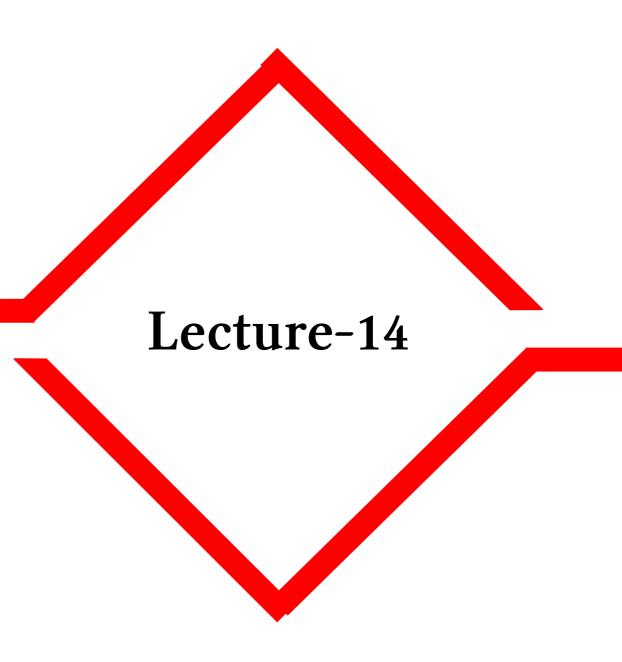
# Computational Physics

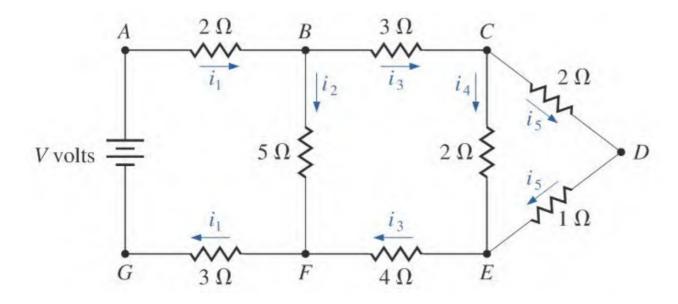
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- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root
- Classical Scattering
- Solving Linear Systems



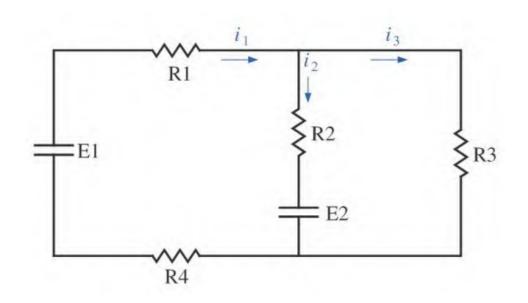
#### Kirchohoff's laws

$$\begin{cases} 5i_1 + 5i_2 = V \\ i_3 - i_4 - i_5 = 0 \\ 2i_4 - 3i_5 = 0 \\ i_1 - i_2 - i_3 = 0 \\ 5i_2 - 7i_3 - 2i_4 = 0 \end{cases}$$

$$Ri = v$$

$$\begin{bmatrix}
5 & 5 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & -1 \\
0 & 0 & 0 & 2 & -3 \\
1 & -1 & -1 & 0 & 0 \\
0 & 5 & -7 & -2 & 0
\end{bmatrix}$$

$$\begin{bmatrix} i_1 \\ i_2 \\ i_3 \\ i_4 \\ i_5 \end{bmatrix} = \begin{bmatrix} V \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$



#### Kirchohoff's laws

$$\begin{cases} (R_1 + R_4)i_1 + R_2i_2 = E_1 + E_2 \\ (R_1 + R_4)i_1 + R_3i_3 = E_1 \\ i_1 - i_2 - i_3 = 0 \end{cases}$$

$$Ri = v \begin{bmatrix} R_1 + R_4 & R_2 & 0 \\ R_1 + R_4 & 0 & R_3 \\ 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} i_1 \\ i_2 \\ i_3 \end{bmatrix} = \begin{bmatrix} E_1 + E_2 \\ E_1 \\ 0 \end{bmatrix}$$

#### • Lower Triangle

$$\begin{bmatrix} a_{11} & 0 & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ a_{31} & a_{32} & a_{33} & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\begin{cases} a_{11}x_1 = b_1 \\ a_{21}x_1 + a_{22}x_2 = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3 \\ a_{41}x_1 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 = b_4 \end{cases} x_1 = b_1/a_{11}$$

$$x_2 = (b_2 - a_{21}x_1)/a_{22}$$

$$x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

$$x_4 = (b_4 - a_{41}x_1 - a_{42}x_2 - a_{43}x_3)/a_{44}$$

#### Lower Triangle

$$\begin{bmatrix} a_{11} & 0 & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ a_{31} & a_{32} & a_{33} & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\begin{cases} x_1 = b_1/a_{11} \\ x_2 = (b_2 - a_{21}x_1)/a_{22} \\ x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33} \\ x_4 = (b_4 - a_{41}x_1 - a_{42}x_2 - a_{43}x_3)/a_{44} \end{cases}$$

$$x_{i} = \frac{1}{a_{ii}} \left( b_{i} - \sum_{j=1}^{i-1} a_{ij} x_{j} \right)$$

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

$$j < i$$

• Upper Triangle

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & 0 & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 = b_1 \\ a_{22}x_2 + a_{23}x_3 + a_{24}x_4 = b_2 \\ a_{33}x_3 + a_{34}x_4 = b_3 \\ a_{44}x_4 = b_4 \end{cases} \Longrightarrow \begin{cases} x_1 = (b_1 - a_{12}x_2 - a_{13}x_3 - a_{14}x_4)/a_{11} \\ x_2 = (b_2 - a_{23}x_3 - a_{24}x_4)/a_{22} \\ x_3 = (b_3 - a_{34}x_4)/a_{33} \\ x_4 = b_4/a_{44} \end{cases}$$

#### Upper Triangle

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & 0 & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\begin{cases} x_1 = (b_1 - a_{12}x_2 - a_{13}x_3 - a_{14}x_4)/a_{11} \\ x_2 = (b_2 - a_{23}x_3 - a_{24}x_4)/a_{22} \\ x_3 = (b_3 - a_{34}x_4)/a_{33} \\ x_4 = b_4/a_{44} \end{cases}$$

$$\begin{vmatrix} x_i = \frac{1}{a_{ii}} \left( b_i - \sum_{j=i+1}^n a_{ij} x_j \right) \\ i = n, n-1, \dots, 1 \\ j > i \end{vmatrix}$$

#### Gaussian Elimination

$$\begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 \\ 2.0 & -2.0 & 3.0 & -3.0 \\ 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -8.0 \\ -20.0 \\ -2.0 \\ 4.0 \end{bmatrix}$$

The basic idea of Gaussian elimination is to transform the original linear equation set to one that has an **upper-triangular** or **lower-triangular** coefficient matrix, but has the same solution. Here we want to transform the coefficient matrix into an **upper triangular** matrix.

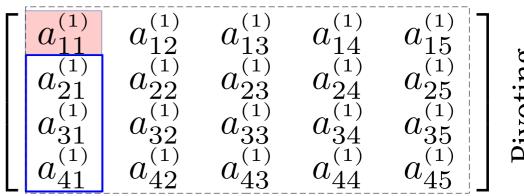
$$\begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 \\ 2.0 & -2.0 & 3.0 & -3.0 \\ 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 \end{bmatrix}_{4\times4} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -8.0 \\ -20.0 \\ -2.0 \\ 4.0 \end{bmatrix}$$

$$\begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 \\ 2.0 & -2.0 & 3.0 & -3.0 \\ 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 \end{bmatrix} -8.0$$

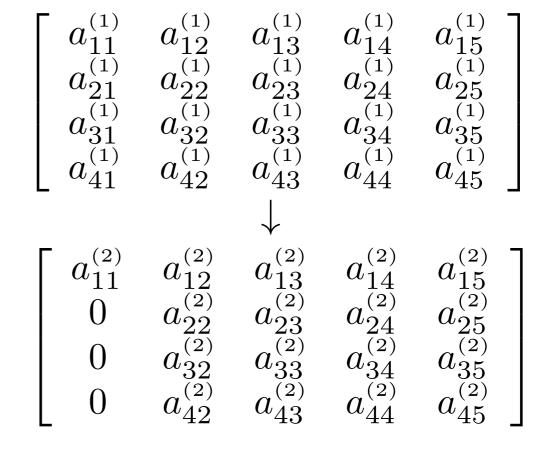
$$\begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 \\ 2.0 & -2.0 & 3.0 & -3.0 \\ 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 \end{bmatrix} \begin{bmatrix} -8.0 \\ -20.0 \\ 4.0 \end{bmatrix}$$

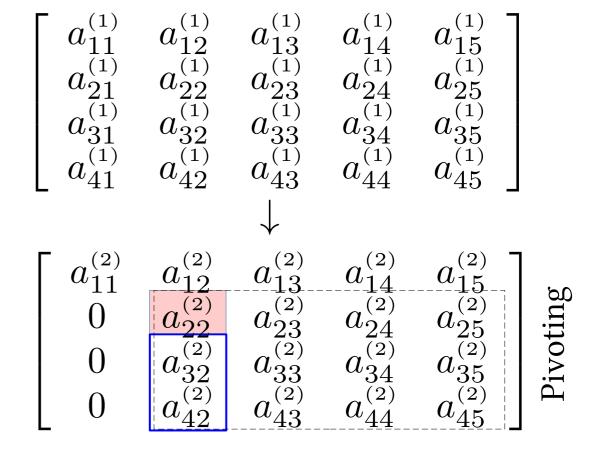
$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & a_{14}^{(1)} & a_{15}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} & a_{24}^{(1)} & a_{25}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} & a_{34}^{(1)} & a_{35}^{(1)} \\ a_{41}^{(1)} & a_{42}^{(1)} & a_{43}^{(1)} & a_{44}^{(1)} & a_{45}^{(1)} \end{bmatrix}$$

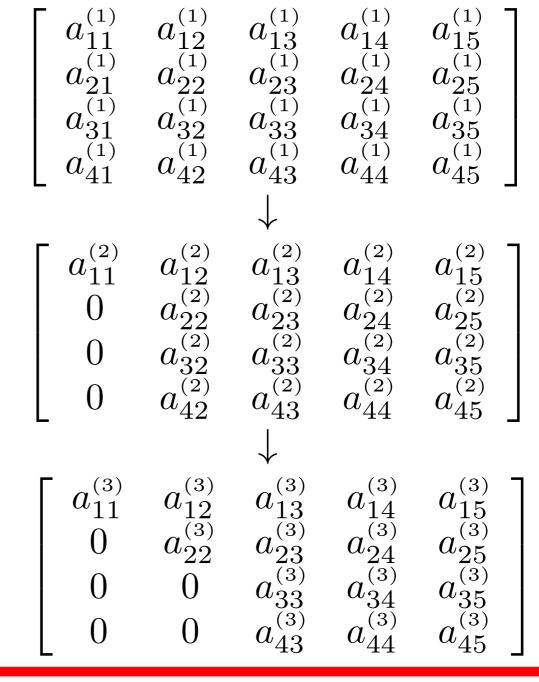
• Gaussian Elimination

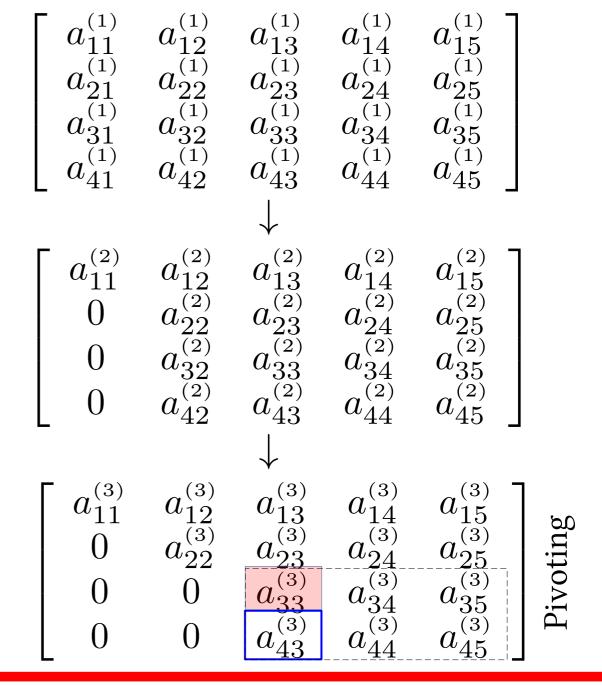


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$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & a_{14}^{(1)} & a_{15}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} & a_{24}^{(1)} & a_{25}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} & a_{34}^{(1)} & a_{44}^{(1)} & a_{42}^{(1)} \\ a_{41}^{(1)} & a_{42}^{(1)} & a_{43}^{(1)} & a_{44}^{(1)} & a_{45}^{(1)} \end{bmatrix} \\ \begin{bmatrix} a_{11}^{(2)} & a_{12}^{(2)} & a_{13}^{(2)} & a_{14}^{(2)} & a_{45}^{(2)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & a_{44}^{(2)} & a_{45}^{(2)} \end{bmatrix} \\ \begin{bmatrix} a_{11}^{(3)} & a_{12}^{(3)} & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & a_{42}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & a_{22}^{(3)} & a_{23}^{(3)} & a_{34}^{(3)} & a_{45}^{(3)} \end{bmatrix} \\ \begin{bmatrix} a_{11}^{(3)} & a_{12}^{(3)} & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & a_{22}^{(3)} & a_{23}^{(3)} & a_{24}^{(3)} & a_{25}^{(3)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{43}^{(3)} & a_{44}^{(3)} & a_{44}^{(3)} \end{bmatrix} \end{bmatrix}$$

$$\begin{bmatrix} a_{11}^{(4)} & a_{12}^{(4)} & a_{13}^{(4)} & a_{14}^{(4)} & a_{15}^{(4)} \\ 0 & a_{22}^{(4)} & a_{23}^{(4)} & a_{24}^{(4)} & a_{25}^{(4)} \\ 0 & 0 & a_{33}^{(4)} & a_{34}^{(4)} & a_{35}^{(4)} \\ 0 & 0 & 0 & a_{44}^{(4)} & a_{45}^{(4)} \end{bmatrix}$$

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & a_{14}^{(1)} & a_{15}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} & a_{24}^{(1)} & a_{25}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} & a_{34}^{(1)} & a_{35}^{(1)} \\ a_{41}^{(1)} & a_{42}^{(1)} & a_{43}^{(1)} & a_{44}^{(1)} & a_{45}^{(1)} \end{bmatrix} \\ & & \downarrow \\ \begin{bmatrix} a_{11}^{(2)} & a_{12}^{(2)} & a_{13}^{(2)} & a_{14}^{(2)} & a_{15}^{(2)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & a_{34}^{(2)} & a_{35}^{(2)} \\ 0 & a_{42}^{(2)} & a_{43}^{(2)} & a_{44}^{(2)} & a_{45}^{(2)} \end{bmatrix} \\ & & \downarrow \\ - \begin{bmatrix} a_{11}^{(3)} & a_{12}^{(3)} & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & a_{22}^{(3)} & a_{23}^{(3)} & a_{24}^{(3)} & a_{25}^{(3)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{43}^{(3)} & a_{44}^{(3)} & a_{45}^{(3)} \end{bmatrix}$$

$$\begin{bmatrix} a_{11}^{(4)} & a_{12}^{(4)} & a_{13}^{(4)} & a_{14}^{(4)} \\ 0 & a_{22}^{(4)} & a_{23}^{(4)} & a_{24}^{(4)} \\ 0 & 0 & a_{33}^{(4)} & a_{34}^{(4)} \\ 0 & 0 & 0 & a_{44}^{(4)} & a_{45}^{(4)} \end{bmatrix} \begin{bmatrix} a_{15}^{(4)} \\ a_{15}^{(4)} \\ a_{25}^{(4)} \\ a_{35}^{(4)} \\ a_{45}^{(4)} \end{bmatrix}$$

#### Gaussian Elimination

Pivot Step

$$\begin{bmatrix} 2.0 & -2.0 & 3.0 & -3.0 & -20.0 \\ \hline 1.0 & -1.0 & 2.0 & -1.0 & -8.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & -2.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 4.0 \end{bmatrix} \begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 & -8.0 \\ 2.0 & -2.0 & 3.0 & -3.0 & -20.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & -2.0 \\ \hline 2.0 & -2.0 & 3.0 & -3.0 & -20.0 \\ \hline 1.0 & 1.0 & 1.0 & 0.0 & -2.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 4.0 \end{bmatrix} \leftarrow \begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 & -8.0 \\ \hline 2.0 & -2.0 & 3.0 & -3.0 & -20.0 \\ \hline 1.0 & 1.0 & 1.0 & 0.0 & -2.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 4.0 \end{bmatrix}$$

#### Gaussian Elimination

Pivot Step

#### Gaussian Elimination

Pivot Step

$$\begin{bmatrix} 2.0 & -2.0 & 3.0 & -3.0 & -20.0 \\ 0.0 & 4.0 & -1.0 & 3.0 & 16.0 \\ 0.0 & 0.0 & 20.0 & 36.0 & 112.0 \\ 0.0 & 0.0 & 0.0 & -64.0 & -128.0 \end{bmatrix}$$

$$\begin{bmatrix} 2.0 & -2.0 & 3.0 & -3.0 \\ 0.0 & 4.0 & -1.0 & 3.0 \\ 0.0 & 0.0 & 20.0 & 36.0 \\ 0.0 & 0.0 & 0.0 & -64.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -20.0 \\ 16.0 \\ 112.0 \\ -128.0 \end{bmatrix}$$

$$x_1 = -7.0, \quad x_2 = 3.0, \quad x_1 = 2.0, \quad x_4 = 2.0$$