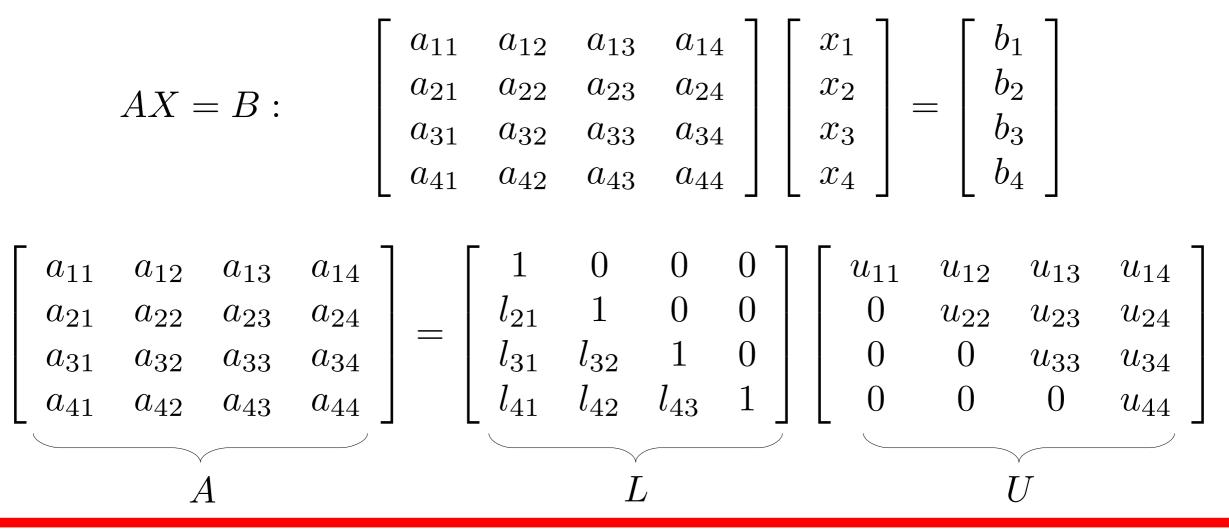# Computational Physics

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Lecture-17

Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root
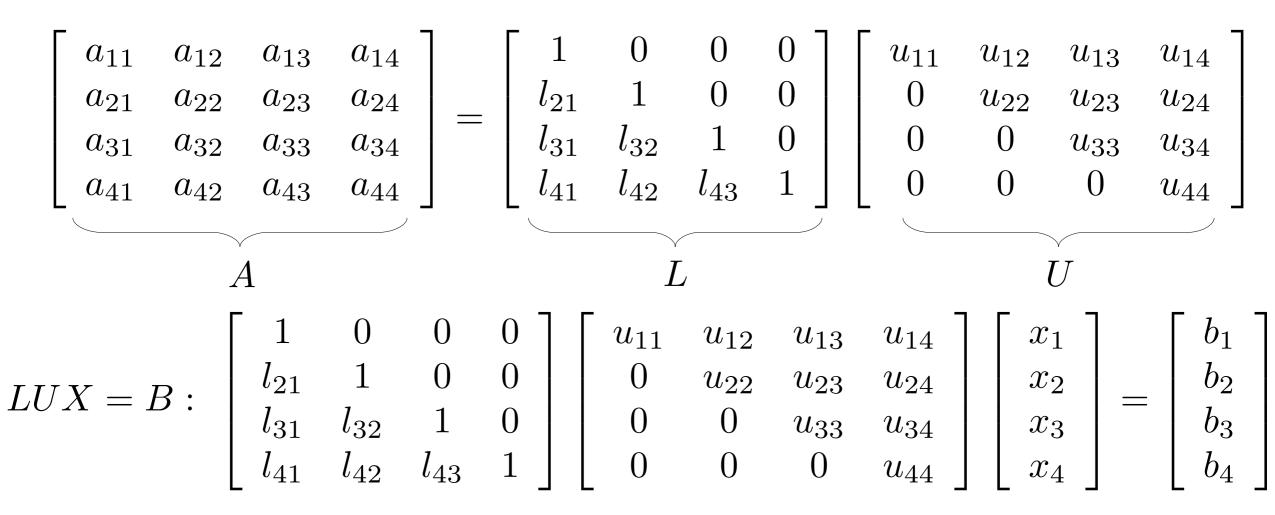- Classical Scattering
- Solving Linear Systems

Solving Linear Systems

- **LU-decomposition**

$$AX = B : \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix}}_{U}$$

Solving Linear Systems

- **LU-decomposition**

$$\left[\begin{array}{cccc} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{array}\right] = \left[\begin{array}{cccc} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{array}\right] \left[\begin{array}{cccc} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{array}\right]$$

$$\underbrace{}_{A} \qquad \underbrace{}_{L} \qquad \underbrace{}_{U}$$

$$LUX = B : \left[\begin{array}{cccc} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{array}\right] \left[\begin{array}{cccc} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \end{array}\right] = \left[\begin{array}{c} b_1 \\ b_2 \\ b_3 \\ b_4 \end{array}\right]$$

Solving Linear Systems

- **LU-decomposition**

$$LUX = B : \begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\text{Let} \quad \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} : \quad UX = Y$$

Solving Linear Systems

- **LU-decomposition**

$$AX = LUX = B, \quad UX = Y \Rightarrow LY = B$$

$$LY = B: \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$
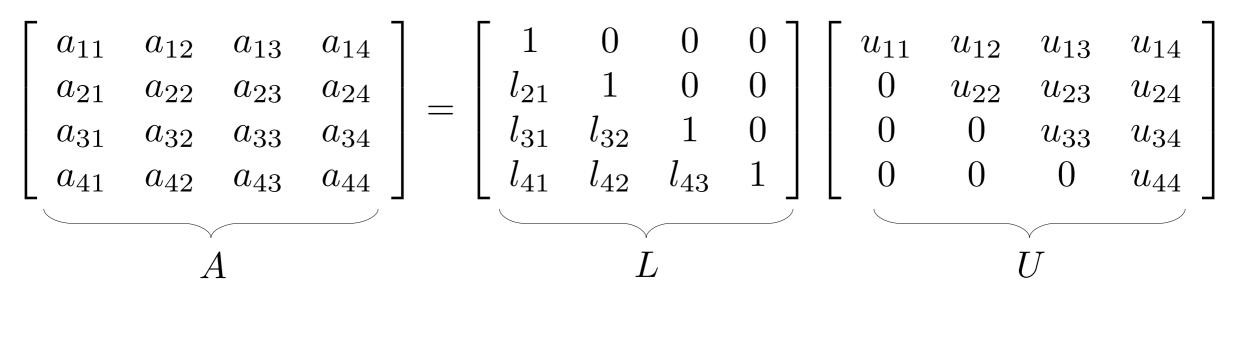
$$UX = Y: \quad \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

Solving Linear Systems

- **LU-decomposition**

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$y_1 = b_1$$

$$l_{21}y_1 + y_2 = b_2 \Rightarrow y_2 = b_2 - l_{21}y_1$$

$$\vdots$$

$$l_{i1}y_1 + l_{i2}y_2 + \cdots + y_i = b_i \Rightarrow \boxed{y_i = b_i - \sum_{j=1}^{i-1} l_{ij}y_j \quad i = 1, 2, \cdots, n}$$

$$\vdots$$

Solving Linear Systems

- **LU-decomposition**

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

$$u_{44}x_4 = y_4 \Rightarrow x_4 = \frac{1}{u_{44}}y_4$$

$$u_{33}x_3 + u_{34}x_4 = y_3 \Rightarrow x_3 = \frac{1}{u_{33}}(y_3 - u_{34}x_4)$$

$$i = n, n-1, \cdots, 1$$

$$\vdots$$

$$u_{i,i}x_i + u_{i,i+1}x_{i+1} + u_{i,i+2}x_{i+2} + \cdots + u_{i,n}x_n = y_i \Rightarrow x_i = \frac{1}{u_{ii}}\left(y_i - \sum_{j=i+1}^{n} u_{ij}x_j\right)$$

$$\vdots$$

Solving Linear Systems

- **LU-decomposition**

$$
\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix}}_{U}
$$

$$
L = ? \quad , \quad U = ?
$$

Solving Linear Systems

- LU-decomposition

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix}$$

$$\begin{cases} u_{11} = a_{11} \\ u_{12} = a_{12} \\ u_{13} = a_{13} \\ u_{14} = a_{14} \end{cases}$$

Solving Linear Systems

- **LU-decomposition**

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} \\
a_{21} & a_{22} & a_{23} & a_{24} \\
a_{31} & a_{32} & a_{33} & a_{34} \\
a_{41} & a_{42} & a_{43} & a_{44}
\end{bmatrix}
=
\begin{bmatrix}
1 & 0 & 0 & 0 \\
l_{21} & 1 & 0 & 0 \\
l_{31} & l_{32} & 1 & 0 \\
l_{41} & l_{42} & l_{43} & 1
\end{bmatrix}
\begin{bmatrix}
u_{11} & u_{12} & u_{13} & u_{14} \\
0 & u_{22} & u_{23} & u_{24} \\
0 & 0 & u_{33} & u_{34} \\
0 & 0 & 0 & u_{44}
\end{bmatrix}
$$

$$
\begin{cases}
l_{21}u_{11} = a_{21} \\
l_{21}u_{12} + u_{22} = a_{22} \\
l_{21}u_{13} + u_{23} = a_{23} \\
l_{21}u_{14} + u_{24} = a_{24}
\end{cases}
\implies
\begin{cases}
l_{21} = a_{21}/u_{11} \\
u_{22} = a_{22} - l_{21}u_{12} \\
u_{23} = a_{23} - l_{21}u_{13} \\
u_{24} = a_{24} - l_{21}u_{14}
\end{cases}
$$

Solving Linear Systems

- **LU-decomposition**

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} \\
a_{21} & a_{22} & a_{23} & a_{24} \\
a_{31} & a_{32} & a_{33} & a_{34} \\
a_{41} & a_{42} & a_{43} & a_{44}
\end{bmatrix}
=
\begin{bmatrix}
1 & 0 & 0 & 0 \\
l_{21} & 1 & 0 & 0 \\
l_{31} & l_{32} & 1 & 0 \\
l_{41} & l_{42} & l_{43} & 1
\end{bmatrix}
\begin{bmatrix}
u_{11} & u_{12} & u_{13} & u_{14} \\
0 & u_{22} & u_{23} & u_{24} \\
0 & 0 & u_{33} & u_{34} \\
0 & 0 & 0 & u_{44}
\end{bmatrix}
$$

$$
\begin{cases}
l_{31}u_{11} = a_{31} \\
l_{31}u_{12} + l_{32}u_{22} = a_{32} \\
l_{31}u_{13} + l_{32}u_{23} + u_{33} = a_{33} \\
l_{31}u_{14} + l_{32}u_{24} + u_{34} = a_{34}
\end{cases}
\implies
\begin{cases}
l_{31} = a_{31}/u_{11} \\
l_{32} = (a_{32} - l_{31}u_{12})/u_{22} \\
u_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23} \\
u_{34} = a_{34} - l_{31}u_{14} - l_{32}u_{24}
\end{cases}
$$

Solving Linear Systems

- **LU-decomposition**

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} \\
a_{21} & a_{22} & a_{23} & a_{24} \\
a_{31} & a_{32} & a_{33} & a_{34} \\
a_{41} & a_{42} & a_{43} & a_{44}
\end{bmatrix}
=
\begin{bmatrix}
1 & 0 & 0 & 0 \\
l_{21} & 1 & 0 & 0 \\
l_{31} & l_{32} & 1 & 0 \\
l_{41} & l_{42} & l_{43} & 1
\end{bmatrix}
\begin{bmatrix}
u_{11} & u_{12} & u_{13} & u_{14} \\
0 & u_{22} & u_{23} & u_{24} \\
0 & 0 & u_{33} & u_{34} \\
0 & 0 & 0 & u_{44}
\end{bmatrix}
$$

$$
\begin{cases}
l_{41}u_{11} = a_{41} \\
l_{41}u_{12} + l_{42}u_{22} = a_{42} \\
l_{41}u_{13} + l_{42}u_{23} + l_{43}u_{33} = a_{43} \\
l_{41}u_{14} + l_{42}u_{24} + l_{43}u_{34} + u_{44} = a_{44}
\end{cases}
\Longrightarrow
\begin{cases}
l_{41} = a_{41}/u_{11} \\
l_{42} = (a_{42} - l_{41}u_{12})/u_{22} \\
l_{43} = (a_{43} - l_{41}u_{13} - l_{42}u_{23})/u_{33} \\
u_{44} = a_{44} - l_{41}u_{14} - l_{42}u_{24} - l_{43}u_{34}
\end{cases}
$$

Solving Linear Systems

- **LU-decomposition**

$$
\begin{bmatrix}
u_{11} & u_{12} & u_{13} & u_{14} \\
0 & u_{22} & u_{23} & u_{24} \\
0 & 0 & u_{33} & u_{34} \\
0 & 0 & 0 & u_{44}
\end{bmatrix}
$$

$$
u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}
$$

$$
i = 1, 2, \cdots, n
$$

$$
j = i, i+1, \cdots, n
$$

$u_{11} = a_{11}$

$u_{12} = a_{12}$

$u_{13} = a_{13}$

$u_{14} = a_{14}$

$u_{22} = a_{22} - l_{21} u_{12}$

$u_{23} = a_{23} - l_{21} u_{13}$

$u_{24} = a_{24} - l_{21} u_{14}$

$u_{33} = a_{33} - l_{31} u_{13} - l_{32} u_{23}$

$u_{34} = a_{34} - l_{31} u_{14} - l_{32} u_{24}$

$u_{44} = a_{44} - l_{41} u_{14} - l_{42} u_{24} - l_{43} u_{34}$

Solving Linear Systems

- **LU-decomposition**

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix}$$

$$l_{ij} = \frac{1}{u_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right)$$

$$j = 1, 2, \cdots, n-1$$

$$i = j+1, \cdots, n$$

$$l_{21} = a_{21}/u_{11}$$

$$l_{31} = a_{31}/u_{11}$$

$$l_{41} = a_{41}/u_{11}$$
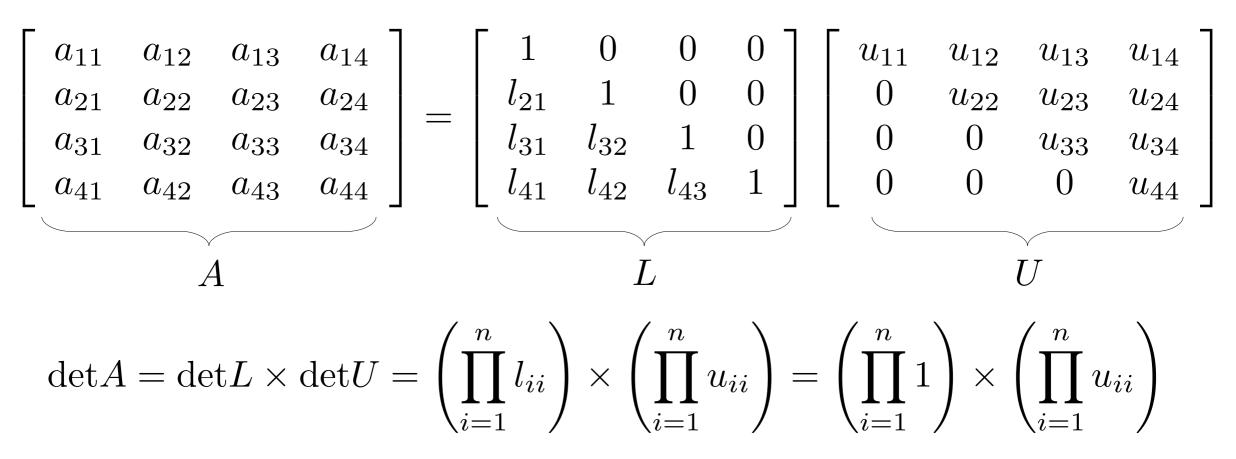
$$l_{32} = (a_{32} - l_{31} u_{12})/u_{22}$$

$$l_{42} = (a_{42} - l_{41} u_{12})/u_{22}$$

$$l_{43} = (a_{43} - l_{41} u_{13} - l_{42} u_{23})/u_{33}$$

Solving Linear Systems

- **Determinant**

$$
\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix}
$$

$$
\underbrace{}_{A} \qquad \underbrace{}_{L} \qquad \underbrace{}_{U}
$$

$$
\det A = \det L \times \det U = \left(\prod_{i=1}^{n} l_{ii} \right) \times \left(\prod_{i=1}^{n} u_{ii} \right) = \left(\prod_{i=1}^{n} 1 \right) \times \left(\prod_{i=1}^{n} u_{ii} \right)
$$

Solving Linear Systems

- **Determinant**

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix}$$

$$\underbrace{\hphantom{xxxxx}}_{A} \qquad \underbrace{\hphantom{xxxxx}}_{L} \qquad \underbrace{\hphantom{xxxxx}}_{U}$$

$$\det A = \det L \times \det U = \left(\prod_{i=1}^{n} u_{ii} \right)$$