Lecture3

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Laplace equation

- Laplacian operator
  - A second-order differentiation

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

- Laplace equation
  - For a function, $\phi(\mathbf{r})$, the Laplace equation reads

$$\nabla^2 \phi(\mathbf{r}) = 0$$

  - Of course, we need boundary conditions.
- Its application?
  - In this course, it is closely related to the Poisson equation.

Analytic solution

- Consider the 1D structure, $[0, a]$.
  - The boundary conditions for $\phi(x)$ are given by $\phi(0) = 0$ and $\phi(a) = 1$.
- It is easy to solve it.
  - In the 1D structure, $\frac{d^2}{dx^2}\phi = 0$.
  - The solution has the form of $\phi(x) = C_1 x + C_0$.
  - Using the boundary conditions, it is found that $\phi(x) = \frac{x}{a}$.

Solution vector

- Let us construct a matrix equation corresponding to the Laplace equation.
  - We assign N points. They are uniformly distributed. For the i-th point, it has the coordinate of

$$x_i = \frac{i-1}{N-1}a$$

  - The solution function, $\phi(x)$, can be approximated by

$$[\phi(x_1) \quad \phi(x_2) \quad \cdots \quad \phi(x_{N-1}) \quad \phi(x_N)]^T$$

  - Therefore, N equations are needed to determine the solution vector.
  - Remember that the Laplacian operator is involved.

Discretization

- How to assign N equations
  - For $2 \leq i \leq N-1$, the discretized Laplacian operator is used.

$$\left.\frac{d^2\phi}{dx^2}\right|_{x=x_i} \approx \frac{\phi(x_{i+1}) - 2\phi(x_i) + \phi(x_{i-1})}{\Delta x^2} = 0$$

  - The Laplace equation at $x = x_i$ can be written as

$$\frac{1}{(\Delta x)^2}\begin{bmatrix} 0 & \cdots & 1 & -2 & 1 & \cdots & 0 \end{bmatrix}\begin{bmatrix} \phi(x_1) \\ \vdots \\ \phi(x_{i-1}) \\ \phi(x_i) \\ \phi(x_{i+1}) \\ \vdots \\ \phi(x_N) \end{bmatrix} = [0]$$

Boundary condition

- How to assign N equations (continued)
  - For $i = 1$ or $i = N$, the boundary condition is applied.
  - For example, for $i = N$, the boundary condition can be written in a matrix form:

$$[0 \quad \cdots \quad 0 \quad 0 \quad 0 \quad \cdots \quad 1] \begin{bmatrix} \phi(x_1) \\ \vdots \\ \phi(x_{i-1}) \\ \phi(x_i) \\ \phi(x_{i+1}) \\ \vdots \\ \phi(x_N) \end{bmatrix} = [1]$$

$N = 5$ example

- Let us collect the previous results explicitly.
  - It is simply given by

$$Ax = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \phi(x_3) \\ \phi(x_4) \\ \phi(x_5) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = b$$

  - How can we solve it numerically?

MATLAB example

- Step-by-step procedure
  - First, set the matrix, A.

```
A = zeros(5,5);
A(1,1) = 1.0;
A(2,1) = 1.0; A(2,2) = -2.0; A(2,3) = 1.0;
A(3,2) = 1.0; A(3,3) = -2.0; A(3,4) = 1.0;
A(4,3) = 1.0; A(4,4) = -2.0; A(4,5) = 1.0;
A(5,5) = 1.0;
```

  - Next , set the vector, b.

```
b = zeros(5,1); b(5,1) = 1.0;
```

  - Finally, get the solution vector, x.

```
x = A \ b
```

Generalized Poisson equation?

- Laplace equation

$$\nabla^2 \phi(\mathbf{r}) = 0$$

- Poisson equation

$$\nabla^2 \phi(\mathbf{r}) = \rho(\mathbf{r})$$

  – Here, $\rho(\mathbf{r})$ is the source function.
  – Therfore, the source-free Poisson equation is the Laplace equation.

- Then, why do we consider the "generalized" Poisson equations?
  – What is the exact meaning of the generalization?

Derivation

- One of the four Maxwell equations

$$\nabla \cdot \mathbf{D} = \rho(\mathbf{r})$$

  $\mathbf{D}(\mathbf{r})$: Displacement vector, which is given by $\epsilon(\mathbf{r})\mathbf{E}(\mathbf{r})$

  $\mathbf{E}(\mathbf{r})$: Electric field

  $\epsilon(\mathbf{r})$: Permittivity (assumed as a scalar)

  $\rho(\mathbf{r})$: Net charge density

- Under the electrostatic approximation, $\mathbf{E}(\mathbf{r}) = -\nabla\phi(\mathbf{r})$.
  - Using the above expression, it is found that

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi(\mathbf{r})] = -\rho(\mathbf{r})$$

  - The above equation is (incorrectly) called as the “Poisson equation.”

Source-free case

- Once again, the "source-free" Poisson equation is the Laplace equation.
  - Since we are (incorrectly) calling the $\nabla \cdot \mathbf{D} = \rho(\mathbf{r})$ as the Poisson equation, the source-free case (no net charge, $\rho(\mathbf{r}) = 0$) is not reduced to the Laplace equation.
  - Instead, (under the electrostatic approximation)

$$\nabla \cdot [\epsilon(\mathbf{r}) \nabla \phi(\mathbf{r})] = 0$$

  - In the 1D strcture,

$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = 0$$

Comparison

- Laplace equation

$$\frac{d}{dx}\left[\frac{d}{dx}\phi(x)\right] = 0$$

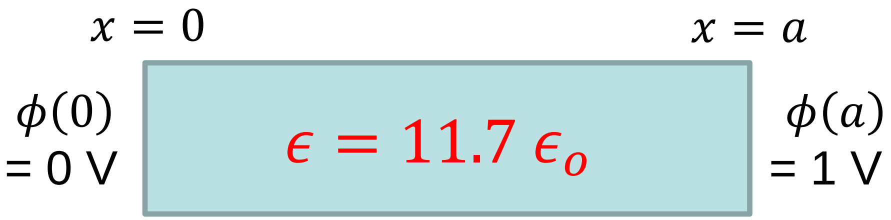
- (Generalized) Poisson equation with the source-free condition

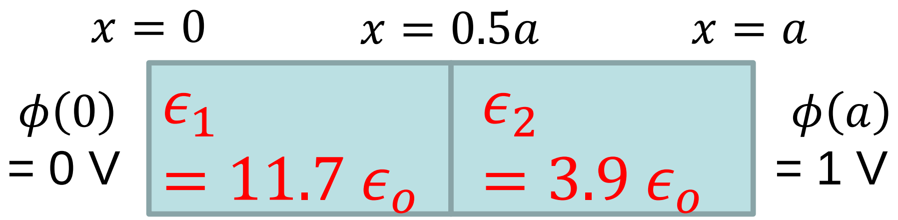
$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = 0$$

  - They look quite similar. However, they are not.

Two capacitors

- Capacitor made of a single dielectric layer
  - Its thickness is 5 nm. Its relative permittivity is 11.7.
- Capacitor made of two dielectric layers
  - Each of them is 2.5 nm thick. Their relative permittivity is 11.7 and 3.9, respectively.





$$\phi(x) = \frac{x}{a}$$

$$\phi(x) = \frac{x}{2a} \qquad \phi(x) = \frac{3x}{2a} - \frac{1}{2}$$

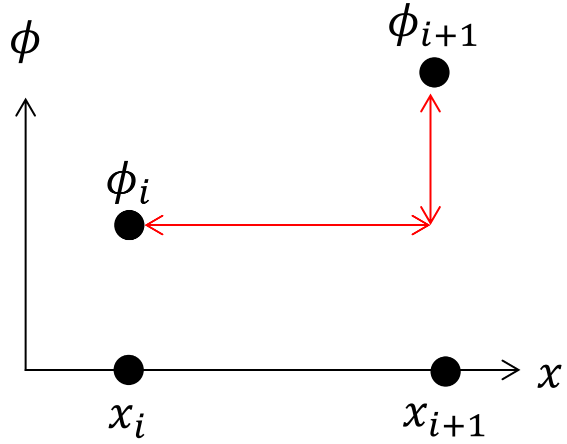
Discretization

- How to treat the position-dependent permittivity
  - For $2 \le i \le N-1$, the integration from $x_{i-0.5}$ to $x_{i+0.5}$ yields

$$\epsilon(x_{i+0.5}) \left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} - \epsilon(x_{i-0.5}) \left.\frac{d\phi}{dx}\right|_{x_{i-0.5}} = 0$$

  - The first derivative is approximated by

$$\left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} \approx \frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}$$



$N = 5$ example

- At x_3, two layers ($\epsilon_1 = 11.7\ \epsilon_0$ and $\epsilon_2 = 3.9\ \epsilon_0$) meet.
  - It is simply given by

$$Ax = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \epsilon_1 & -2\epsilon_1 & \epsilon_1 & 0 & 0 \\ 0 & \epsilon_1 & -\epsilon_2 - \epsilon_1 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_2 & -2\epsilon_2 & \epsilon_2 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \phi(x_3) \\ \phi(x_4) \\ \phi(x_5) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = b$$

  - Note that the third row has different coefficients.
  - When $\epsilon_1 = \epsilon_2$, it is reduced to the Laplace equation.

MATLAB example (1)

- Step-by-step procedure
  - First, set the number of points, N.

```
N = 51; % An odd number
mid = (N+1)/2;
eps1 = 11.7; eps2 = 3.9; % Relative permittivity
```

  - Next, set the matrix, A.

```
A = zeros(N,N);
A(1,1) = 1.0;
for ii=2:N-1
   if (ii< mid) A(ii,ii-1) = eps1; A(ii,ii) = -2*eps1;    A(ii,ii+1) = eps1; end
   if (ii==mid) A(ii,ii-1) = eps1; A(ii,ii) = -eps1-eps2; A(ii,ii+1) = eps2; end
   if (ii> mid) A(ii,ii-1) = eps2; A(ii,ii) = -2*eps2;    A(ii,ii+1) = eps2; end
end
A(N,N) = 1.0;
```

MATLAB example (2)

- Step-by-step procedure (continued)
  - Next , set the vector, b.

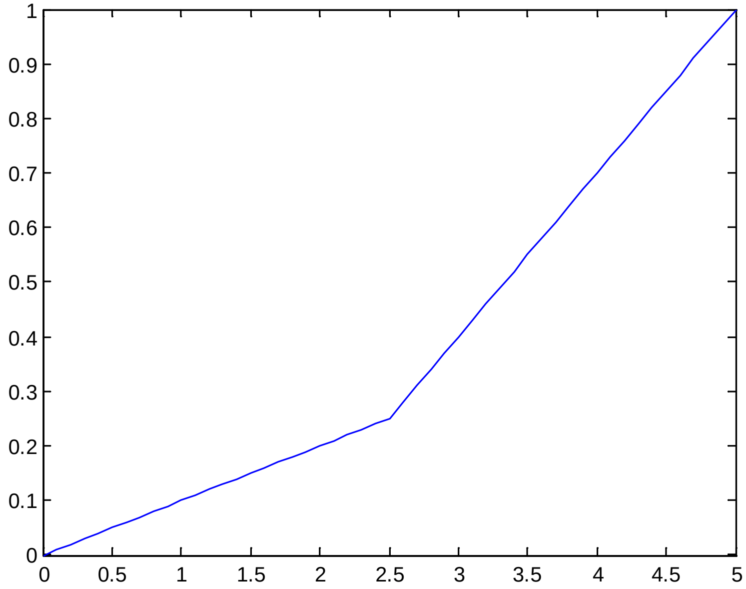
```
b = zeros(N,1); b(N,1) = 1.0;
```

  - Finally, get the solution vector, x.

```
x = A \ b
```

  - Why don’t we plot it?

```
plot(5/(N-1)*[0:N-1],x)
```



Homework#3

- Due: AM08:00, September 12
- Problem#1
  - In your own research work, you may consider a heterostructure.
  - Specify your own hetrostructure. Specify the thickness and the relative permittivity of each layer. (Ignore mobile carriers.)
  - Then, calculate the capacitance per area. (F/cm^2)
  - Compare your result with the analytic expression.

  - (When you have no idea about the heterostructure, please select any one available to you.)