Key Concepts for this section

1: Lorentz force law, Field, Maxwell's equation

2: Ion Transport, Nernst-Planck equation

3: (Quasi)electrostatics, potential function,

4: Laplace's equation, Uniqueness

5: Debye layer, electroneutrality

Goals of Part II:

(1) Understand when and why electromagnetic (E and B) interaction is relevant (or not relevant) in biological systems.

(2) Be able to analyze quasistatic electric fields in 2D and 3D.

$$\vec{E} = -\nabla\Phi \qquad \nabla\cdot(\varepsilon\vec{E}) = \nabla\cdot(-\varepsilon\nabla\Phi) = \rho_e$$

$$\nabla^2\Phi = -\frac{\rho_e}{\varepsilon} \quad (Poisson's\ Equation)$$

However, biomolecules in the system do not generate E-field, since they are shielded by counterions (electroneutrality)…….

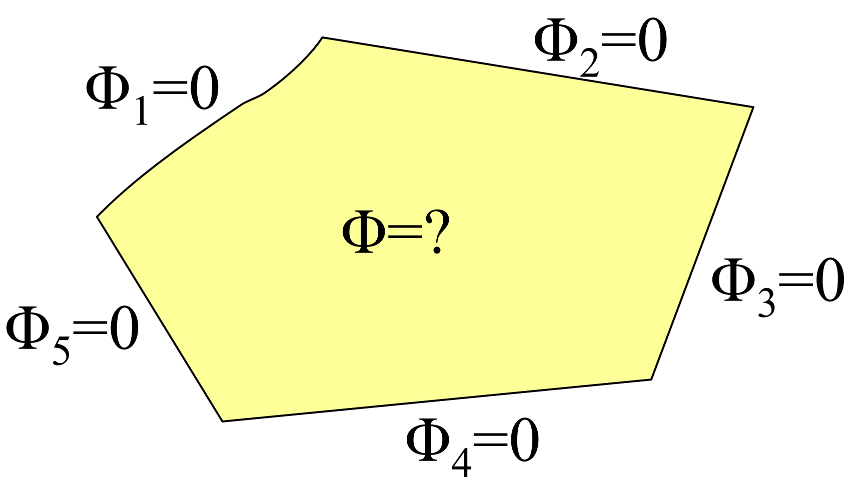
It all comes down to solving….. $\nabla^2\Phi = 0 \quad (Laplace's\ Equation)$

$$\nabla^2 c = \frac{\partial c}{\partial t}$$ (Fick's second law) → $\nabla^2 c = 0$ (steady-state diffusion)

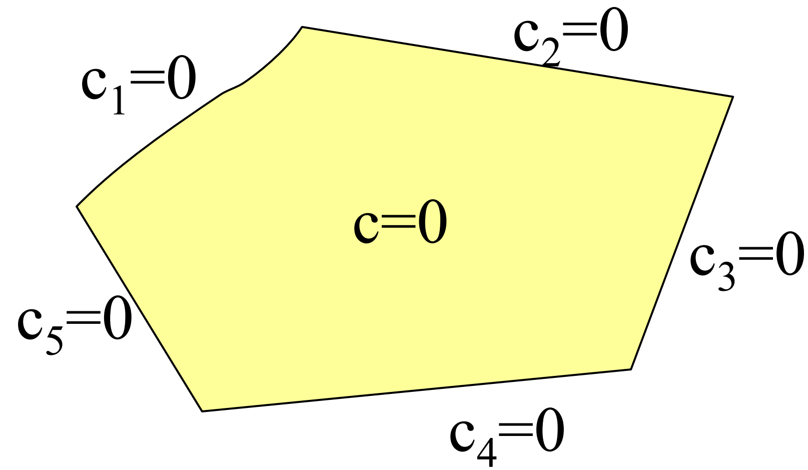
$$\vec{q} = -k\nabla T$$ (Fourier's law for heat conduction)

$$\nabla\cdot\vec{q} = 0$$ (conservation law for heat) → $\nabla^2 T = 0$ (steady heat flow)

Electrostatics

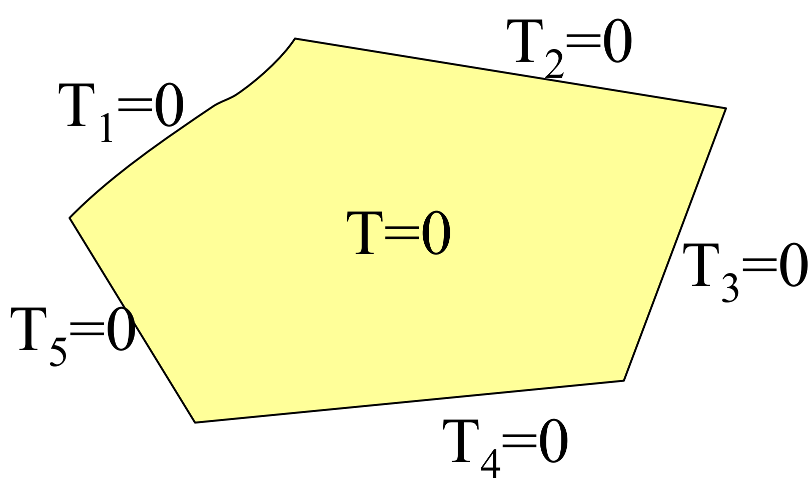


Steady state diffusion $\nabla^2 c = 0$



Thermal conduction

$$\nabla^2 T = 0$$



Uniqueness of Solution

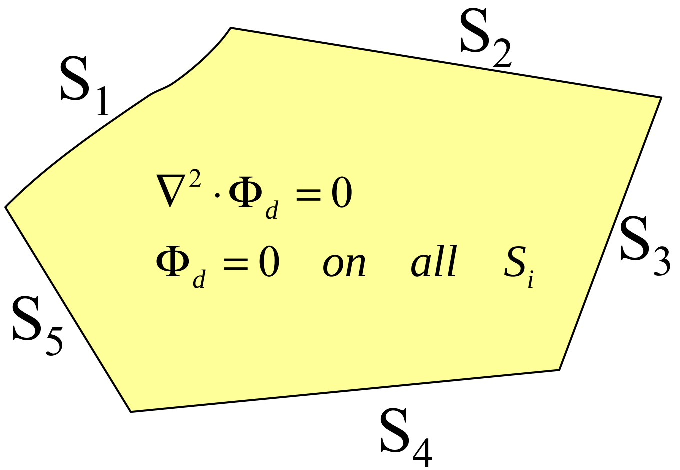
Let's assume two different solutions, Φ_a and Φ_b

$$\nabla^2 \cdot \Phi_a = -\frac{\rho_e}{\varepsilon}; \quad \Phi_a = \Phi_i \quad on \quad S_i$$

$$\nabla^2 \cdot \Phi_b = -\frac{\rho_e}{\varepsilon}; \quad \Phi_b = \Phi_i \quad on \quad S_i$$

Then define $\Phi_d = \Phi_a - \Phi_b$

$$\nabla^2 \cdot \Phi_d = 0; \quad \Phi_d = 0 \quad on \quad S_i$$ (satisfy Laplace Eq.)

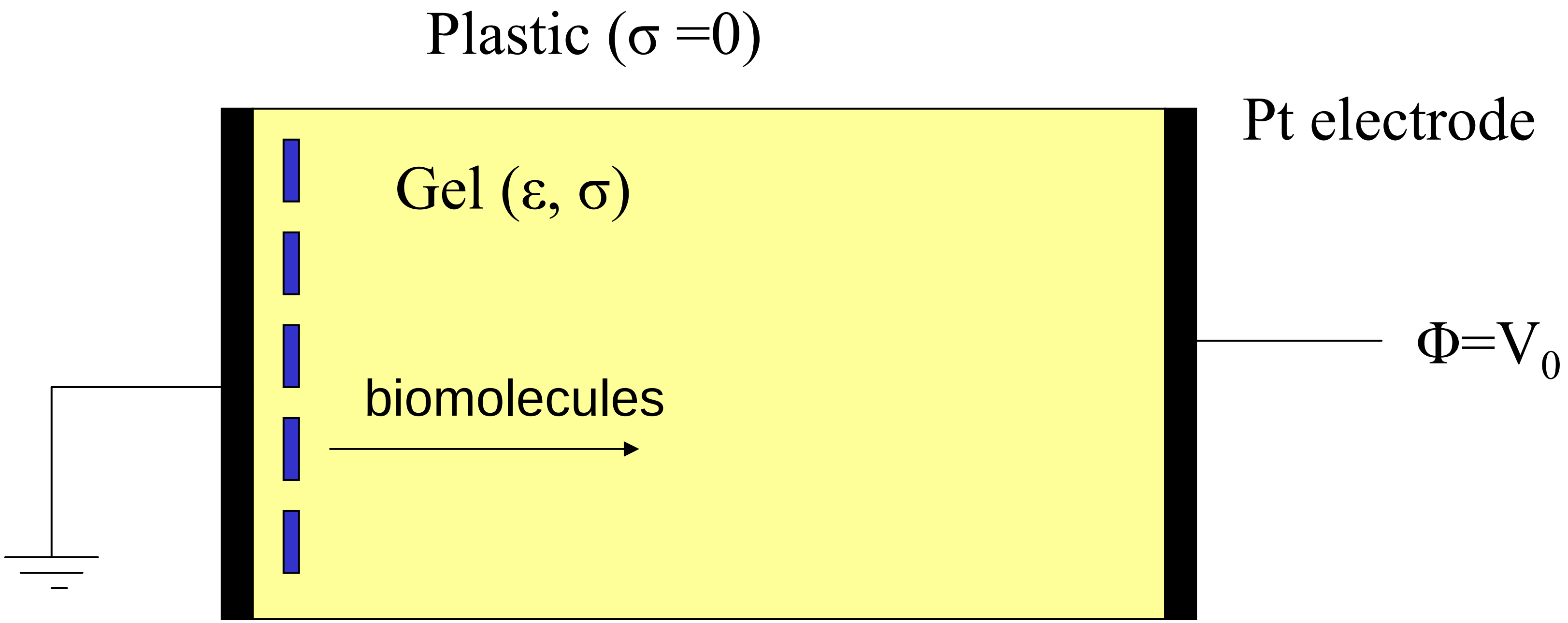


Answer:

$$\Phi_d = 0$$ for everywhere

$$\therefore \quad \Phi_a - \Phi_b = 0$$

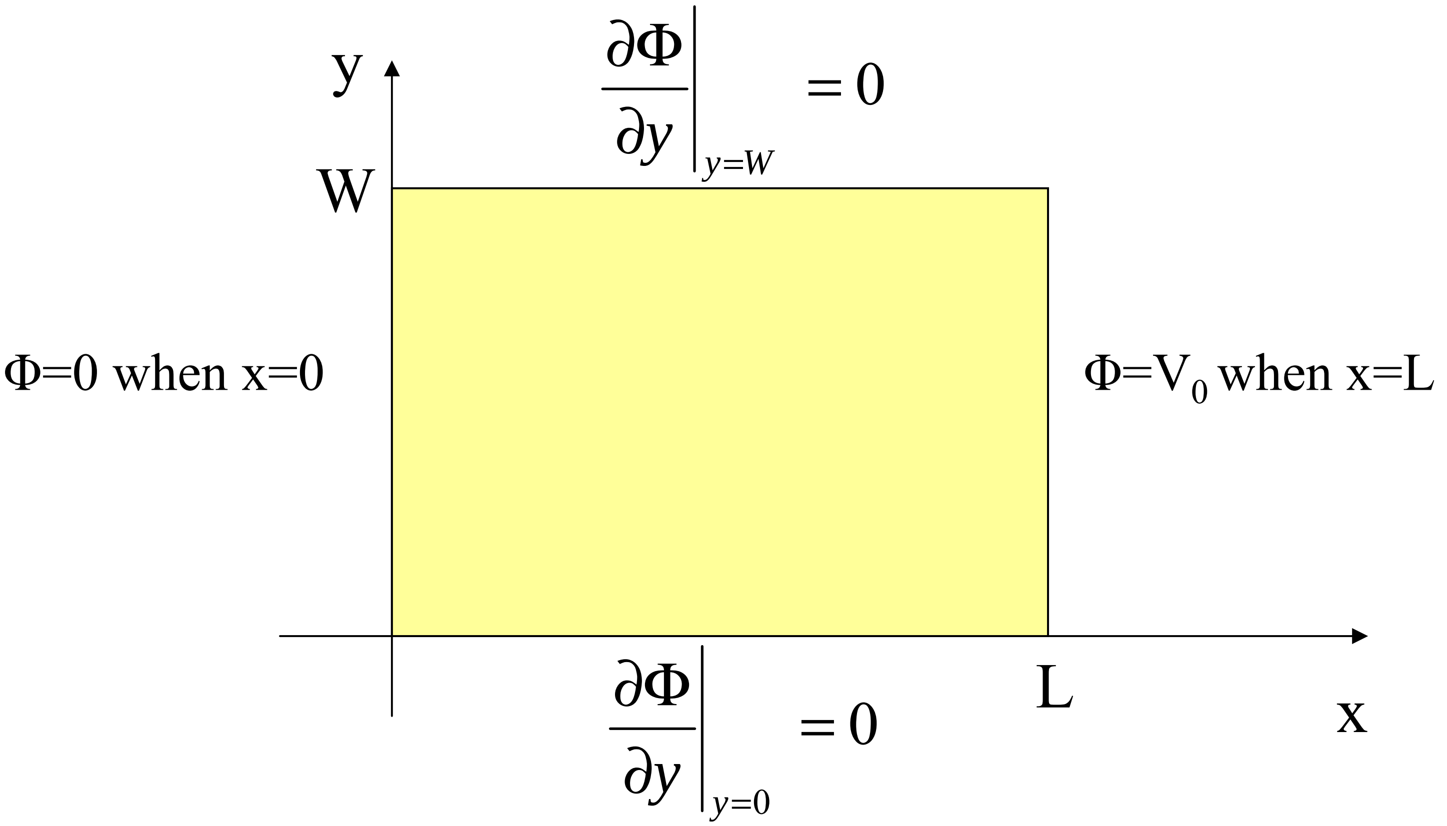
Gel Electrophoresis



$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} = 0 \; (electrostatics) \quad \Rightarrow \quad \vec{E} = -\nabla \Phi$$

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t} = 0 \quad \text{(steady state, no charge accumulation)}$$

$$\nabla \cdot \vec{J} = \nabla \cdot \left(\sigma \vec{E} \right) = 0 \quad \Rightarrow \quad \nabla \cdot \vec{E} = 0 \quad \Rightarrow \quad \nabla^2 \Phi = 0$$



$\nabla \cdot \vec{J} = 0$ ⇒ (no charge accumulation)

$\vec{J} = J_x \hat{x}$ ⇒ $J_y = \sigma E_y = 0 = \left.\frac{\partial \Phi}{\partial y}\right|_{y=0 \text{ or } W}$

J=0 (insulator)

Boundary Conditions (For EQS approximation)

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon} \quad \Rightarrow \quad \hat{n} \cdot (\varepsilon_1 \vec{E}_1 - \varepsilon_2 \vec{E}_2) = \sigma_s$$

$$\nabla \times \vec{E} = 0 \quad \Rightarrow \quad \hat{n} \times \vec{E}_1 = \hat{n} \times \vec{E}_2 \quad (\vec{E}_1\big|_{\text{tangential}} = \vec{E}_2\big|_{\text{tangential}})$$

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t} \quad \Rightarrow \quad \hat{n} \cdot (\sigma_1 \vec{E}_1 - \sigma_2 \vec{E}_2) = -\frac{\partial \sigma_s}{\partial t}$$

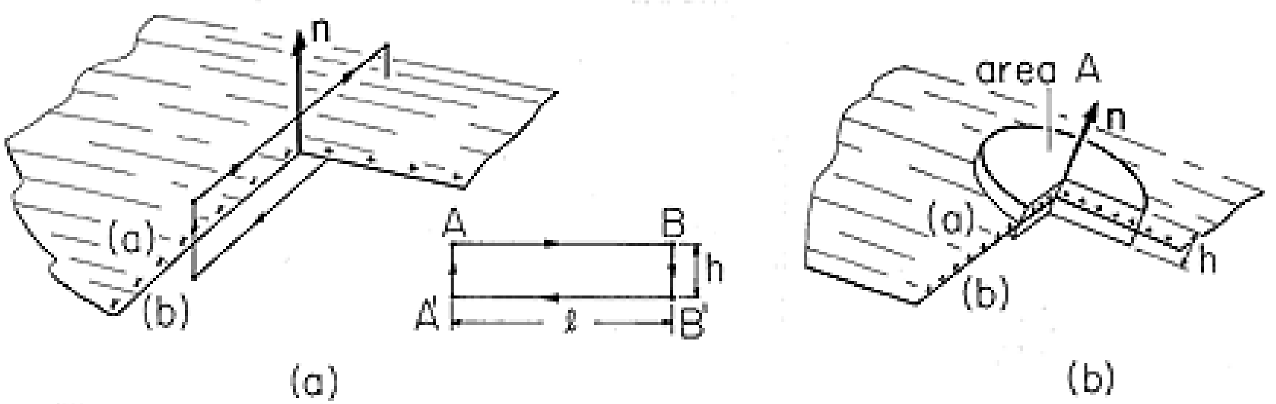
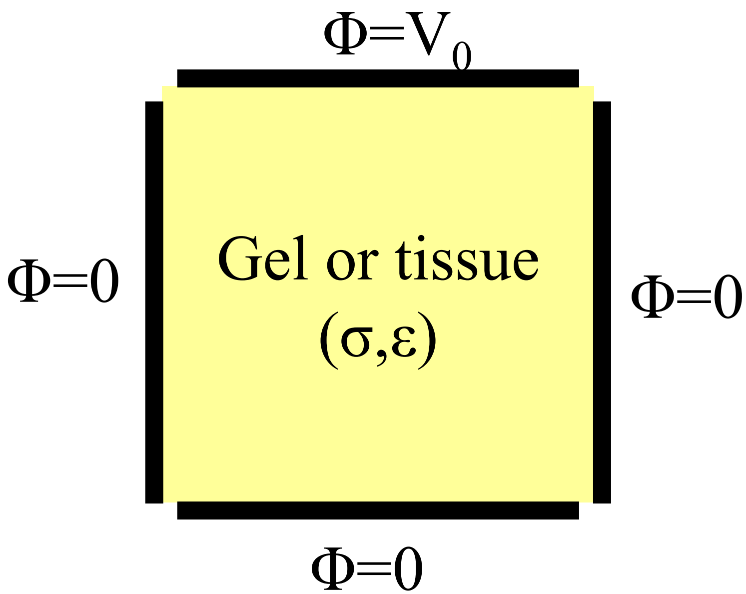


Figure 5.3.1 (a) Differential contour intersecting surface supporting surface charge density. (b) Differential volume enclosing surface charge on surface having normal **n**.

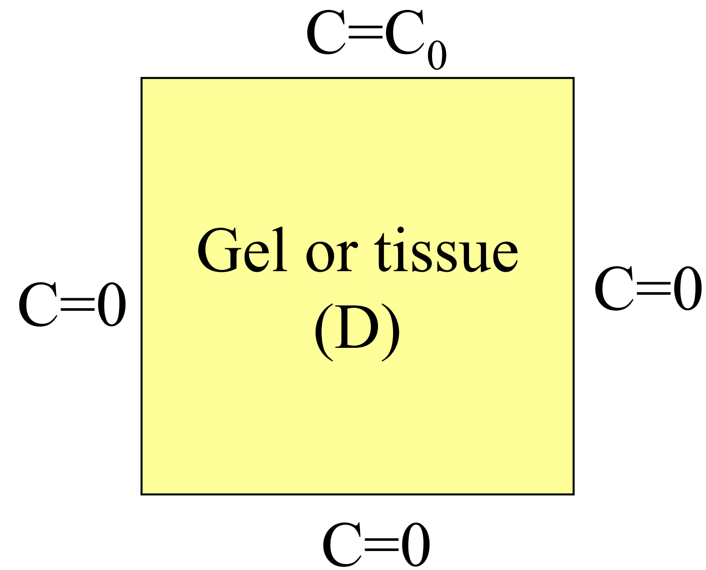
Electrostatics



$$\nabla^2 \Phi = 0$$

$$\vec{J}_e = -\sigma \nabla \Phi$$

Steady Diffusion



$$\nabla^2 C = 0$$

$$\vec{J}_i = -D_i \nabla c_i$$

$$\Phi = A \sin kx \sinh ky$$

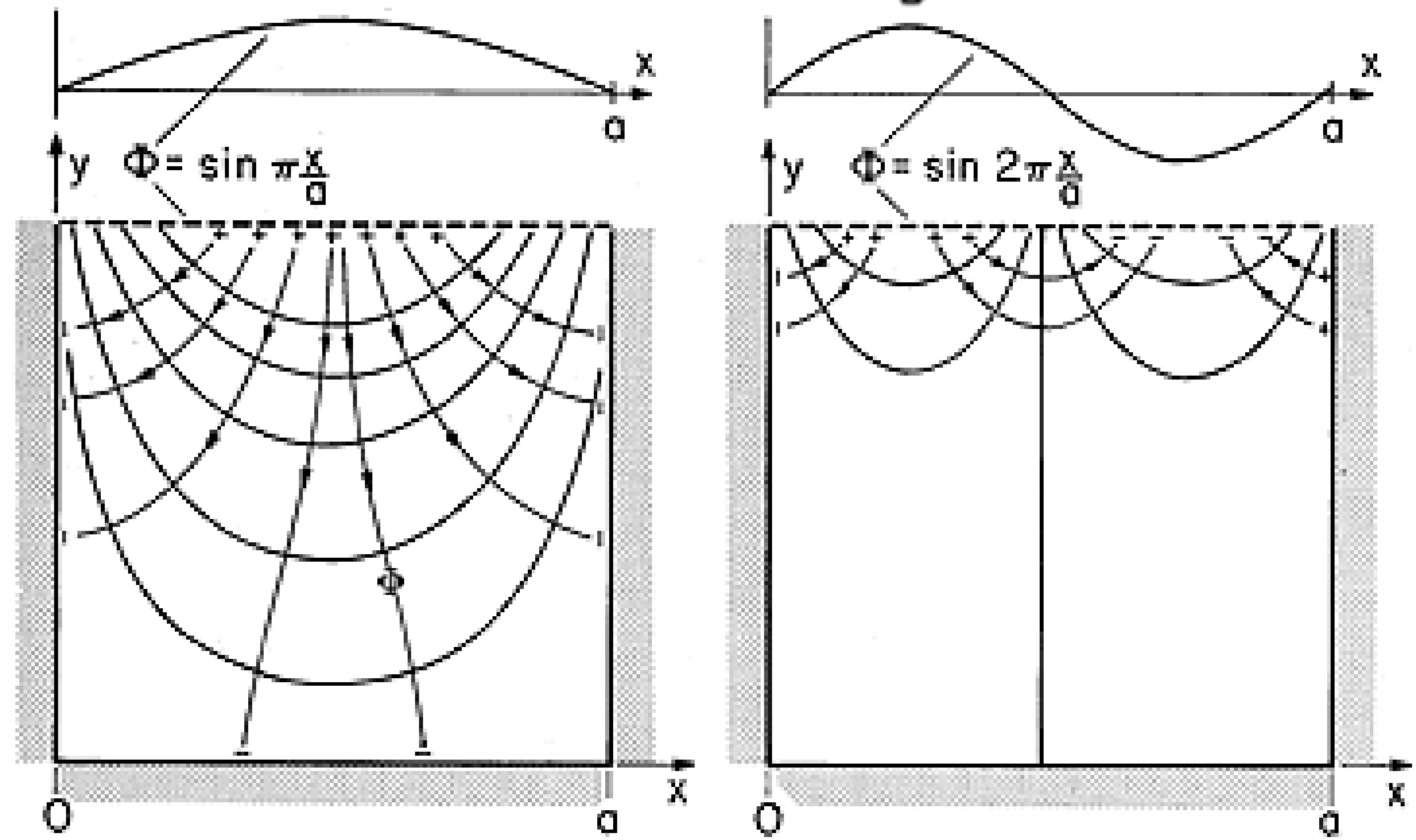
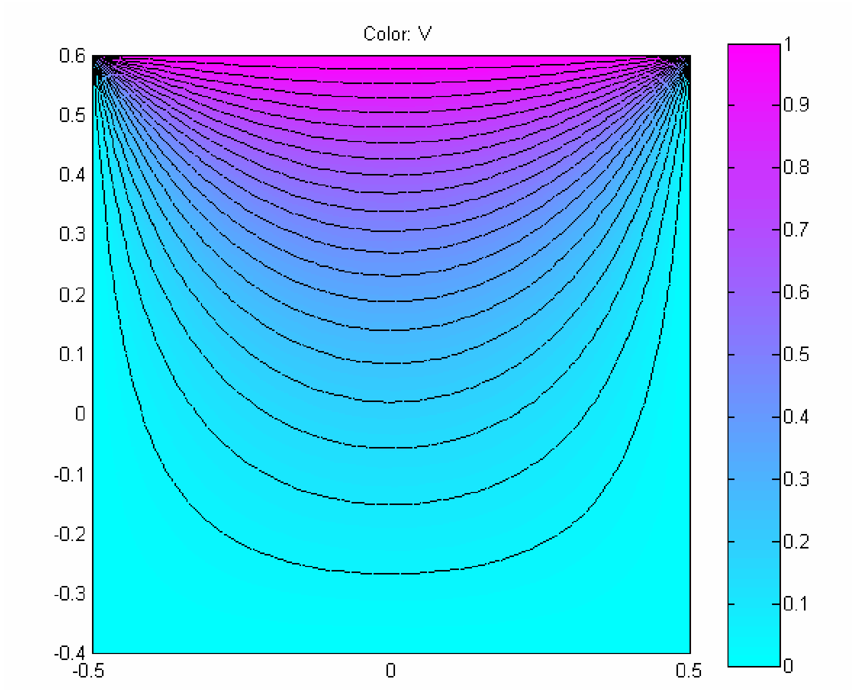


Figure 5.5.1 Two of the infinite number of potential functions having the form of (1) that will fit the boundary conditions $\Phi = 0$ at $y = 0$ and at $x = 0$ and $x = a$.

Solution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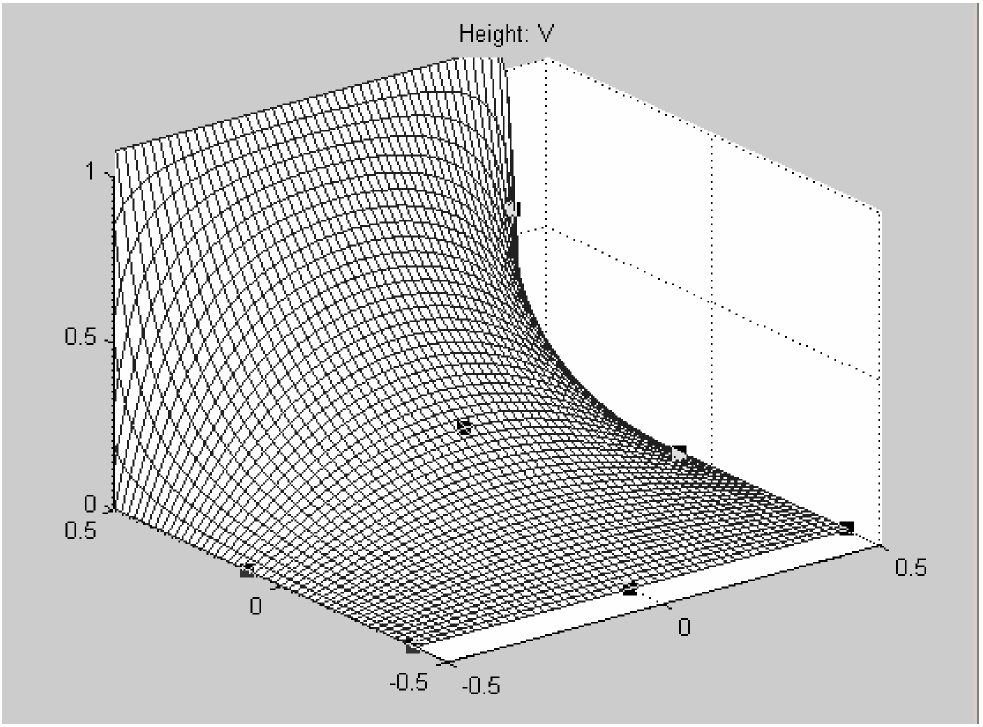
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Known Solutions for Laplace equations

Cylindrical Coordinates

$$\nabla^2\Phi(\rho,\varphi,z)=0 \quad \Rightarrow \quad \frac{\partial^2\Phi}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\Phi}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2\Phi}{\partial\varphi^2}+\frac{\partial^2\Phi}{\partial z^2}=0$$

$$\Phi(\rho,\varphi,z)=R(\rho)\Psi(\varphi)Z(z)$$

$$R(\rho) \quad \Rightarrow \quad \textit{Bessel Functions}\ (J_n, N_n, I_n, K_n)$$

$$\Psi(\varphi) \quad \Rightarrow \quad \textit{Trigonometric}\ (\sin, \cos, \sinh, \cosh)$$

$$Z(z) \quad \Rightarrow \quad \textit{Trigonometric}\ (\sin, \cos, \sinh, \cosh)$$

Spherical Coordinates

$$\nabla^2\Phi(r,\theta,\varphi)=0 \quad \Rightarrow \quad \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\varphi^2}=0$$

$$\Phi(r,\theta,\varphi)=R(r)\Theta(\theta)\Psi(\varphi)$$

$$R(r) \quad \Rightarrow \quad \textit{Spherical Bessel Functions}$$

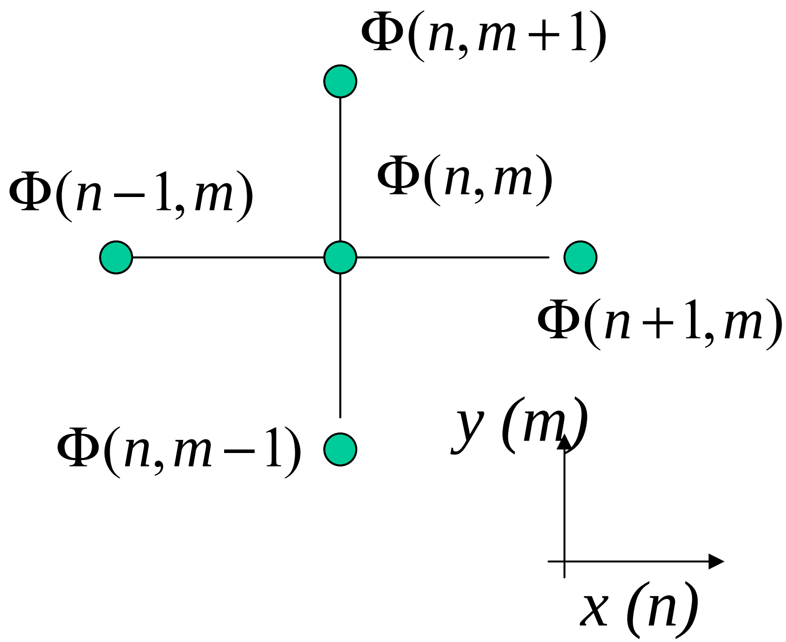
$$\Theta(\theta) \quad \Rightarrow \quad \textit{Legendre Functions}\ (P_n(\cos\theta))$$

$$\Psi(\varphi) \quad \Rightarrow \quad \textit{Trigonometric}\ (\sin\varphi, \cos\varphi)$$

Solving Laplace's Equation (Numerically)

1D case: $\dfrac{d^2\Phi}{dx^2} = 0 \quad \rightarrow \quad \Phi(x) = ax + b$

2D case: $\dfrac{\partial^2\Phi}{\partial x^2} + \dfrac{\partial^2\Phi}{\partial y^2} = 0$

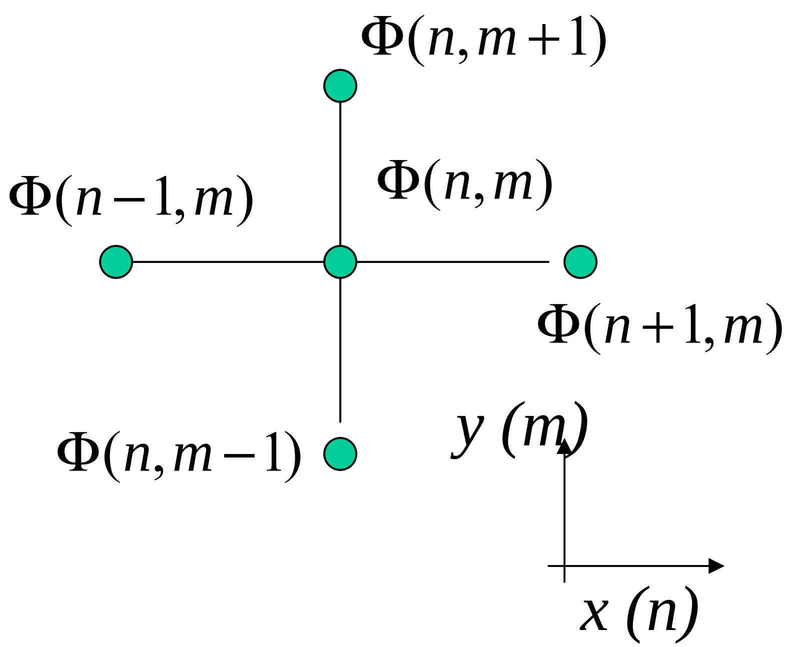


$$\frac{\partial\Phi}{\partial x}\left(n+\frac{1}{2}, m\right) = \Phi(n+1, m) - \Phi(n, m)$$

$$\frac{\partial\Phi}{\partial x}\left(n-\frac{1}{2}, m\right) = \Phi(n, m) - \Phi(n-1, m)$$

$$\frac{\partial^2\Phi}{\partial x^2}(n, m) = \frac{\partial\Phi}{\partial x}\left(n+\frac{1}{2}, m\right) - \frac{\partial\Phi}{\partial x}\left(n-\frac{1}{2}, m\right) = \Phi(n+1, m) + \Phi(n-1, m) - 2\Phi(n, m)$$

Laplace’s equation
In discretized form



$$\frac{\partial^2 \Phi}{\partial x^2}(n,m) + \frac{\partial^2 \Phi}{\partial y^2}(n,m) =$$

$$\Phi(n+1,m) + \Phi(n-1,m) + \Phi(n,m+1) + \Phi(n,m-1) - 4\Phi(n,m) = 0$$

$$\Phi(n,m) = \frac{\Phi(n+1,m) + \Phi(n-1,m) + \Phi(n,m+1) + \Phi(n,m-1)}{4}$$

Value in the middle = average of surrounding values

Finite Element Method