# Computational Microelectronics L11

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# Laplace equation

# Discretization of $\nabla^2\phi$ in 1D

- It is just $\frac{d^2\phi}{dx^2}$.
  - For uniform spacing of $\Delta x$, at $x = x_i$,

$$\left.\frac{d^2\phi}{dx^2}\right|_{x_i} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2}$$

  - Integration from $x_{i-0.5}$ to $x_{i+0.5}$

$$\left.\frac{d^2\phi}{dx^2}\right|_{x_i} \approx \frac{1}{x_{i+0.5} - x_{i-0.5}} \int_{x_{i-0.5}}^{x_{i+0.5}} \frac{d}{dx}\left[\frac{d\phi}{dx}\right] dx$$

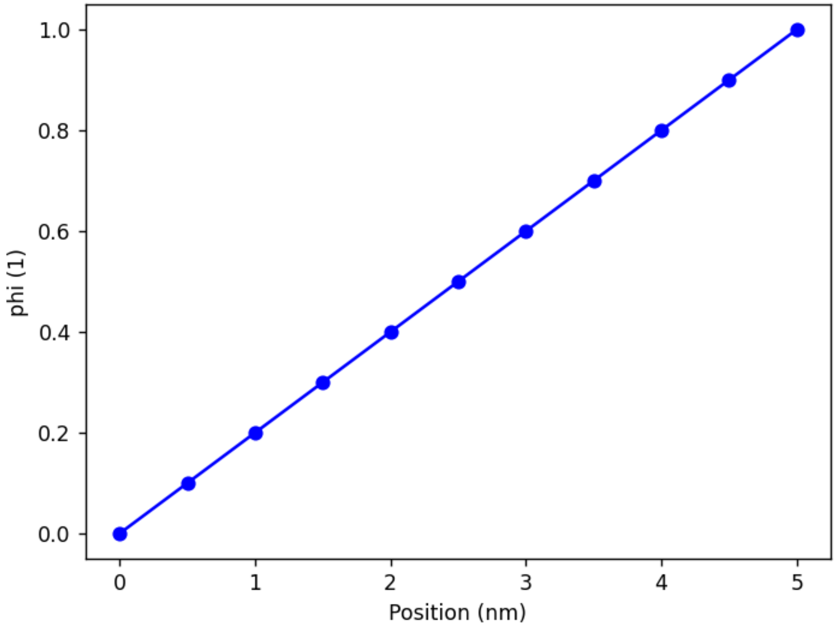
$$= \frac{1}{x_{i+0.5} - x_{i-0.5}} \left[\left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} - \left.\frac{d\phi}{dx}\right|_{x_{i-0.5}}\right]$$

# Laplace equation in 1D

- The Laplace equation, $\frac{d^2\phi}{dx^2} = 0$ (in its integrated form)
  - At $x = x_i$,

$$\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} = 0$$

- Of course, we need the boundary condition.
  - Specify $\phi$ at the leftmost and rightmost points.



# Divergence theorem

- Volume integral of $\nabla \cdot \mathbf{F}$ over a domain $\Omega$ ($\mathbf{F}$ is a vector field.)

$$\int_{\Omega} \nabla \cdot \mathbf{F} d^3 r$$

- Surface integral of the normal component of $\mathbf{F}$ over the surface of $\Omega$, $\partial\Omega$

$$\int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n}\, da$$

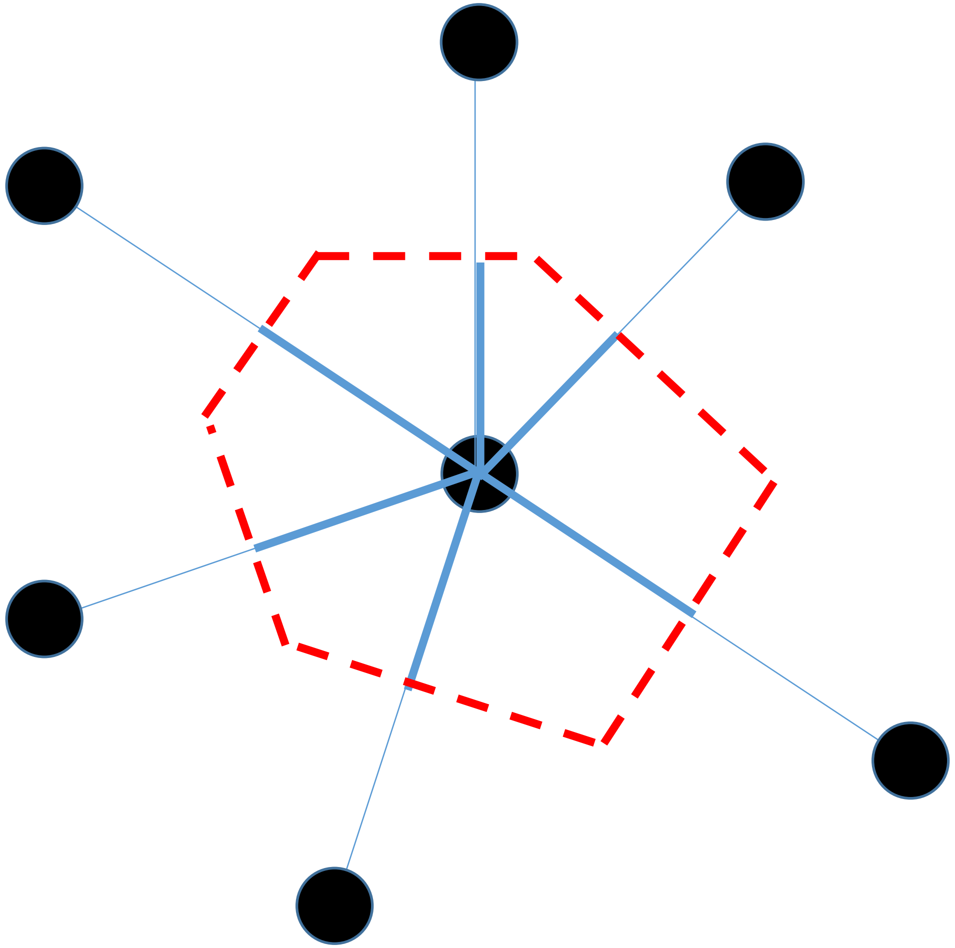
  – Here, $\mathbf{n}$ is the outer normal unit vector.

- Divergence theorem states that

$$\int_{\Omega} \nabla \cdot \mathbf{F} d^3 r = \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n}\, da$$

# Control volume, $\Omega_i$

- Set of points, whose nearest vertex is $\mathbf{r}_i$



# In 2D or 3D,

- Integration runs over $\Omega_i$.
  - Then, following the divergence theorem,

$$\int_{\Omega_i} \nabla^2 \phi \, d^3 r = \int_{\partial\Omega_i} \nabla\phi \cdot \mathbf{n} \, da$$

  - At $\mathbf{r} = \mathbf{r}_i$,

$$\int_{\partial\Omega_i} \nabla\phi \cdot \mathbf{n} \, da \approx \sum_j \nabla\phi \cdot \mathbf{n}_{ji} \, A_{ij}$$

Area

Neighboring vertices

Unit vector from $\mathbf{r}_i$ to $\mathbf{r}_j$

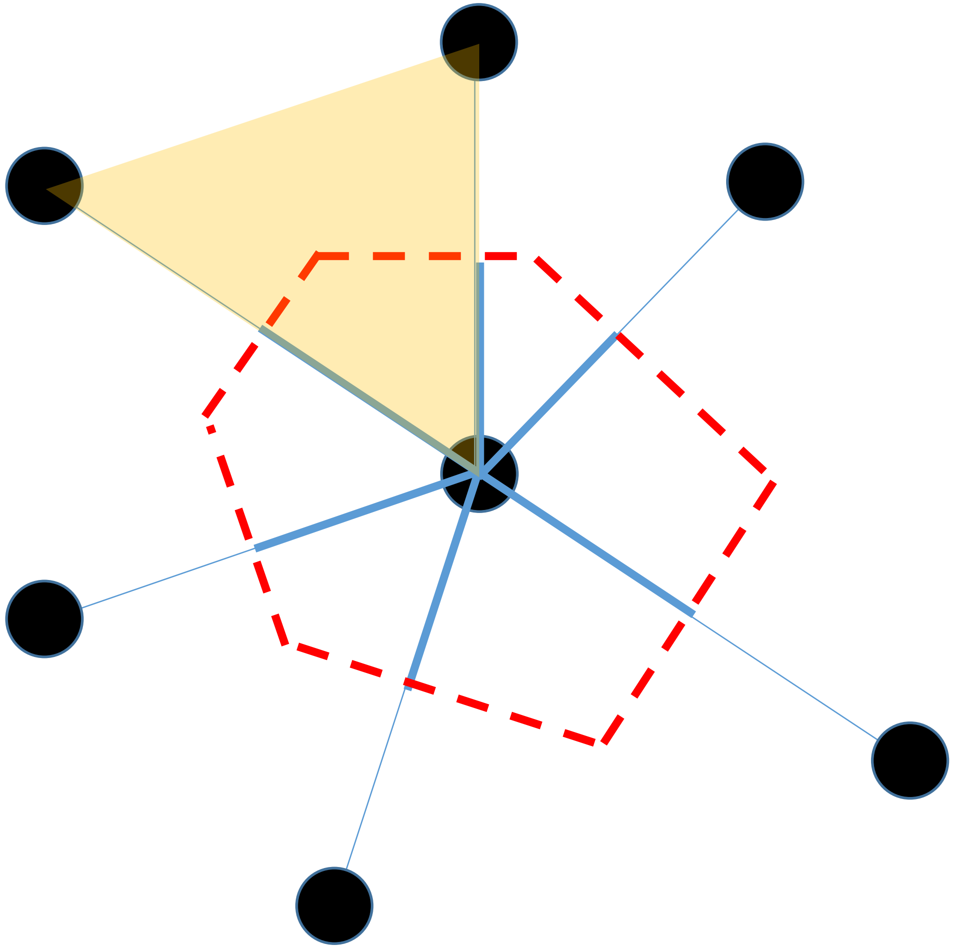
# Directional approximation

- We need to evaluate $\nabla\phi \cdot \mathbf{n}_{ji}$.
  - It is well approximated as $\frac{\phi_j - \phi_i}{|\mathbf{r}_j - \mathbf{r}_i|}$.
  - Therefore, the (integrated and discretized) Laplacian operator at $\mathbf{r} = \mathbf{r}_i$ reads

$$\int_{\Omega_i} \nabla^2 \phi \, d^3 r = \sum_j \frac{\phi_j - \phi_i}{|\mathbf{r}_j - \mathbf{r}_i|} A_{ij}$$

# How can we calculate $A_{ij}$?

- The distance, $|\mathbf{r}_j - \mathbf{r}_i|$, is easy to calculate.
  - Then, we must calculate $A_{ij}$.
  - In 2D structures, find
  the circumcenter of each triangle.



# Laplace equation in 2D or 3D

- The Laplace equation, $\nabla^2 \phi = 0$ (in its integrated form)
  - At $\mathbf{r} = \mathbf{r}_i$,

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

- Of course, we need the boundary condition.
  - Specify $\phi$ at the some contact points. (Dirichlet boundary condition)
  - For other boundary points, leave them without modification. (Neumann boundary condition)

# Homework#11

- Due: AM08:00, October 22
- Problem#1
  - Set two surface contacts in the BJT example. (Their positions are specified by you.) Solve the Laplace equation with a boundary condition, where one contact has 1 and the other 0.
  - Once after you get the solution, swap the contact values. Then, calculate the solution again.
  - Show the first solution, the second solution, and their sum (over the domain).

# Thank you for your attention!