_3 = c_3$
4. $c_2 = c_2 - \tilde{U}_2 \cdot \begin{bmatrix} x_3 \\ x_4 \end{bmatrix}$
5. Solve $U_2 x_2 = c_2$
6. $c_1 = c_1 - \tilde{U}_1 \cdot \begin{bmatrix} x_2 \\ x_3 \\ x_4 \end{bmatrix}$
7. Solve $U_1 x_1 = c_1$

Forward Substitution

$$\begin{bmatrix} I & & & \\ L_2 & I & & \emptyset \\ \multicolumn{2}{c}{L_3} & I & \\ \multicolumn{3}{c}{L_4} & I \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

1. $c_1 = b_1$
2. $c_2 = b_2 - L_2 \cdot c_1$
3. $c_3 = b_3 - L_3 \cdot \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$
4. $c_4 = b_4 - L_4 \cdot \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$