Computational Microelectronics
Lecture 12 Multi-Dimensional Device

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Box Method

A general form

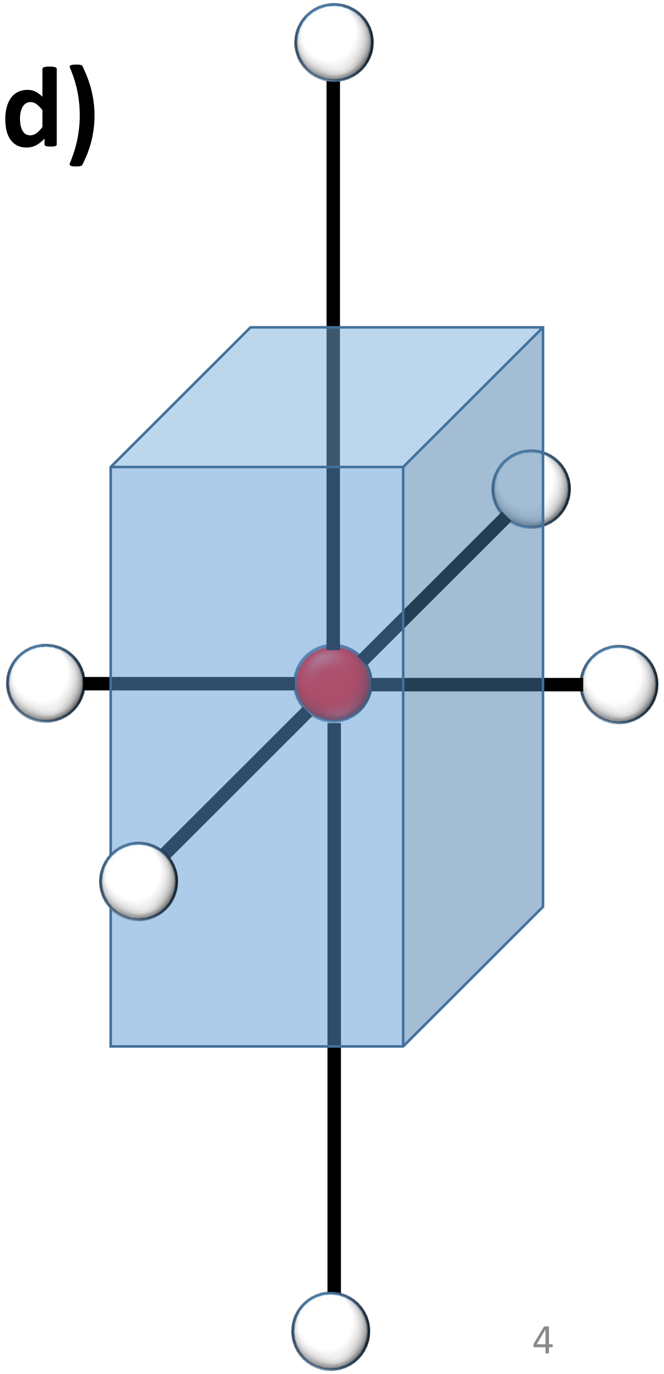
- Equations
  - Steady-state diffusion equation:
$$\nabla \cdot \mathbf{F} = 0$$
  - Poisson equation:
$$\nabla \cdot \mathbf{D} - \rho(\mathbf{r}) = 0$$
  - Steady-state continuity equation:
$$\nabla \cdot \mathbf{F} - G(\mathbf{r}) + R(\mathbf{r}) = 0$$
  - They can be written in a general form:
$$\nabla \cdot \mathbf{F} - s(\mathbf{r}) = 0$$
- Beyond the 1D structure?

Box method (Finite volume method)

- Consider a set of vertices. (Dots)
  - A box, Ω_i, surrounding a vertex node (Red dot, $\mathbf{r}_i$)
  - Its surface, A_i
  - A_i can be decomposed into multiple pieces, A_{ij}

$$A_i = \bigcup_j A_{ij}$$

  (Here, j runs over the neighboring vertex nodes.)
  - A face is perpendicular to an edge.



Key idea

- Integration over a box
  - Then,

$$\int_{\Omega_i} [\nabla \cdot \mathbf{F} - s(\mathbf{r})] d^3 r = 0$$

  - By applying the divergence theorem,

$$\int_{A_i} \mathbf{F} \cdot d\boldsymbol{a} - \int_{\Omega_i} s(\mathbf{r}) d^3 r = 0$$

  - Discretization of the volume integral

$$\int_{\Omega_i} s(\mathbf{r}) d^3 r \approx s(\mathbf{r}_i) \Omega_i$$

Discretization of surface integral

- Surface, A_i, can be decomposed into multiple pieces, A_{ij}'s.
  - Then,

$$\int_{A_i} \mathbf{F} \cdot d\boldsymbol{a} = \sum_j \int_{A_{ij}} \mathbf{F} \cdot d\boldsymbol{a}$$

  - From $\mathbf{F} \cdot d\boldsymbol{a}$, we need a component of $\mathbf{F}$, which is perpendicular to $d\boldsymbol{a}$. In other words, the edge-directional component is needed.

$$\int_{A_{ij}} \mathbf{F} \cdot d\boldsymbol{a} \approx F_{ji} A_{ij}$$

(Note that F_{ji} is aligned with $\hat{\mathbf{a}}_{ji}$, a unit vector starting at the i-th node.)

Summary

- For the i-th vertex node,
  - The original equation

$$\nabla \cdot \mathbf{F} - s(\mathbf{r}) = 0$$

  - Discretizated equation

$$\sum_j F_{ji} A_{ij} - s(\mathbf{r}_i)\Omega_i = 0$$

  - Remaining task? Finding out an appropriate form of F_{ji}

Laplace Equation

Laplace equation

- In our notation, the Laplace equation has the following terms.
  - The flux

$$\mathbf{F} = \nabla\phi$$

  - The source

$$s(\mathbf{r}) = 0$$

  - Therefore, we need to calculate $F_{ji} = \nabla\phi \cdot \hat{\mathbf{a}}_{ji}$, which is written as

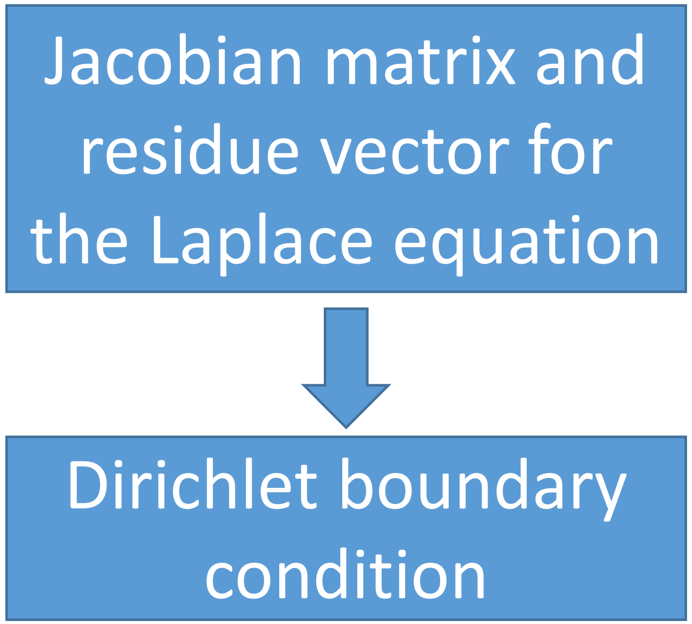
$$F_{ji} = \frac{\phi_j - \phi_i}{|\mathbf{r}_j - \mathbf{r}_i|}$$

  - Discretized Laplace equation reads

$$\sum_j \frac{\phi_j - \phi_i}{|\mathbf{r}_j - \mathbf{r}_i|} A_{ij} = 0$$

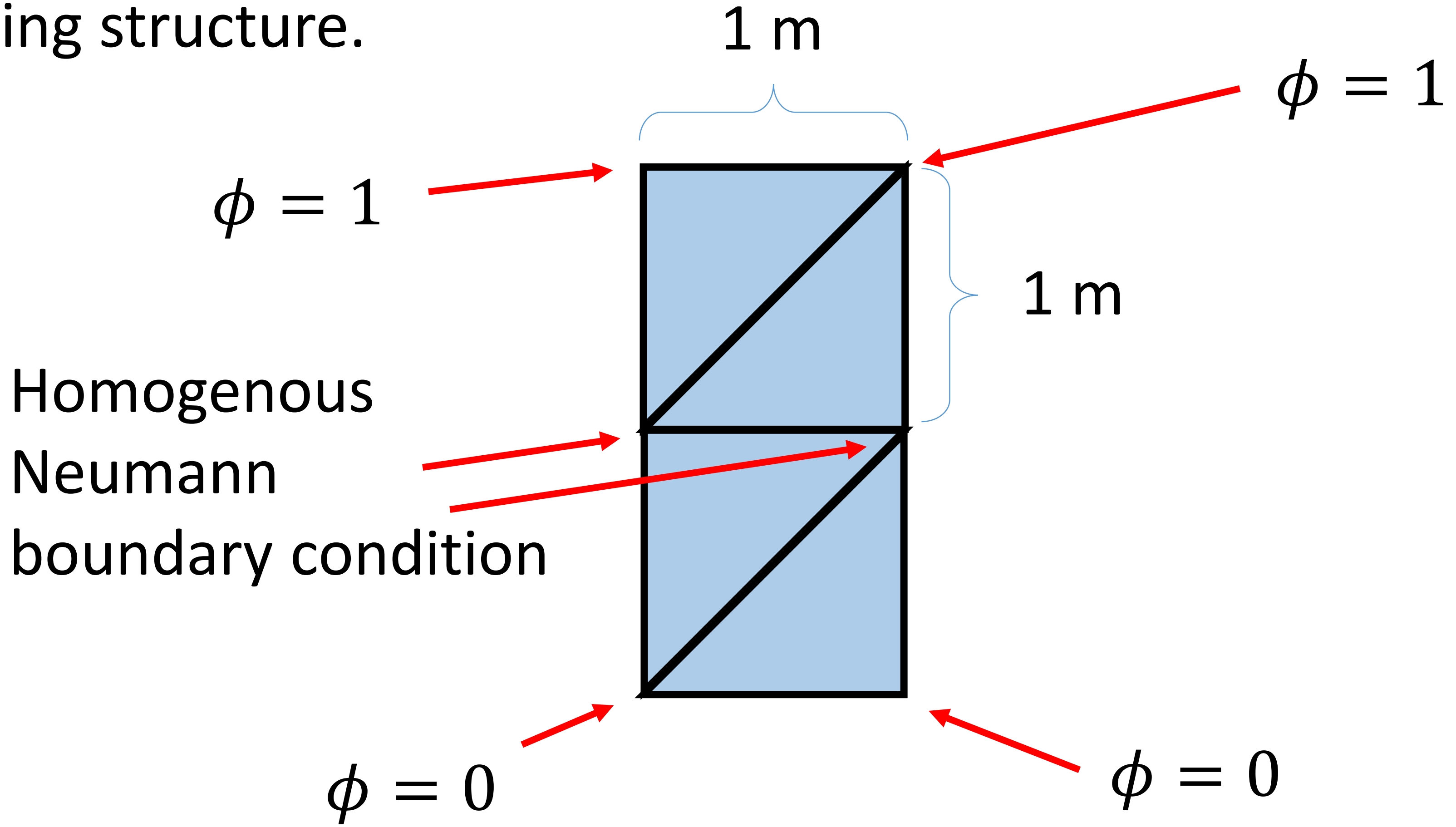
Boundary condition

- Dirichlet condition
  - At vertex nodes for the Dirichlet boundary condition, just impose it. (We don’t have to solve the Laplace equation at those nodes.)
  - It is better to consider the boundary condition, after considering the Laplace equation.
- Homogeneous Neumann condition
  - Nothing to do



An easy example

- 2D problem with 6 vertex nodes
  - Consider the following structure.



HW#11

- Due: AM08:00, October 16
- Problem#1
  - This problem is not for numerical results. Instead, explicitly write down the Jacobian matrix.
  - First, identify each node with a unique index. Then,
- Problem#2
  - Implement the above matrix

Thank you!