# Parallel Scientific Computing Course AMS301 - Fall 2023 - Lecture 5 

Direct methods for linear systems

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## Solution procedures for linear systems - Recap

$$
\text { Find } \mathbf{x} \in \mathbb{R}^{n} \text { such that } \mathbf{A x}=\mathbf{b} \text { with } \mathbf{A} \in \mathbb{R}^{n \times n} \text { and } \mathbf{b} \in \mathbb{R}^{n} \text {. }
$$

## Solution procedures

- Direct methods: Factorization of $\mathbf{A}$ into triangular and diagonal matrices (ex. $\mathbf{A}=\mathbf{L U}$ ) and solution of simpler problems.

$$
\mathbf{A x}=\mathbf{b} \quad \Leftrightarrow \quad \mathbf{L U x}=\mathbf{b} \quad \Leftrightarrow \quad \begin{array}{r}
\mathbf{L y}=\mathbf{b} \\
\mathbf{U x}=\mathbf{y}
\end{array}
$$

Advantages: exact solution known after a given number of operations Difficulties: heavy computational cost (operations/memory), hard to parallelize

- Iterative methods: Iterative procedure to minimizing an error $\left\|\mathbf{x}^{(\ell)}-\mathbf{x}_{\text {ref }}\right\|$ and/or a residual $\left\|\mathbf{A x} \mathbf{x}^{(\ell)}-\mathbf{b}\right\|$.

$$
\begin{aligned}
\mathbf{x}^{(0)} & =\operatorname{Iter}_{(0)}(\mathbf{A}, \mathbf{b}) \\
\mathbf{x}^{(\ell+1)} & =\operatorname{Iter}^{(\ell+1)}\left(\mathbf{x}^{(\ell)}, \mathbf{x}^{(\ell-1)}, \ldots, \mathbf{A}, \mathbf{b}\right), \quad \text { pour } \ell \geq 0
\end{aligned}
$$

Advantages: limited cost per iteration (operations/memory), easy to parallelize Difficulties: approximate solution, control of the convergence of the process

# Direct methods for linear systems 

Solution of triangular systems
Gaussian elimination
Matrix factorization

## Triangular systems - Approaches by points

## Definitions

- Lower triangular matrix: $\mathbf{L} \in \mathbb{R}^{n \times n}$ with $L_{i j}=0$ if $i<j$
- Upper triangular matrix: $\mathbf{U} \in \mathbb{R}^{n \times n}$ with $U_{i j}=0$ if $i>j$

$$
\mathbf{L}=\left[\begin{array}{ccc}
L_{11} & 0 & 0 \\
L_{21} & L_{22} & 0 \\
L_{31} & L_{32} & L_{33}
\end{array}\right] \quad \mathbf{U}=\left[\begin{array}{ccc}
U_{11} & U_{12} & U_{13} \\
0 & U_{22} & U_{23} \\
0 & 0 & U_{33}
\end{array}\right]
$$

## Properties

- The determinant of a triangular matrix is the product of the diagonal elements:

$$
\operatorname{det}(\mathbf{L})=\prod_{i=1}^{n} L_{i i} \quad \operatorname{det}(\mathbf{U})=\prod_{i=1}^{n} U_{i i}
$$

- A triangular matrix is invertible if, and only if, its diagonal elements are nonzero.


## Triangular systems - Approaches by points [2/2]

## Procedure to solve $\mathbf{L x}=\mathbf{b} \quad$ (Forward substitution)

Data: $\mathbf{L}$ and $\mathbf{b}$
Initialization: $\mathbf{x} \leftarrow 0$
for $i=1, \ldots, n$ do
$x_{i} \leftarrow\left[b_{i}-\sum_{j=1}^{i-1} L_{i j} x_{j}\right] / L_{i i}$
end

## Procedure to solve $\mathbf{U x}=\mathbf{b} \quad$ (Backward substitution)

Data: $\mathbf{U}$ et $\mathbf{b}$
Initialization: $\mathbf{x} \leftarrow 0$
for $i=n, \ldots, 1$ do
$x_{i} \leftarrow\left[b_{i}-\sum_{j=i+1}^{n} U_{i j} x_{j}\right] / U_{i i}$
end

## Algorithmic aspects

- Cost: $n^{2}$ operations
- Weak parallelization (computation of sums in parallel)


## Triangular systems - Approaches by blocks

## Definitions

- Lower triangular matrix by blocks: $\mathbf{L} \in \mathbb{R}^{n \times n}$ with $\mathbf{L}_{I J}=0$ si $I<J$
- Upper triangular matrix by blocks: $\mathbf{U} \in \mathbb{R}^{n \times n}$ with $\mathbf{U}_{I J}=0$ si $I>J$

$$
\mathbf{L}=\left[\begin{array}{ccc}
\mathbf{L}_{11} & 0 & 0 \\
\mathbf{L}_{21} & \mathbf{L}_{22} & 0 \\
\mathbf{L}_{31} & \mathbf{L}_{32} & \mathbf{L}_{33}
\end{array}\right] \quad \mathbf{U}=\left[\begin{array}{ccc}
\mathbf{U}_{11} & \mathbf{U}_{12} & \mathbf{U}_{13} \\
0 & \mathbf{U}_{22} & \mathbf{U}_{23} \\
0 & 0 & \mathbf{U}_{33}
\end{array}\right]
$$

The diagonal blocks are square. The other blocks may not be square.

## Properties

- The determinant of a triangular matrix by blocks is the product of the determinants of the diagonal blocks:

$$
\operatorname{det}(\mathbf{L})=\prod_{I=1}^{N} \operatorname{det}\left(\mathbf{L}_{I I}\right) \quad \operatorname{det}(\mathbf{U})=\prod_{I=1}^{N} \operatorname{det}\left(\mathbf{U}_{I I}\right)
$$

- A diagonal or triangular matrix by blocks is invertible if, and only if, the diagonal blocks are invertible.


## Triangular systems - Approaches by blocks

## Procedure to solve $\mathbf{L x}=\mathbf{b} \quad$ (Forward substitution)

Data: $\mathbf{L}$ and $\mathbf{b}$
Initialization: $\mathbf{x} \leftarrow 0$
for $I=1, \ldots, N$ do
$\mathbf{x}_{I} \leftarrow \mathbf{L}_{I I}^{-1}\left[\mathbf{b}_{I}-\sum_{J=1}^{I-1} \mathbf{L}_{I J} \mathbf{x}_{J}\right]$
end

## Procedure to solve $\mathbf{U x}=\mathbf{b} \quad$ (Backward substitution)

Data: $\mathbf{U}$ and $\mathbf{b}$
Initialization: $\mathbf{x} \leftarrow 0$
for $I=N, \ldots, 1$ do
$\mathbf{x}_{I} \leftarrow \mathbf{U}_{I I}^{-1}\left[\mathbf{b}_{I}-\sum_{J=I+1}^{N} \mathbf{U}_{I J} \mathbf{x}_{J}\right]$
end

## Algorithmic aspects

- Cost: $N$ small system to solve and $N(N-1) / 2$ matrix-vector products
- Better for parallel computing (computation of matrix-vector products in parallel)


# Direct methods for linear systems 

Solution of triangular systems
Gaussian elimination
Matrix factorization

## General systems — Gaussian elimination [1/5]

Goal: Transform $\mathbf{A x}=\mathbf{b}$ into an equivalent system $\mathbf{U x}=\mathbf{b}^{\prime}$.

## Procedure

- Initialization:

$$
\left[\begin{array}{cccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1 n}^{(1)} \\
A_{21}^{(1)} & A_{22}^{(1)} & \cdots & A_{2 n}^{(1)} \\
\vdots & \vdots & & \vdots \\
A_{n 1}^{(1)} & A_{n 2}^{(1)} & \cdots & A_{n n}^{(1)}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
x_{n}
\end{array}\right]=\left[\begin{array}{c}
b_{1}^{(1)} \\
b_{2}^{(1)} \\
\vdots \\
b_{n}^{(1)}
\end{array}\right]
$$

- Iteration 1 :

$$
\left[\begin{array}{cccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1 n}^{(1)} \\
0 & A_{22}^{(2)} & \cdots & A_{2 n}^{(2)} \\
\vdots & \vdots & & \vdots \\
0 & A_{n 2}^{(2)} & \cdots & A_{n n}^{(2)}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
x_{n}
\end{array}\right]=\left[\begin{array}{c}
b_{1}^{(1)} \\
b_{2}^{(2)} \\
\vdots \\
b_{n}^{(2)}
\end{array}\right]
$$

with

$$
\begin{aligned}
\alpha_{i 1} & =A_{i 1}^{(1)} / A_{11}^{(1)} & & i=2, \ldots, n \\
A_{i j}^{(2)} & =A_{i j}^{(1)}-\alpha_{i 1} A_{1 j}^{(1)} & & i, j=2, \ldots, n \\
b_{i}^{(2)} & =b_{i}^{(1)}-\alpha_{i 1} b_{1}^{(1)} & & i=2, \ldots, n
\end{aligned}
$$

## General systems - Gaussian elimination [2/5]

Goal: Transform $\mathbf{A x}=\mathbf{b}$ into an equivalent system $\mathbf{U x}=\mathbf{b}^{\prime}$.

## Procedure

- Iteration $k$ :

$$
\left[\begin{array}{cccccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & \cdots & A_{1 n}^{(1)} \\
0 & A_{22}^{(2)} & & & & A_{2 n}^{(2)} \\
\vdots & & \ddots & & & \vdots \\
0 & \cdots & 0 & A_{k+1, k+1}^{(k)} & \cdots & A_{k+1, n}^{(k)} \\
\vdots & & \vdots & \vdots & & \vdots \\
0 & \cdots & 0 & A_{n, k+1}^{(k)} & \cdots & A_{n, n}^{(k)}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
x_{k+1} \\
\vdots \\
x_{n}
\end{array}\right]=\left[\begin{array}{c}
b_{1}^{(1)} \\
b_{2}^{(2)} \\
\vdots \\
b_{k+1}^{(k)} \\
\vdots \\
b_{n}^{(k)}
\end{array}\right]
$$

- Iteration $n-1$ :

$$
\left[\begin{array}{ccccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & A_{1 n}^{(1)} \\
0 & A_{22}^{(2)} & & & A_{2 n}^{(2)} \\
\vdots & & \ddots & & \vdots \\
0 & & & \ddots & \vdots \\
0 & & & & A_{n n}^{(n)}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
\vdots \\
x_{n}
\end{array}\right]=\left[\begin{array}{c}
b_{1}^{(1)} \\
b_{2}^{(2)} \\
\vdots \\
\vdots \\
b_{n}^{(n)}
\end{array}\right]
$$

## General systems — Gaussian elimination [3/5]

## Gaussian elimination

Data: A and b
Initialization: $\mathbf{A}^{(1)}=\mathbf{A}$ and $\mathbf{b}^{(1)}=\mathbf{b}$
for $k=1, \ldots, n-1$ do
for $i=k+1, \ldots, n$ do
$\alpha_{i k}=A_{i k}^{(k)} / A_{k k}^{(k)}$
Si $A_{k k}^{(k)} \neq 0$ !
$A_{i j}^{(k+1)}=A_{i j}^{(k)}-\alpha_{i k} A_{k j}^{(k)} \quad(j=k+1, \ldots, n)$
$b_{i}^{(k+1)}=b_{i}^{(k)}-\alpha_{i k} b_{k}^{(k)}$
end
end

## Gaussian elimination (Rewriting)

Data: A and b
for $k=1, \ldots, n-1$ do
for $i=k+1, \ldots, n$ do
$\alpha \leftarrow A_{i k} / A_{k k} \quad$ Si $A_{k k} \neq 0$ !
$A_{i j} \leftarrow A_{i j}-\alpha A_{k j} \quad(j=k+1, \ldots, n)$
$A_{i k} \leftarrow 0$
$b_{i} \leftarrow b_{i}-\alpha b_{k}$
end
end

## General systems — Gaussian elimination [4/5]

$$
\left[\begin{array}{lll}
A_{11} & A_{12} & A_{13} \\
A_{21} & A_{22} & A_{23} \\
A_{31} & A_{32} & A_{33}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{l}
b_{1} \\
b_{2} \\
b_{3}
\end{array}\right] \Leftrightarrow\left[\begin{array}{ccc}
A_{11}^{\prime} & A_{12}^{\prime} & A_{13}^{\prime} \\
0 & A_{22}^{\prime} & A_{23}^{\prime} \\
0 & 0 & A_{33}^{\prime}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{l}
b_{1}^{\prime} \\
b_{2}^{\prime} \\
b_{3}^{\prime}
\end{array}\right]
$$

## Cost

- Gaussian elimination: $2(n-1) n(n+1) / 3+n(n-1)$ flop
- Backward substitution: $n^{2}$ flop
- Largest term: $2 / 3 n^{3}$ flop


## Conditions of use

- The method must be modified if, at one step, $A_{k k}^{(k)}=0$.
- The method can be used without modification...
- if $\mathbf{A}$ is diagonally dominant per line or per column
- if $\mathbf{A}$ is symmetric positive definite
- For the other cases $\Rightarrow$ Permutation of lines and/or columns


## General systems - Gaussian elimination [5/5]

## Gaussian elimination with pivoting

Data: A and b
for $k=1, \ldots, n-1$ do
Find $r \in[k, \ldots, n]$ such that $\left|A_{r k}\right|$ is $\max$. (if $\max _{r}\left|A_{r k}\right|=0$, then $\mathbf{A}$ not invert.) Swap the $r^{\text {th }}$ and $k^{\text {th }}$ lines of $\mathbf{A}$ and $\mathbf{b}$ for $i=k+1, \ldots, n$ do $\alpha \leftarrow A_{i k} / A_{k k}$ $A_{i j} \leftarrow A_{i j}-\alpha A_{k j} \quad(j=k+1, \ldots, n)$ $A_{i k} \leftarrow 0$ $b_{i} \leftarrow b_{i}-\alpha b_{k}$ end
end

## Possible pivoting strategies

- Find $r \in[k, \ldots, n]$ such that $\left|A_{k r}\right|$ is maximum (partial pivoting)
- Find $r \in[k, \ldots, n]$ and $s \in[k, \ldots, n]$ such that $\left|A_{r s}\right|$ is maximum (total pivoting)

One can always find $r \in[k, \ldots, n]$ such that $\left|A_{r k}\right|>0$, otherwise $\mathbf{A}$ is not invertible.
$\Rightarrow$ The Gaussian elimination with pivoting is applicable to every invertible matrix!

# Direct methods for linear systems 

Solution of triangular systems
Gaussian elimination
Matrix factorization

## Generalities on matrix factorization [1/2]

## Principle

- Factorize A into triangular matrices:

$$
\underbrace{\left[\begin{array}{ccc}
\times & \times & \times \\
\times & \times & \times \\
\times & \times & \times
\end{array}\right]}_{\text {A }}=\underbrace{\left[\begin{array}{ccc}
\times & 0 & 0 \\
\times & \times & 0 \\
\times & \times & \times
\end{array}\right]}_{\mathbf{L}} \underbrace{\left[\begin{array}{ccc}
\times & \times & \times \\
0 & \times & \times \\
0 & 0 & \times
\end{array}\right]}_{\mathbf{U}}
$$

- Rewrite the problem with triangular matrices:

$$
\mathbf{A} \mathbf{x}=\mathbf{b} \quad \Leftrightarrow \quad \mathbf{L U x}=\mathbf{b} \quad \Leftrightarrow \quad\left\{\begin{array}{l}
\mathbf{L y}=\mathbf{b} \\
\mathbf{U} \mathbf{x}=\mathbf{y}
\end{array}\right.
$$

and solve these problems with forward/back substitutions.

## Comments

- A priori, same cost than Gaussian elimination.
- If the system must be solved with several right-hand sides, only one factorization is necessary.


## Generalities on matrix factorization [2/2]

## Several factorizations

If $\mathbf{A}$ is invertible and factorizable (to define later), one has:

$$
\begin{array}{lll}
\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U} & \text { (Gauss) } & \\
\mathbf{A}=\mathbf{L} \tilde{\mathbf{U}} & \text { (Gauss) } & \\
\mathbf{A}=\tilde{\mathbf{L}} \mathbf{D} \tilde{\mathbf{U}} & \text { (Gauss-Jordan) } & \\
\mathbf{A}=\tilde{\mathbf{L}} \tilde{\mathbf{L}}^{T} & \text { (Crout) } & \text { Si } \mathbf{A} \text { symétrique. } \\
\mathbf{A}=\mathbf{L L}^{T} & \text { (Cholesky) } & \text { Si } \mathbf{A} \text { symétrique définie positive (SDP). }
\end{array}
$$

with
D - diagonal matrix
L - lower triangular matrix
$\tilde{\mathbf{L}}$ - lower triangular matrix with unit diagonal
U - upper triangular matrix
$\tilde{\mathbf{U}}$ - upper triangular matrix with unit diagonal

## Gaussian factorization $(\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U})$

## Procedure

- Initialization:

$$
\mathbf{A}=\left[\begin{array}{cccc}
1 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 \\
\vdots & \vdots & & \vdots \\
0 & 0 & \cdots & 1
\end{array}\right]\left[\begin{array}{cccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1 n}^{(1)} \\
A_{21}^{(1)} & A_{22}^{(1)} & \cdots & A_{2 n}^{(1)} \\
\vdots & \vdots & & \vdots \\
A_{n 1}^{(1)} & A_{n 2}^{(1)} & \cdots & A_{n n}^{(1)}
\end{array}\right]
$$

- Iteration 1:

$$
\mathbf{A}=\left[\begin{array}{ccccc}
1 & 0 & \cdots & \cdots & 0 \\
\alpha_{21} & 1 & & & 0 \\
\alpha_{31} & 0 & 1 & & 0 \\
\vdots & \vdots & & \ddots & \vdots \\
\alpha_{n 1} & 0 & \cdots & \cdots & 1
\end{array}\right]\left[\begin{array}{cccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1 n}^{(1)} \\
0 & A_{22}^{(2)} & \cdots & A_{2 n}^{(2)} \\
0 & A_{32}^{(2)} & \cdots & A_{3 n}^{(2)} \\
\vdots & \vdots & & \vdots \\
0 & A_{n 2}^{(2)} & \cdots & A_{n n}^{(2)}
\end{array}\right]
$$

with

$$
\begin{aligned}
\alpha_{i 1} & =A_{i 1}^{(1)} / A_{11}^{(1)} & & i=2, \ldots, n \\
A_{i j}^{(2)} & =A_{i j}^{(1)}-\alpha_{i 1} A_{1 j}^{(1)} & & i, j=2, \ldots, n
\end{aligned}
$$

## Gaussian factorization ( $\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U}$ )

Procedure (continuation)

- Iteration $k$ :

$$
\left[\begin{array}{cccccc}
1 & 0 & \cdots & \cdots & \cdots & 0 \\
\alpha_{21} & \ddots & & & & 0 \\
\vdots & \ddots & 1 & & & \vdots \\
\vdots & & \vdots & 1 & & \vdots \\
\vdots & & \vdots & & \ddots & \vdots \\
\alpha_{n 1} & \cdots & \alpha_{n k} & 0 & \cdots & 1
\end{array}\right]\left[\begin{array}{cccccc}
A_{11}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & \cdots & A_{1 n}^{(1)} \\
0 & A_{22}^{(2)} & & & & A_{2 n}^{(2)} \\
\vdots & & \ddots & & & \vdots \\
0 & \cdots & 0 & A_{k+1, k+1}^{(k)} & \cdots & A_{k+1, n}^{(k)} \\
\vdots & & \vdots & \vdots & & \vdots \\
0 & \cdots & 0 & A_{n, k+1}^{(k)} & \cdots & A_{n n}^{(k)}
\end{array}\right]
$$

- Iteration $n-1$ :
$\left[\begin{array}{ccccc}1 & 0 & \cdots & \cdots & 0 \\ \alpha_{21} & 1 & & & 0 \\ \vdots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & 1 & \vdots \\ \alpha_{n 1} & \cdots & \cdots & \alpha_{n(n-1)} & 1\end{array}\right]\left[\begin{array}{ccccc}A_{11}^{(1)} & A_{12}^{(1)} & \cdots & \cdots & A_{1 n}^{(1)} \\ 0 & A_{22}^{(2)} & & & A_{2 n}^{(2)} \\ \vdots & & \ddots & & \vdots \\ 0 & & & \ddots & \vdots \\ 0 & & & & A_{n n}^{(n)}\end{array}\right]$


## Gaussian factorization $(\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U})[$ [3/4]

## Gaussian factorization

Data: A
Initialization: $\tilde{\mathbf{L}}=\mathbf{I}$ and $\mathbf{U}=\mathbf{A}$
for $k=1, \ldots, n-1$ do
for $i=k+1, \ldots, n$ do
$\tilde{L}_{i k} \leftarrow U_{i k} / U_{k k} \quad$ Si $U_{k k} \neq 0$ !
$U_{i j} \leftarrow U_{i j}-\tilde{L}_{i k} U_{k j} \quad(j=k+1 \ldots n)$
$U_{i k} \leftarrow 0$
end
end

## Gaussian factorization (Rewriting)

Data: A
for $k=1, \ldots, n-1$ do
for $i=k+1, \ldots, n$ do
$A_{i k} \leftarrow A_{i k} / A_{k k} \quad$ Si $A_{k k} \neq 0$ !
$A_{i j} \leftarrow A_{i j}-A_{i k} A_{k j} \quad(j=k+1 \ldots n)$
end
end

## Gaussian factorization $(\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U})$ [4/4]

Theorem - Unicity of the Gaussian factorization ( $\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U}$ )
The Gaussian factorization, if it exists, is unique.
Theorem - Existence of the Gaussian factorization ( $\mathbf{A}=\tilde{\mathbf{L}} \mathbf{U}$ )
(not necessary)
Every matrix that is symmetric positive definite (SPD) is factorizable.

Theorem - Existence of the Gaussian factorization after permutation (PA = $\mathbf{L} \mathbf{U}$ )
For every invertible matrix, there exists a sequence of elementary permutations such that the permuted matrix admits a Gaussian factorization.

## Permutation matrix

- An elementary permutation matrix $\mathbf{P}^{\left(i_{1}, i_{2}\right)}$ is a matrix which the application on a matrix A permutes the lines $i_{1}$ and $i_{2}$ :

$$
\left[\begin{array}{llll}
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1
\end{array}\right]\left[\begin{array}{llll}
A_{11} & A_{12} & A_{13} & A_{14} \\
A_{21} & A_{22} & A_{23} & A_{24} \\
A_{31} & A_{32} & A_{33} & A_{34} \\
A_{41} & A_{42} & A_{43} & A_{44}
\end{array}\right]=\left[\begin{array}{llll}
A_{\mathbf{3 1}} & A_{\mathbf{3 2}} & A_{\mathbf{3 3}} & A_{\mathbf{3 4}} \\
A_{21} & A_{22} & A_{23} & A_{24} \\
A_{\mathbf{1 1}} & A_{\mathbf{1 2}} & A_{13} & A_{\mathbf{1 4}} \\
A_{41} & A_{42} & A_{43} & A_{44}
\end{array}\right]
$$

- The permutation matrix $\mathbf{P}^{\left(i_{1}, i_{2}\right)}$ is obtained by swapping the lines $i_{1}$ and $i_{2}$ and the columns $i_{1}$ and $i_{2}$ from the identity matrix.


## Solution after factorization

## Gaussian factorization (Rewriting)

Data: A
for $k=1, \ldots, n-1$ do for $i=k+1, \ldots, n$ do

$$
A_{i k} \leftarrow A_{i k} / A_{k k} \quad \text { Si } A_{k k} \neq 0!
$$

$A_{i j} \leftarrow A_{i j}-A_{i k} A_{k j} \quad(j=k+1 \ldots n)$
end
end

## Cost of the entire solution procedure

- Gaussian or Gauss-Jordan factorization: $2 / 3 n^{3}$ operations
- Crout or Cholesky factorization: $1 / 3 n^{3}$ operations
- Forward and back substitution: $2 n^{2}$ operations
- Additional operations with pivoting strategies


## Parallelization

- Parallelization not easy for problems with dense matrices
- Strategies are possible with blocks approaches.
- Strategies are possible with sparse matrices.


## Summary

- Triangular systems
- Simple computational procedures, but not suited for parallel computing!
- Computational cost:
- By points: $n^{2}$ scalar operations
- By blocks: $N$ small systems to solve and $\mathcal{O}\left(N^{2}\right)$ matrix-vector products
- Parall. comp.: by-block strategy (dense mat.) or ad-hoc strategy (sparse mat.)
- General systems
- Approaches:
- Gaussian elimination $\Rightarrow$ Gives the solution for a given vector b
- LU factorization + Two triangular systems to solve $\Rightarrow$ Factorization computed once and used for any vector b
- For any invertible matrix $\mathbf{A}, \exists$ permutation matrix $\mathbf{P}$ such that $\mathbf{P A}=\tilde{\mathbf{L}} \mathbf{U}$
- Different factorizations: $\tilde{\mathbf{L}} \mathbf{U}, \tilde{\mathbf{L}} \mathbf{D} \tilde{\mathbf{U}}$ (Gen), $\tilde{\mathbf{L}} \mathbf{D} \tilde{\mathbf{L}}^{\top}(\mathrm{Sym}), \mathbf{L L}^{\top}$ (SDP)
- Computational cost: $\mathcal{O}\left(n^{3}\right)$ operations
- Parall. comp.: by-block strategy (dense mat.) or ad-hoc strategy (sparse mat.)


## Resources

- Méthodes Numériques: Algorithmes, analyse et applications A. Quarteroni, R. Sacco, F. Saleri (2007), Springer
- Calcul scientifique parallèle
F. Magoulès et F.-X. Roux (2017), Dunod
- Calcul scientifique parallèle
P. Ciarlet et E. Jamelot, polycopié de cours

