Lecture13

Sung-Min Hong (smhong@gist.ac.kr)

Semiconductor Device Simulation Lab.
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology

GIST Lecture on October 24, 2018

Laplace equation in 2D

- Laplacian operator in 2D (yz-plane)
  - A second-order differentiation

$$\nabla^2 = \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

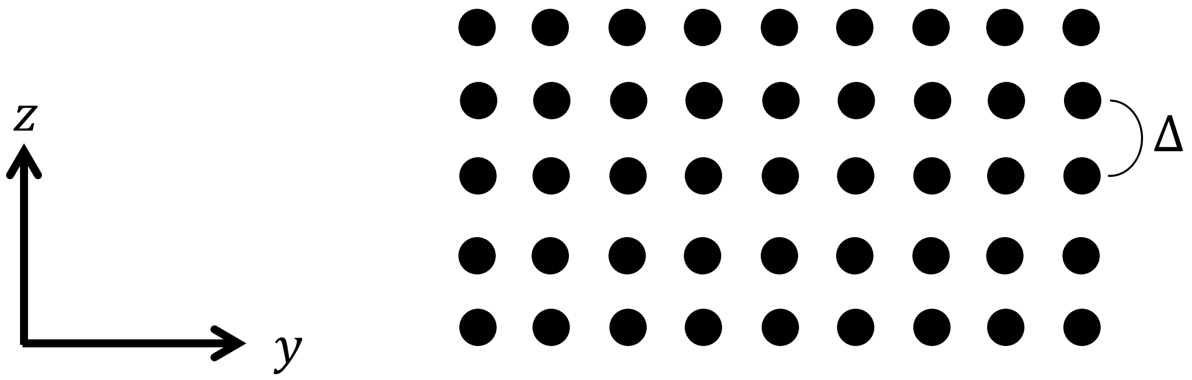
- Laplace equation in 2D (yz-plane)
  - For a function, $\psi(y,z)$, the Laplace equation reads

$$\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(y,z) = 0$$

  - Of course, we need boundary conditions.

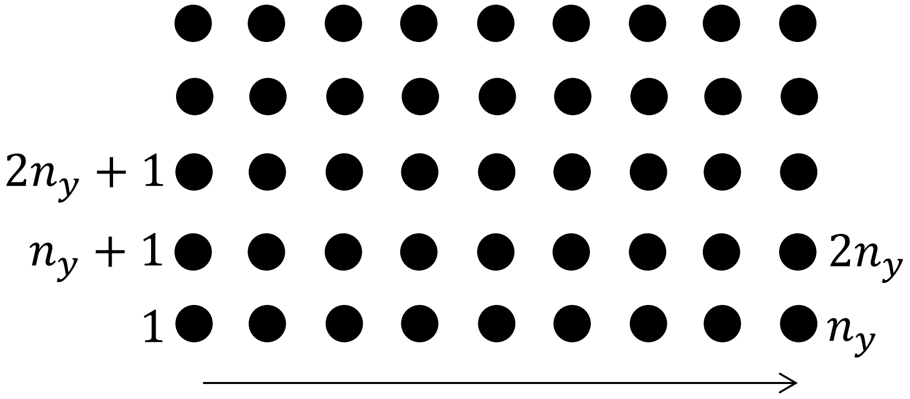
An example

- Consider a rectangle.
  - A common spacing of Δ is assumed.
  - Along the y-direction, n_y points are assigned.
  - Along the z-direction, n_z points are assigned.
  - Mixed boundary condition will be considered later.



Solution vector

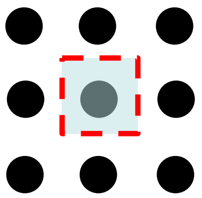
- The solution vector is a vector.
  - We must assign an integer to each node.
  - There can be many different ways to assign the index.
  - In this example, we change y more frequently.
  - The index is given by `(iz-1)*ny+iy`.



Discretization

- How to assign equations
  - Basically, the Laplace equation for a given node is integrated over its control volume.

$$\int_{Volume} \nabla^2 \psi d\mathbf{r} = \oint_{Surface} \nabla \psi \cdot d\mathbf{a}$$



  - The integrated form can be discretized as

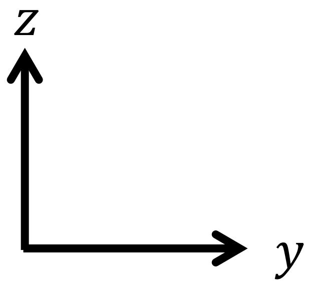
$$\psi_{i+1,j} + \psi_{i,j+1} - 4\psi_{i,j} + \psi_{i-1,j} + \psi_{i,j-1}$$

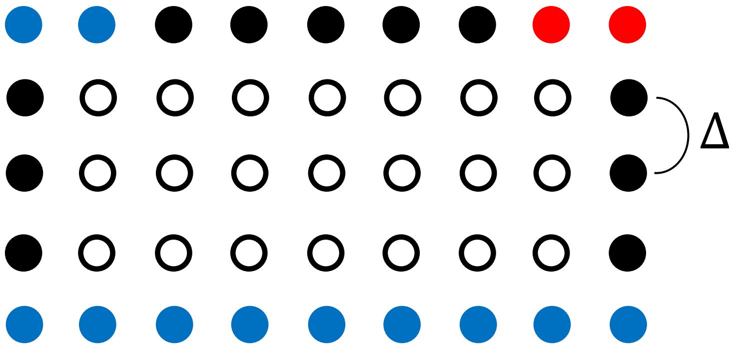
(Thickness along the x-direction is assumed to be unity)

  - Special care for the boundary nodes is required.

Our example

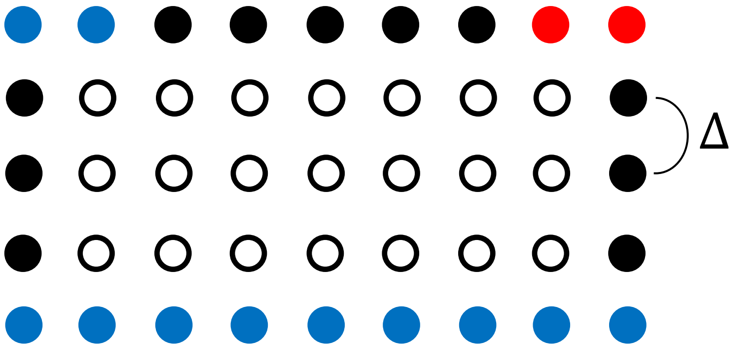
- Consider a toy problem.
  - Here, $n_y = 9$ and $n_z = 5$.
  - Empty circles: Bulk nodes. Their discretization is already studied.
  - Black circles: Homogeneous Neumann boundary condition
  - Blue circles: The function is zero.
  - Red circles: The function is unity.



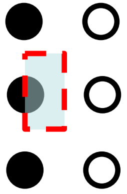


Boundary condition (1)

- Dirichlet boundary condition
  - It is not difficult to consider the Dirichlet boundary condition.
  - For a (ix, iy) node, we simply have $\psi_{ix,iy} = 0$ (for blue circles) or $\psi_{ix,iy} = 1$ (for red circles).



Boundary condition (2)



- Consider a node in the left boundary
  - Now, the integrated form of the Laplacian operator reads

$$\underbrace{\psi_{2,j} + 0.5\,\psi_{1,j+1} - 2\psi_{1,j} + 0.5\,\psi_{1,j-1}}_{\text{Jacobian-related}} + \underbrace{\Delta}_{\text{Residue-related}}$$

  - Similar expressions hold for other boundary nodes.
  - When you build the Jacobian matrix, you should be careful.
  - An edge-wise construction would be beneficial.

Homework#8

- Due: AM08:00, October 31
- Problem#1 (Counted as two problems)
  - Now, you have two tools: the nonlinear Poisson solver and the Schrödinger-Poisson solver.
  - Calculate the integrated electron density as a function of the gate voltage (from 0 V to 1 V).
  - Compare the results from the two tools.
  - Also compare the electron densities (cm^{-3}) calculated by two tools.
  - In your report, instead of just showing your results, add some "discussion" pragraphs.

Homework#9

- Due: AM08:00, November 5
- Problem#1
  - Solve our toy problem. (Laplace equation in the 2D space)
  - Consider four cases:
  - 1) The red circles are located in the original position.
  - 2) The red circles are located in the top/left position.
  - 3) The red circles are located in the bottom position.
  - 4) At all three positions above, the function is unity.
  - Draw 3D graphs for each of them.