
Lecture13

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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)

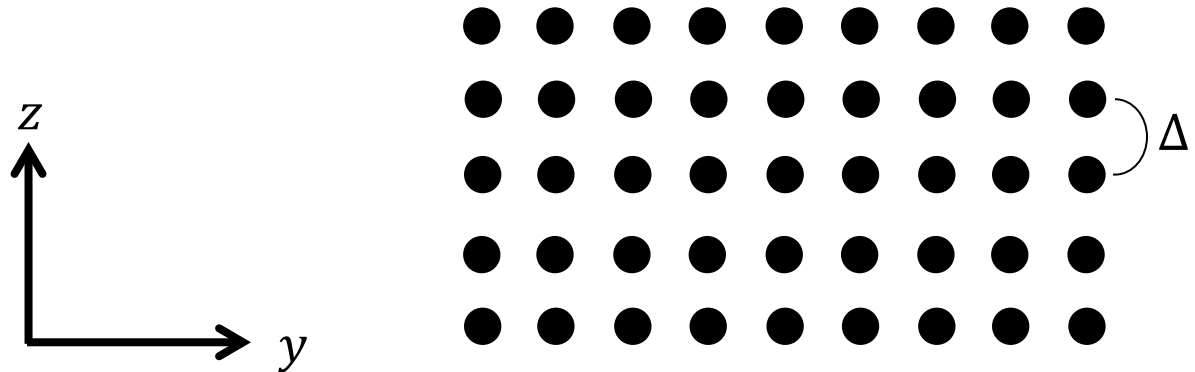
- For a function, $\psi(y, z)$, the Laplace equation reads

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

- Of course, we need boundary conditions.

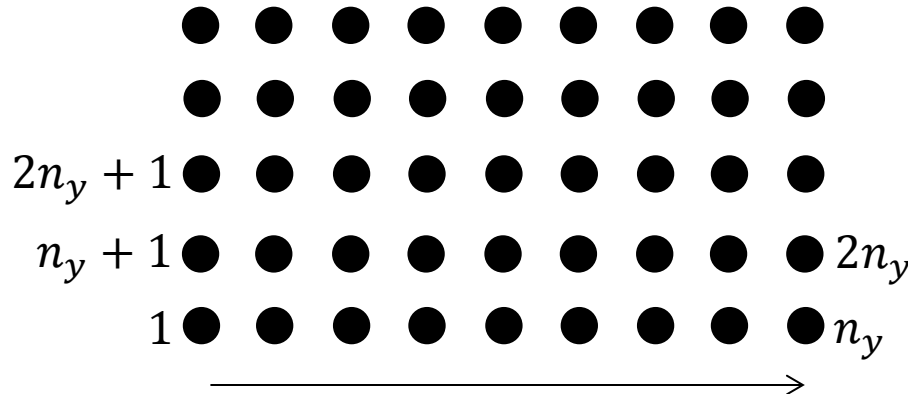
An example

- 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

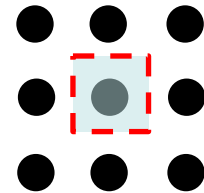
- The solution vector is a vector.
 - We must assign an integer to each node.
 - There can be many different ways to assign the index.
 - In this example, we change y more frequently.
 - The index is given by $(i_z - 1) * n_y + i_y$.



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

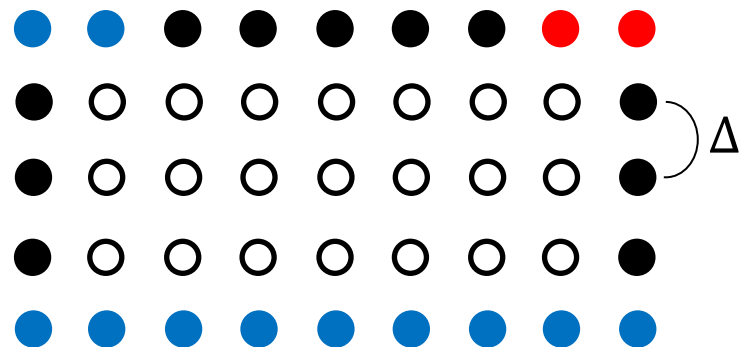
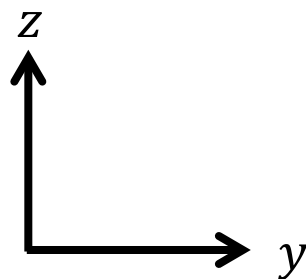
$$\psi_{i+1,j} + \psi_{i,j+1} - 4\psi_{i,j} + \psi_{i-1,j} + \psi_{i,j-1}$$

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

- Special care for the boundary nodes is required.

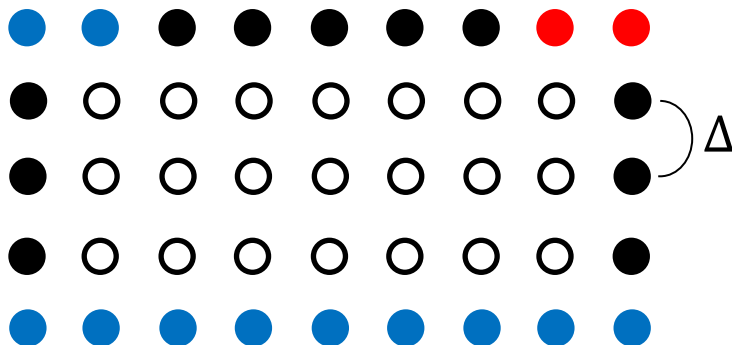
Our example

- 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).

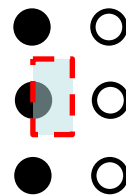


Boundary condition (2)

- Consider a node in the left boundary
 - Now, the integrated form of the Laplacian operator reads
$$\psi_{2,j} + 0.5 \psi_{1,j+1} - 2\psi_{1,j} + 0.5 \psi_{1,j-1} + 0$$

Jacobian-related

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” paragraphs.

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.