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

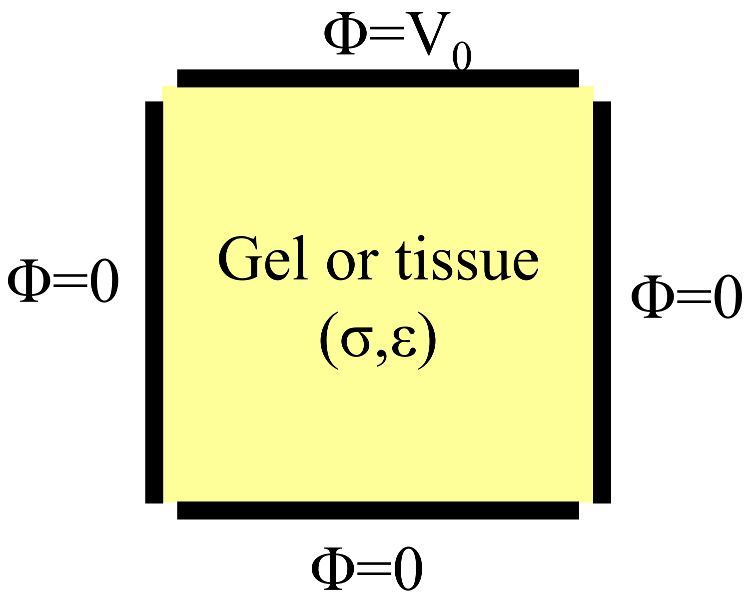
5: Debye layer, electroneutrality

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.

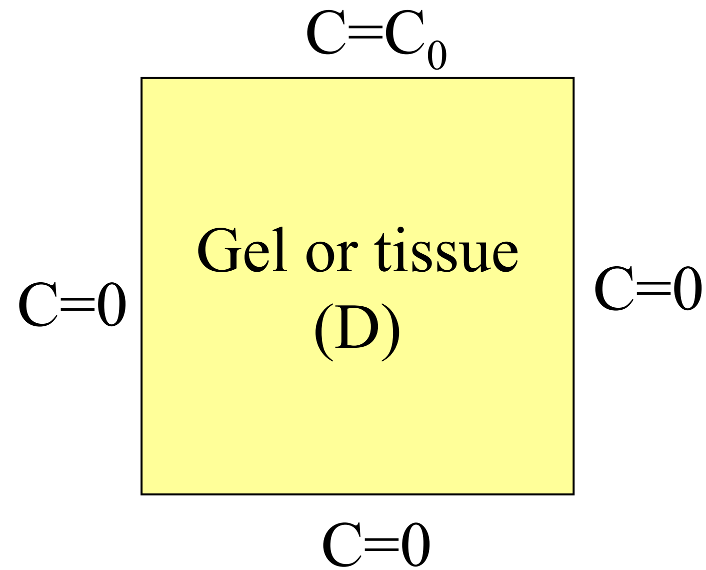
Electrostatics



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

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

Steady Diffusion



$$\nabla^2 C = 0$$

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

$$\nabla^2\Phi = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2} = 0$$

Assume $\Phi(x, y, z) = \mathrm{X}(x)\Upsilon(y)\mathrm{Z}(z)$

$$\nabla^2\Phi = \Upsilon \mathrm{Z}\frac{\partial^2 \mathrm{X}}{\partial x^2} + \mathrm{X}\mathrm{Z}\frac{\partial^2\Upsilon}{\partial y^2} + \mathrm{X}\Upsilon\frac{\partial^2 \mathrm{Z}}{\partial z^2} = 0$$

$$\underbrace{\frac{1}{\mathrm{X}}\frac{\partial^2 \mathrm{X}}{\partial x^2}}_{\substack{function\\ of\ x}} + \underbrace{\frac{1}{\Upsilon}\frac{\partial^2\Upsilon}{\partial y^2}}_{\substack{function\\ of\ y}} + \underbrace{\frac{1}{\mathrm{Z}}\frac{\partial^2 \mathrm{Z}}{\partial z^2}}_{\substack{function\\ of\ z}} = 0$$

Three possibilities

$$\frac{1}{\mathrm{X}}\frac{\partial^2 \mathrm{X}}{\partial x^2} = k_x{}^2 \quad \Rightarrow \quad \mathrm{X}(x) = e^{+k_x x},\ e^{-k_x x}$$

$$or = -k_x{}^2 \quad \Rightarrow \quad \mathrm{X}(x) = \sin(k_x x), \cos(k_x x)$$

$$or = 0 \quad \Rightarrow \quad \mathrm{X}(x) = ax + b \quad (a, b : constants)$$

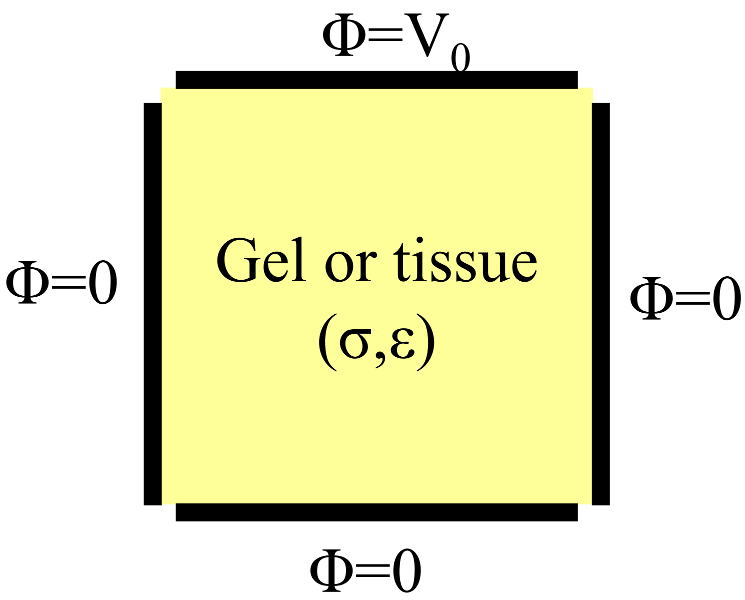
$$\nabla^2\Phi = 0, \quad \Phi(x,y) = \mathrm{X}(x)\Upsilon(y)$$

$$\frac{1}{\mathrm{X}}\frac{\partial^2 \mathrm{X}}{\partial x^2} + \frac{1}{\Upsilon}\frac{\partial^2 \Upsilon}{\partial y^2} = 0$$

$$\frac{1}{\mathrm{X}}\frac{\partial^2 \mathrm{X}}{\partial x^2} = -k^2 \quad X(x) \sim \sin(kx)$$

$$\sin(kL) = 0 \Rightarrow kL = n\pi \quad (n: \text{integer})$$

$$\textit{Eigenvalue}: \quad k_n = \frac{n\pi}{L}$$



expand X(x) using Fourier sine series

$$\mathrm{X}(x) = \sum_n A_n \sin\left(\frac{n\pi x}{L}\right) \quad \text{(This satisfies B. C. at x=0, L)}$$

$$\text{then, } \frac{\partial^2 \Upsilon(y)}{\partial y^2} - k_n^2 \Upsilon(y) = 0 \quad \Rightarrow \quad \Upsilon(y) \sim \sinh\left(\frac{n\pi y}{L}\right) \quad \textit{or} \quad \cosh\left(\frac{n\pi y}{L}\right)$$

$$\Upsilon(y) = \sinh\left(\frac{n\pi y}{L}\right) \quad \text{since } \Phi(x,0) = 0 \quad \therefore \quad \Phi(x,y) = \sum_n A_n \sin\left(\frac{n\pi x}{L}\right)\sinh\left(\frac{n\pi y}{L}\right)$$

Determining $\mathrm{A_n}$: use boundary condition

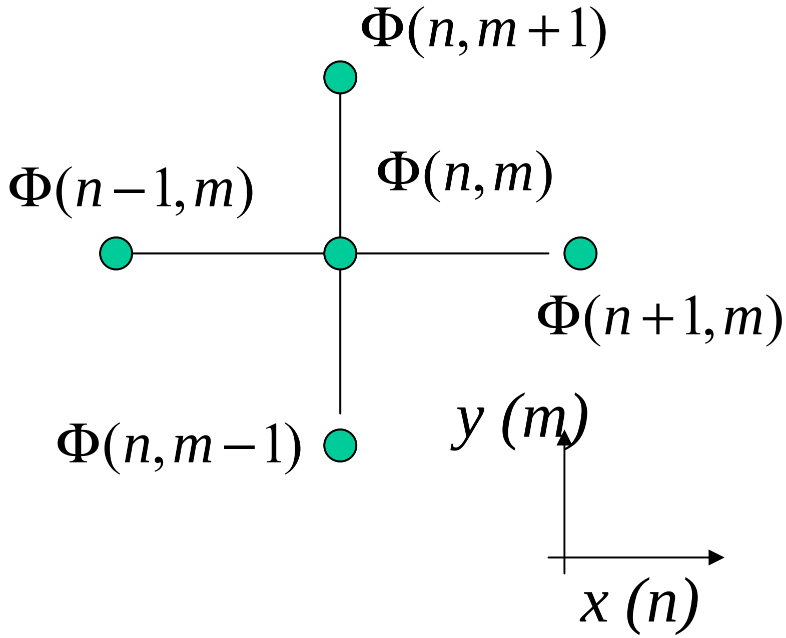
$$\Phi(x,L) = V_0 = \sum_n A_n \sin\left(\frac{n\pi x}{L}\right)\sinh(n\pi)$$

$$\textit{operate} \quad \int_0^L \sin\left(\frac{m\pi x}{L}\right) \quad \textit{on both sides} \Rightarrow A_n = \frac{2V_0}{n\pi}\frac{(1-\cos(n\pi))}{\sinh(n\pi)}$$

Solving Laplace's Equation (Numerically)

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

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

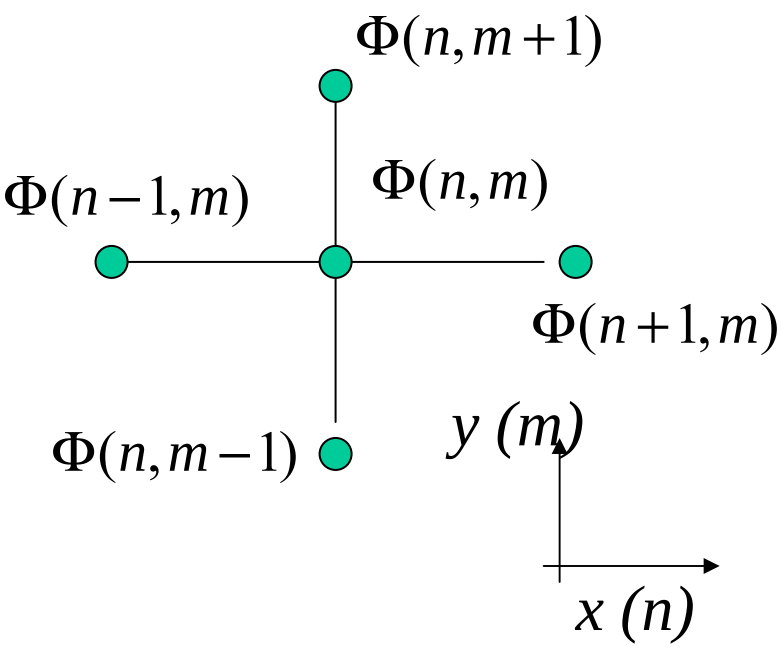


$$\frac{\partial\Phi}{\partial x}(n+\frac{1}{2},m) = \Phi(n+1,m) - \Phi(n,m)$$

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

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

Laplace's equation
In discretized form



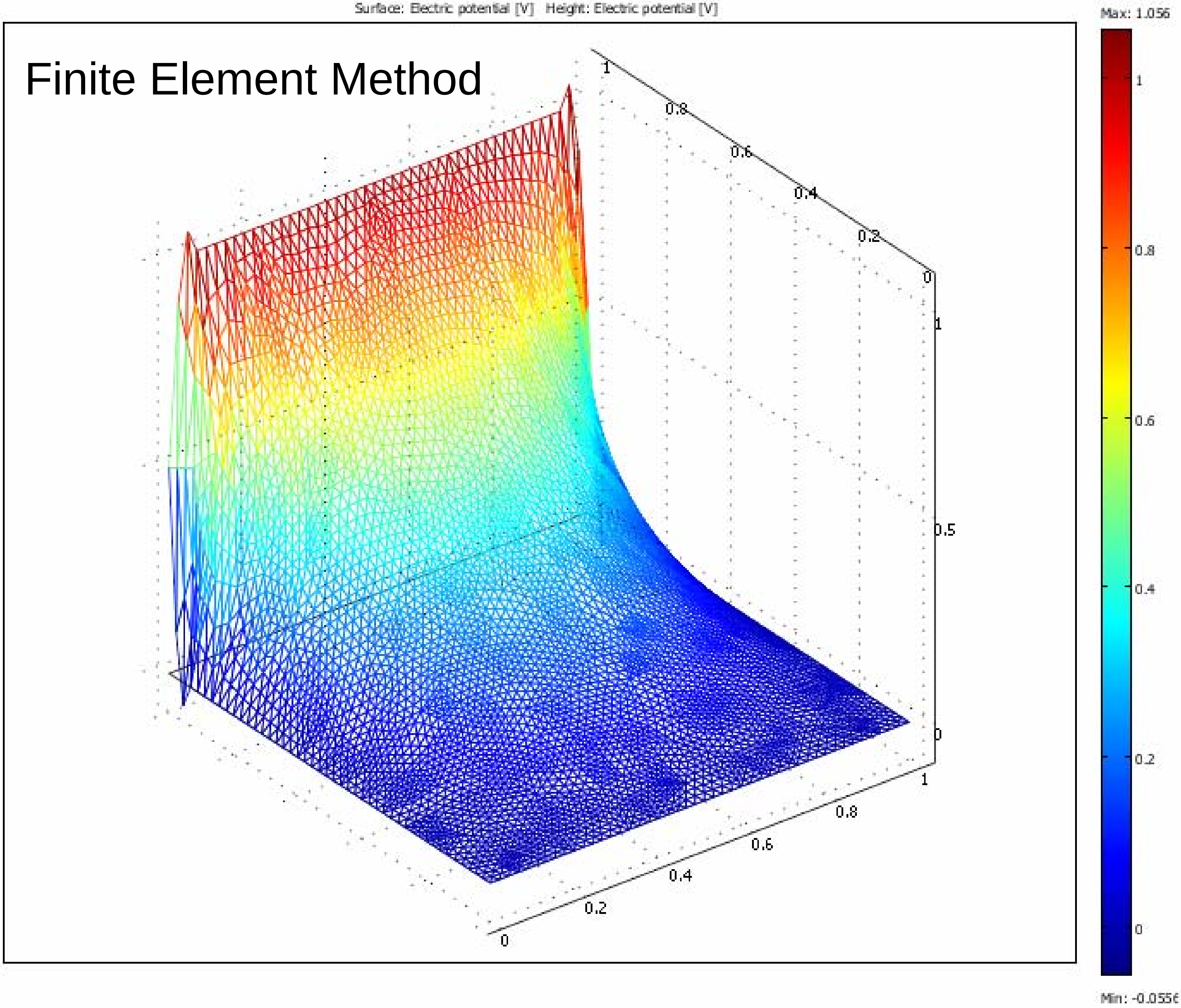
$$\frac{\partial^2 \Phi}{\partial x^2}(n,m) + \frac{\partial^2 \Phi}{\partial y^2}(n,m) =$$

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

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

Value in the middle = average of surrounding values

Finite Element Method



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

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

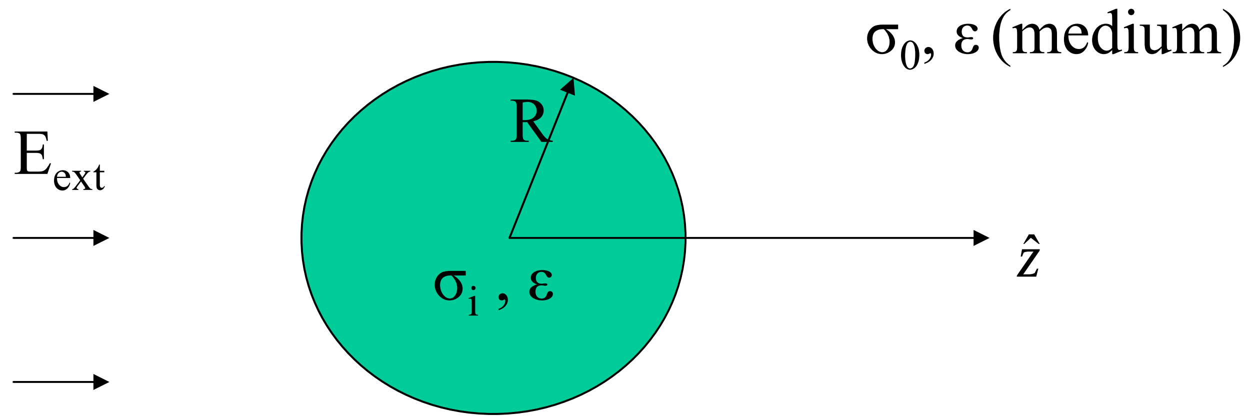
$$\Phi(r,\theta,\varphi)=R(r)\Theta(\theta)\Psi(\varphi)$$

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

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

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

Cell in a field



Equation to solve :

$$\nabla \cdot \vec{J}_e = \nabla \cdot (\sigma \vec{E}) = -\nabla \cdot (\sigma \nabla \Phi) = 0 \quad \therefore \nabla^2 \Phi = 0 \quad (\textit{Laplace's Equation})$$

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

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

separate and solve,

$$R(r) \quad \Rightarrow \quad Ar^n + B\frac{1}{r^{n+1}}$$

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

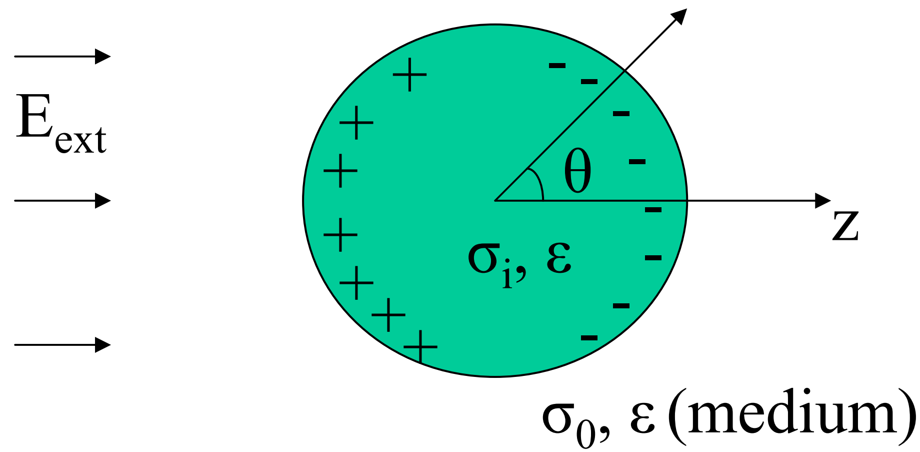
Guessing the solution

$$\vec{E} \to E_{ext}\hat{z} \quad as \quad r \to \infty \quad \Rightarrow \quad \Phi = -E_{ext} z = -E_{ext} r\cos\theta \quad as \quad r \to \infty$$

$P_n(\cos\theta) \sim \cos n\theta$

Only n =1 term contributes

(should be “dipole” field)



Trial Solution:

$$\Phi_o = Ar\cos\theta + B\frac{1}{r^2}\cos\theta \quad \text{(for r } \geq \text{ R)}$$

$$\Phi_i = Cr\cos\theta + D\frac{1}{r^2}\cos\theta \quad \text{(for r } \leq \text{ R)}$$

$$D = 0 \quad (\Phi_i \text{ finite at r=0})$$

$$A = -E_{ext} \quad (\Phi_o \to -E_{ext} r\cos\theta \text{ when r} \to \infty)$$

Boundary Conditions (For EQS approximation)

$$\nabla \cdot (\varepsilon \vec{E}) = \rho_e \quad \Rightarrow \quad \hat{n} \cdot (\varepsilon_1 \vec{E_1} - \varepsilon_2 \vec{E_2}) = \sigma_s$$

$$\nabla \times \vec{E} = 0 \quad \Rightarrow \quad \hat{n} \times \vec{E_1} = \hat{n} \times \vec{E_2} \quad (\vec{E}_1\big|_{\text{tangential}} = \vec{E}_2\big|_{\text{tangential}})$$

$$\nabla \cdot \vec{J_e} = -\frac{\partial \rho}{\partial t} \quad \Rightarrow \quad \hat{n} \cdot (\sigma_1 \vec{E_1} - \sigma_2 \vec{E_2}) = -\frac{\partial \sigma_s}{\partial t}$$

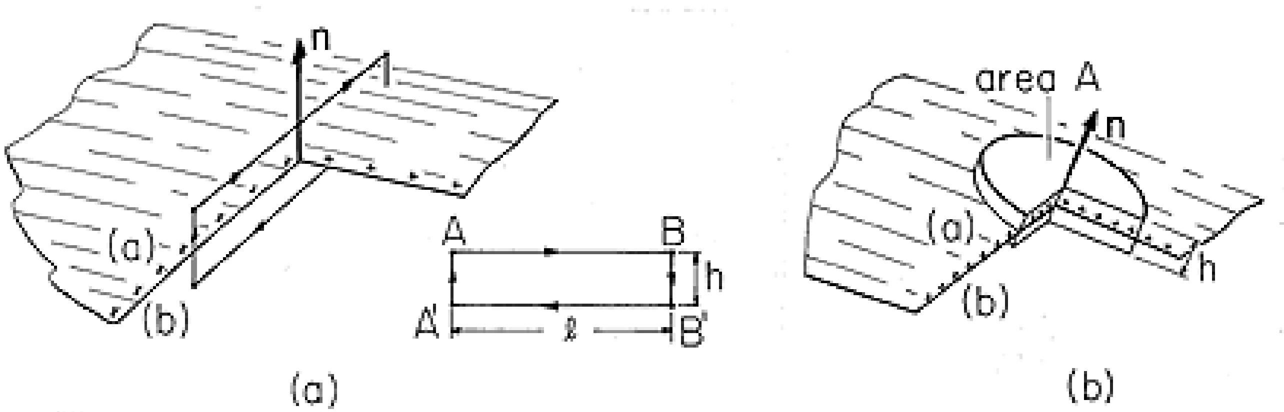


Figure 5.3.1 (a) Differential contour intersecting surface supporting surface charge density. (b) Differential volume enclosing surface charge on surface having normal **n**.

Some plots for the solution

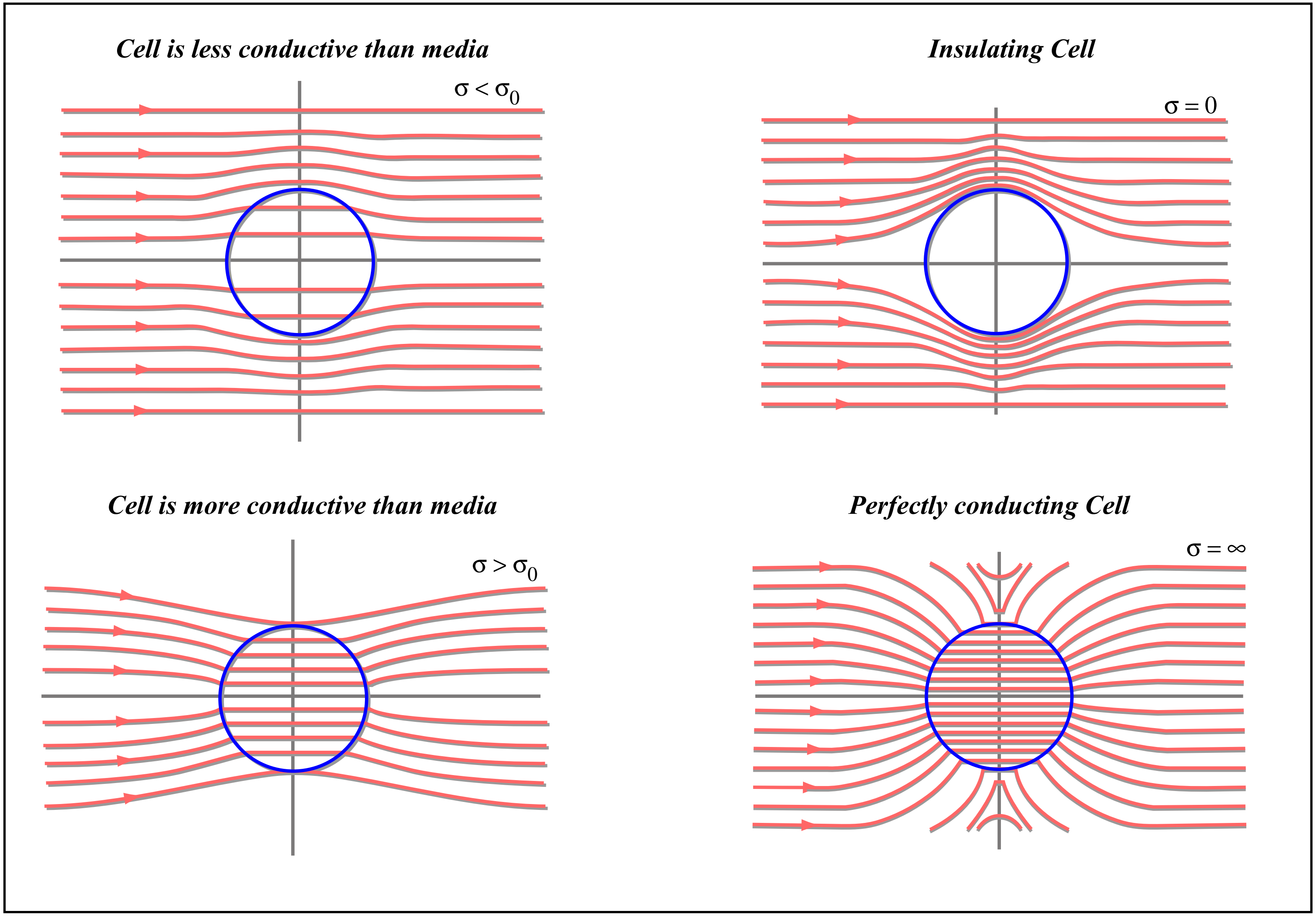


Figure by MIT OCW.