Lecture 8: Fast Linear Solvers (Part 1)

LU Factorization

Solve

$$
\begin{aligned}
E_1: &\quad a_{11}x_1 + a_{12}x_2 + \cdots a_{1n}x_n = b_1 \\
E_2: &\quad a_{21}x_1 + a_{22}x_2 + \cdots a_{2n}x_n = b_2 \\
&\quad \vdots \\
E_n: &\quad a_{n1}x_1 + a_{n2}x_2 + \cdots a_{nn}x_n = b_n
\end{aligned}
$$

for $x_1, x_2, \dots, x_n$.

- Matrix form $A\boldsymbol{x} = \boldsymbol{b}$:

$$
\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}
$$

- Direct method for solving $A\boldsymbol{x} = \boldsymbol{b}$ is by computing **LU factorization** $A = LU$

  Where L is lower triangular and U is upper triangular.

Solve $$\begin{aligned} x_1 + x_2 + 2x_3 &= 6 \\ 2x_2 + x_3 &= 4 \\ 2x_1 + x_2 + x_3 &= 7 \end{aligned}$$

$$\left[\begin{array}{ccc|c} 1 & 1 & 2 & 6 \\ 0 & 2 & 1 & 4 \\ 2 & 1 & 1 & 7 \end{array}\right]$$

$$l_{21} = 0; l_{31} = 2 \rightarrow (E_3 - 2 * E_1) \rightarrow (E_3) \left[\begin{array}{ccc|c} 1 & 1 & 2 & 6 \\ 0 & 2 & 1 & 4 \\ 0 & -1 & -3 & -5 \end{array}\right] \quad l_{32} = -0.5 \rightarrow (E_3 + 0.5 * E_2) \rightarrow (E_3) \left[\begin{array}{ccc|c} 1 & 1 & 2 & 6 \\ 0 & 2 & 1 & 4 \\ 0 & 0 & -\frac{5}{2} & -3 \end{array}\right]$$

Theorem If Gaussian elimination can be performed on the linear system $A\boldsymbol{x} = \boldsymbol{b}$ *without row interchange,* A can be factored into the product of *lower triangular* matrix L and *upper triangular* matrix U as $A = LU$:

$$U = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \dots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & \dots & a_{2n}^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn}^{(n)} \end{bmatrix}, \qquad L = \begin{bmatrix} 1 & 0 & \dots & 0 \\ l_{21} & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & \cdots & l_{n,n-1} & 1 \end{bmatrix}$$

1. LU decomposition: $\mathrm{A} = LU$ so that $A\boldsymbol{x} = \boldsymbol{b}$ becomes

$$LU\boldsymbol{x} = \boldsymbol{b}$$

2. Solve $L\boldsymbol{y} = \boldsymbol{b}$ by forward substitution to obtain vector $\boldsymbol{y}$
3. Solve $U\boldsymbol{x} = \boldsymbol{y}$ backward for $\boldsymbol{x}$

Gaussian Elimination Algorithm

- (n-1) stages of elimination are needed to obtain U. Assume all pivots at every stage are not 0.
- At the last stage, U overwrites A.
- We assume that pivoting (row interchange) is not needed for simplicity.

```
for k = 1 to n − 1                    // loop over columns
   for i = k + 1 to n
      l_ik = a_ik / a_ii              // multipliers for kth column
      b_i = b_i − l_ik b_k
   end;
   for j = k + 1 to n
      for i = k + 1 to n
         a_ij = a_ij − l_ik a_kj      // elimination step
      end;
   end;
end;
```

Gaussian elimination requires about $n^3/3$ paired additions and multiplications, and about $n^2/2$ divisions.

Backward Substitution

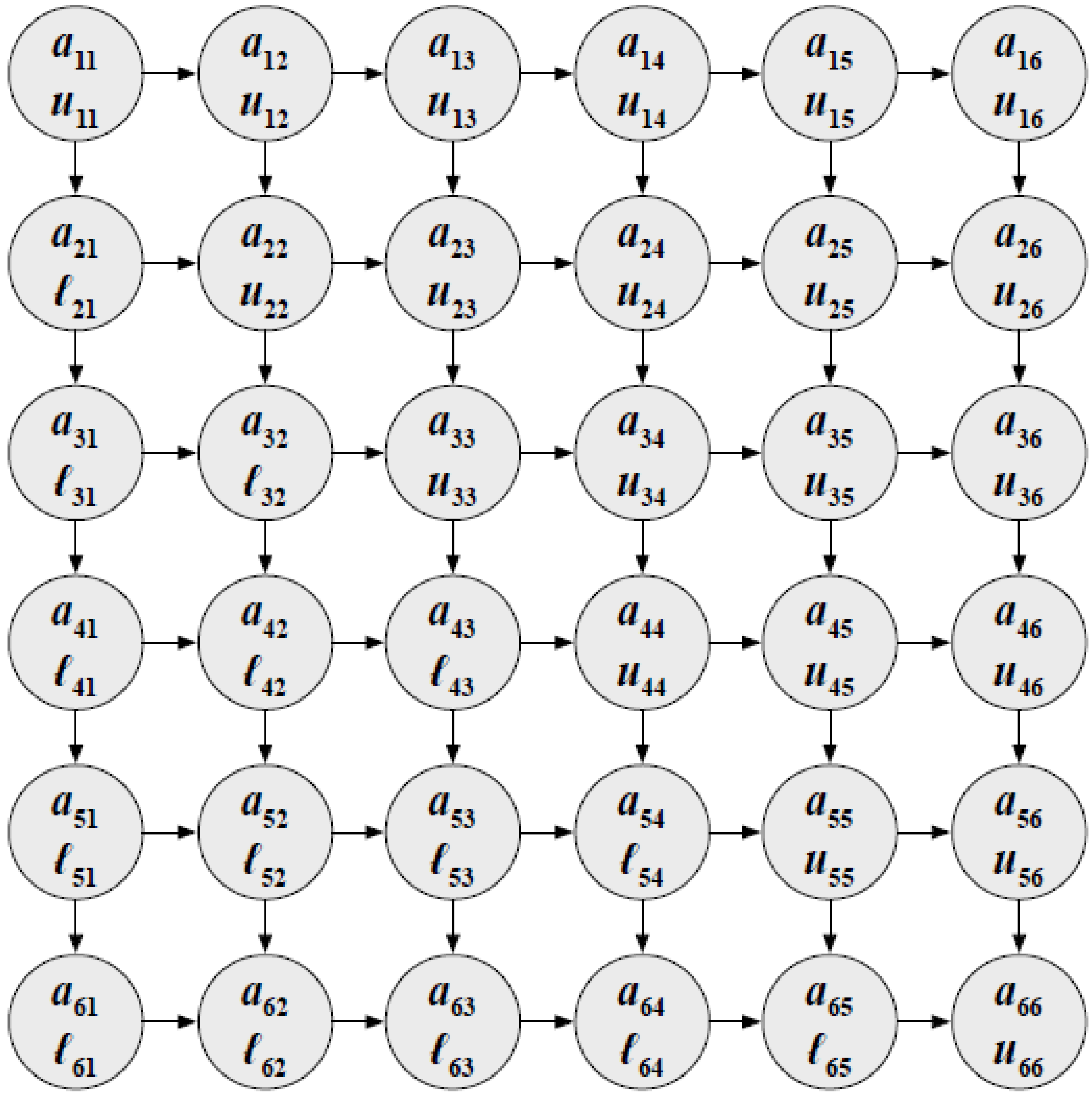
After elimination, we obtain upper triangular $U\boldsymbol{x} = \boldsymbol{b}^{(n-1)}$.

for $k = n$ **to** 1
    $x_k = b_k$
    for $i = k + 1$ **to** n
        $x_k = x_k - u_{ki}x_i$
    end;
    $x_k = x_k / u_{kk}$
end;

Parallel Algorithm Design

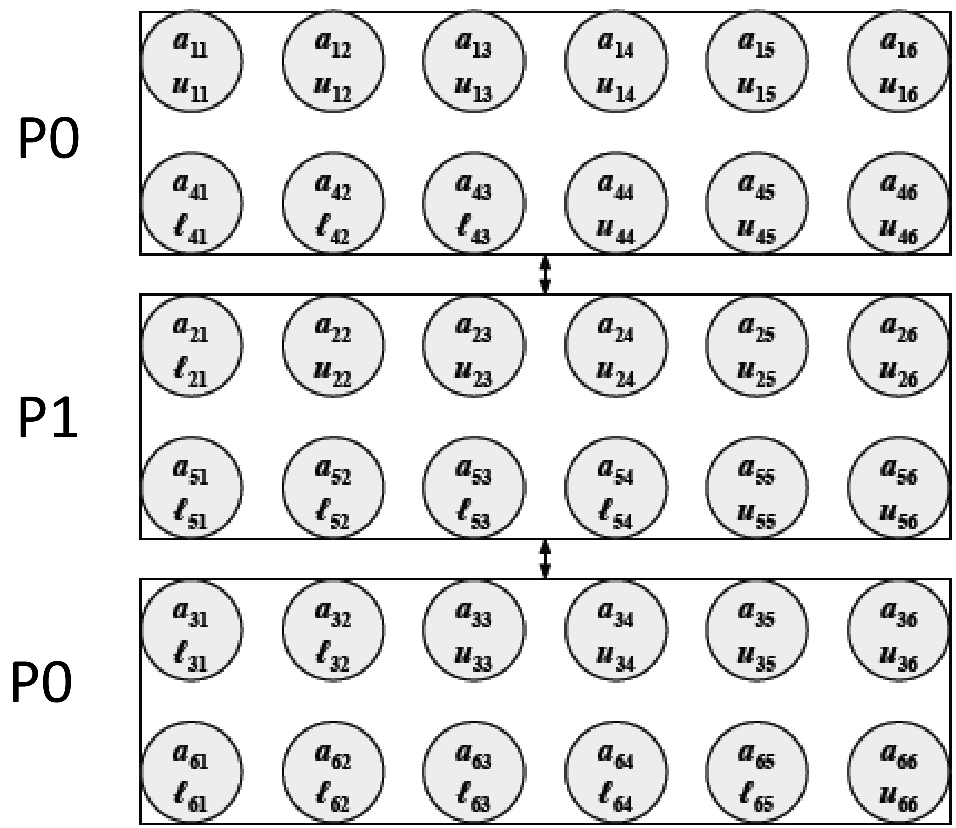
- Assume a fine-grained decomposition, i.e., a_{ij} is assigned to process P_{ij}.
- **Outer** loop can not be executed in parallel; while the **inner** loop can be executed in parallel.
- Communications:
  - Broadcast row of A vertically below
  - Broadcast l_{ik} horizontally to tasks to right

Fine-Grained Tasks and Communication



Row-wise Cyclic Mapping Parallel Algorithm

- A few contiguous rows of A (2 or 3 or more rows) are grouped into blocks. Distribute blocks to processes in a wraparound manner.
- Also associate corresponding elements of $\boldsymbol{b}$ and $\boldsymbol{x}$ of blocks to processes, respectively.



- Multipliers need not to be broadcasted horizontally, since any row of matrix is held entirely in one process.
- Vertical communications are still needed to broadcast a row of matrix to processes holding rows below it for updating.

Row-wise Parallel Algorithm

for $k = 1$ **to** $n - 1$ // loop over columns
  broadcast kth row to processes holding $k + 1, \dots, n$ rows
  for processes holding ith row, $i > k$,
    $l_{ik} = a_{ik}/a_{ii}$ // multipliers for kth column
  end;
  for processes holding ith row, $i > k$
    for j $= k + 1$ **to** n
      $a_{ij} = a_{ij} - l_{ik}a_{kj}$ // elimination step
    end;
  end;
end;

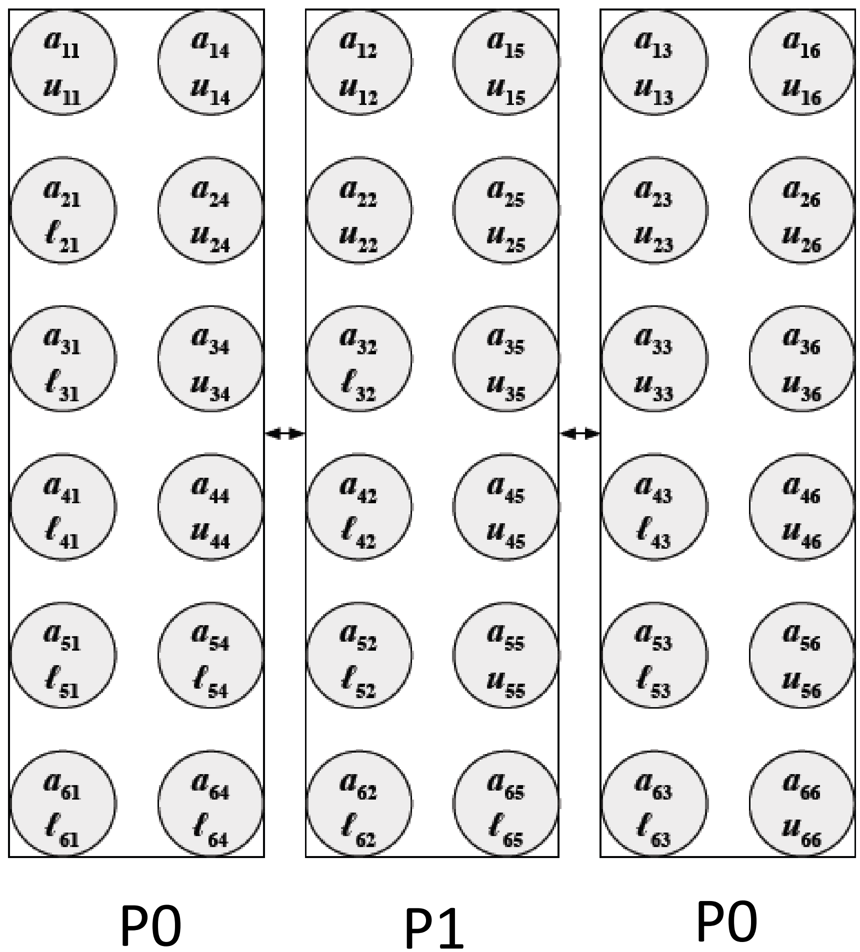
Performance Analysis

Assume each row of matrix is assigned to a process.

- The inner loop at step k involves $n - k$ multiplications and subtractions for processes holding ith rows, $k < i < n$.
- At step k, there are $n - k$ divisions to compute multiplier $(\frac{a_{ik}}{a_{ii}})$
- At step k, the one-to-all broadcast times time: $t_s + t_w(n - k)logn$
- Overall complexity: $3\sum_{k=1}^{n}(n - k) + \sum_{k=1}^{n}(t_s + t_w(n - k)logn) = \frac{3}{2}n(n - 1) + t_snlogn + \frac{1}{2}n(n - 1)t_wlogn$

Column-wise Cyclic Mapping Parallel Algorithm

- A few contiguous columns of A (2 or 3 or more columns) are grouped into blocks. Distribute blocks to processes in a wraparound manner.

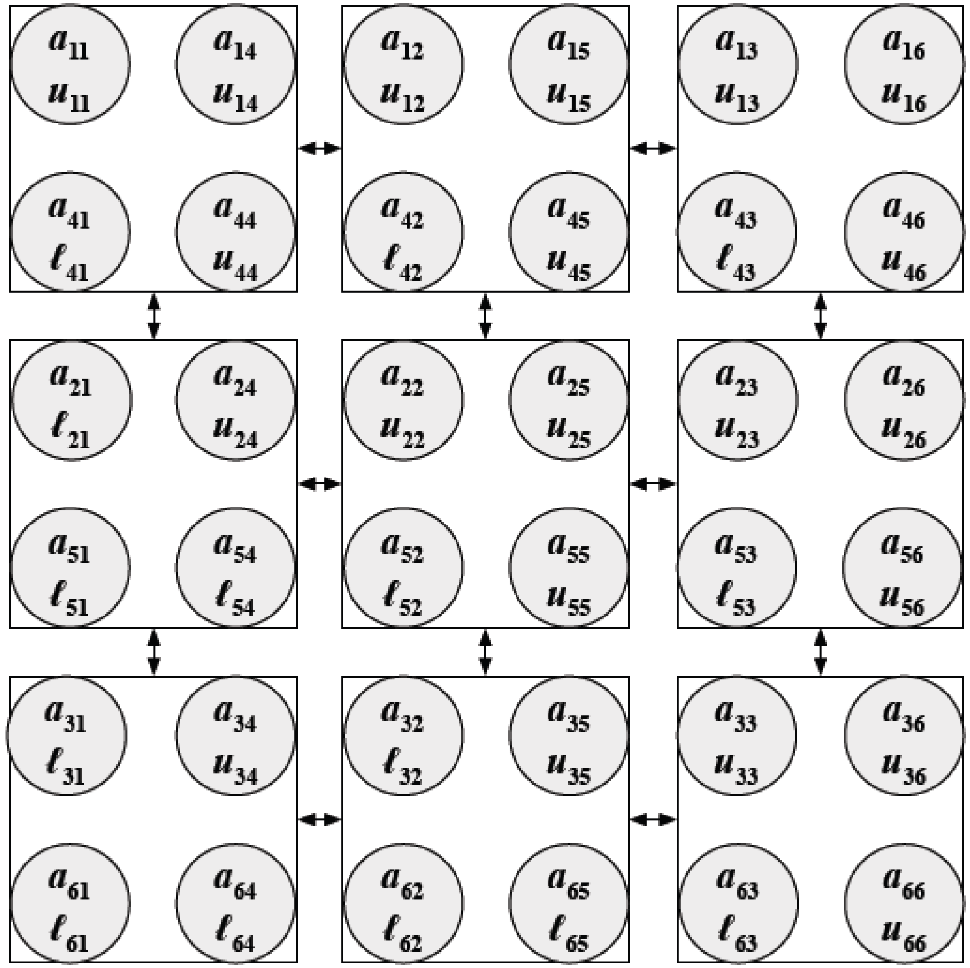


- Horizontal communications are needed to broadcast multipliers for updating.
- Vertical communications are not needed to broadcast a row of matrix, since any column is assigned to one process.

Column-wise Parallel Algorithm

```
for k = 1 to n − 1                                          // loop over columns
   if process holds kth column, then
      for i = k + 1  to n
         l_ik = a_ik / a_ii                                 // multipliers for kth column
      endfor;
   endif;
   broadcast {l_ik : k < i ≤ n} to processes holding k, … , n columns
   for processes holds jth column,   j > k
      for i = k + 1 to n
         a_ij = a_ij − l_ik a_kj                            // elimination step
      end;
   end;
end;
```

2D Block Cyclic Mapping Parallel Algorithm



- With cyclic block mapping, each process holds several submatrices assembled globally. This improves both concurrency and load balance.
- Horizontal communications are needed to broadcast multipliers for updating.
- Vertical communications are also needed to broadcast a row of matrix, since any column is assigned to one process.

2D Block Cyclic Mapping Parallel Algorithm

```
for k = 1 to n − 1                                          // loop over columns
   broadcast {a_kj : k < j ≤ n} among columns of processes
   if process holds kth column, then
      for processes hold ith row, i > k
         l_ik = a_ik / a_ii                                 // multipliers for kth column
      endfor;
   endif;
   broadcast {l_ik : k < i ≤ n} to rows of processes
   for processes hold jth column,  j > k
      for processes hold ith row, i > k
         a_ij = a_ij − l_ik a_kj                            // elimination step
      end;
   end;
end;
```

Gaussian Elimination with Partial Pivoting

- If pivot element ≈ 0, significant round-off errors can occur.
- Partial pivoting finds the smallest $p \geq k$ such that $\left|a_{pk}^{(k)}\right| = \max_{k \leq i \leq n} |a_{ik}^{(k)}|$ and interchanges the rows $(E_k) \leftrightarrow (E_p)$.
- Partial pivoting is required for numerical stability of LU factorization

Gaussian Elimination with Partial Pivoting Parallel Algorithm

- With 1D row algorithm or 2D block algorithm, searching pivot requires communication.
- With 1D column algorithm, searching pivot is local operation.
- Once pivot is found, index of pivot row must be communicated to all processes. Row interchange communication must be called.

Pivot Searching

- Use MPI_Allreduce(), operator MPI_MAXLOC and derived data type MPI_DOUBLE_INT (struct {double, int}).

```
struct {
   double value;
   int    index;
} local, global;
...
local.value = fabs(a[j][i]);
local.index = j;
...
MPI_Allreduce (&local, &global, 1,
   MPI_DOUBLE_INT, MPI_MAXLOC,
   MPI_COMM_WORLD);
```