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

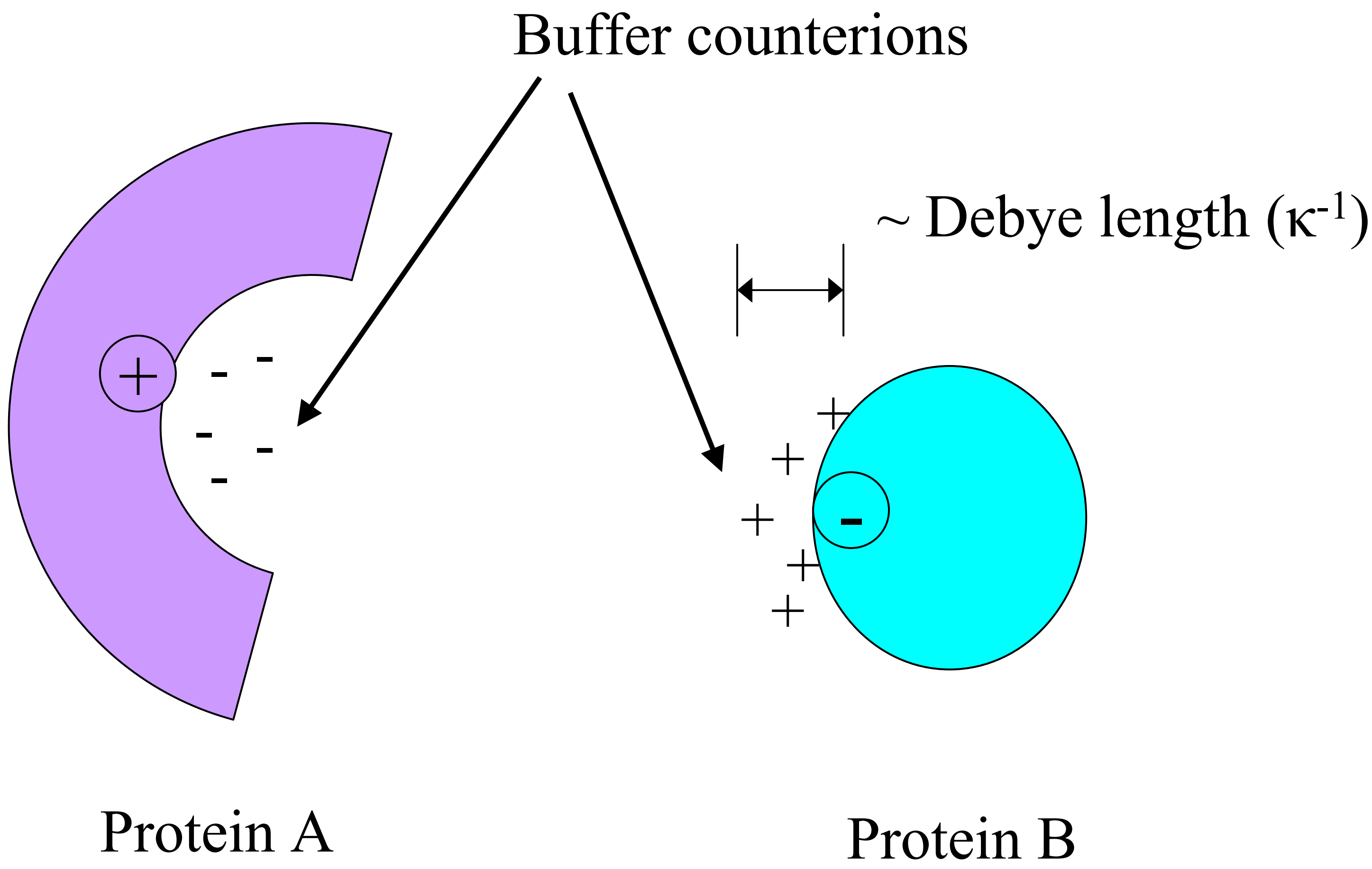
5: Debye layer, electroneutrality

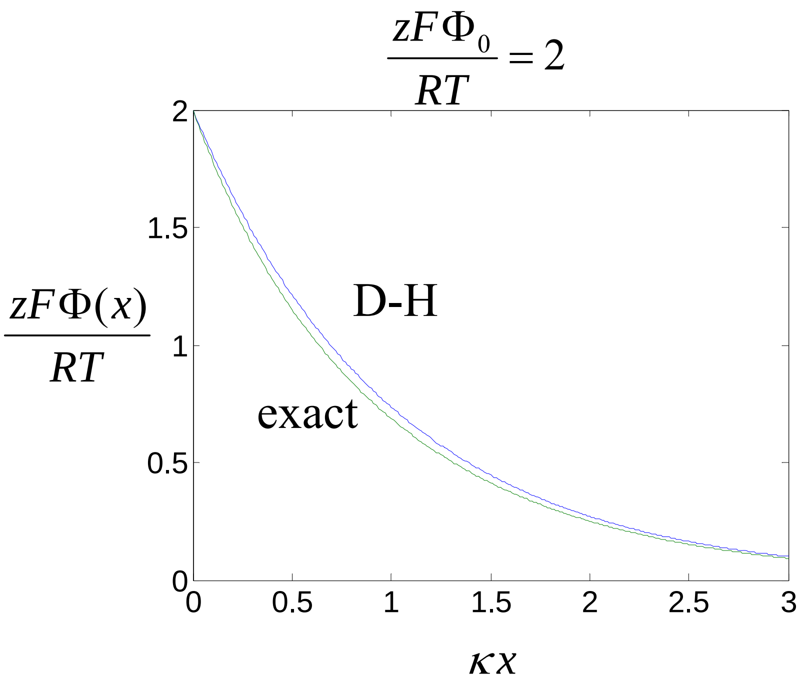
Goals of Part II:

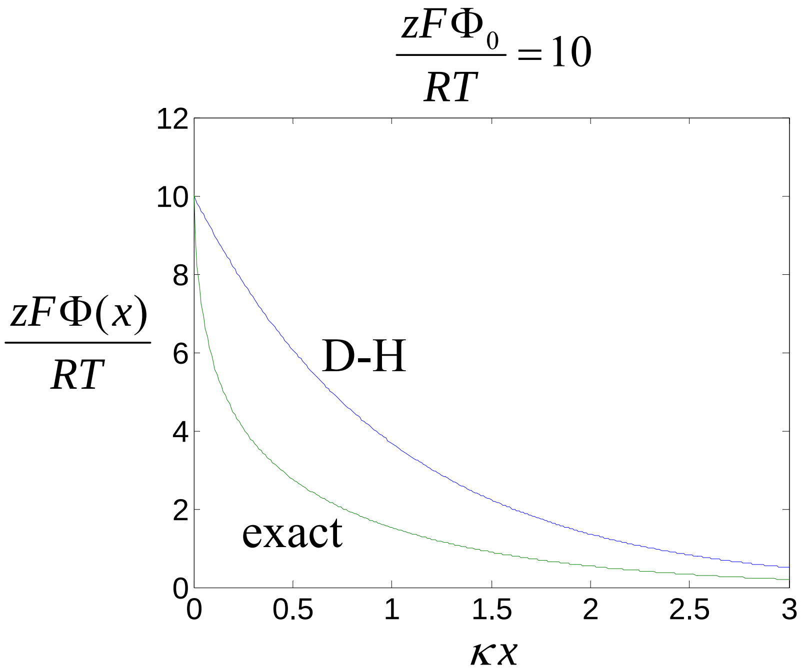
(1) Understand when and why electromagnetic (E and B) interaction is relevant (or not relevant) in biological systems.

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

Electroneutrality





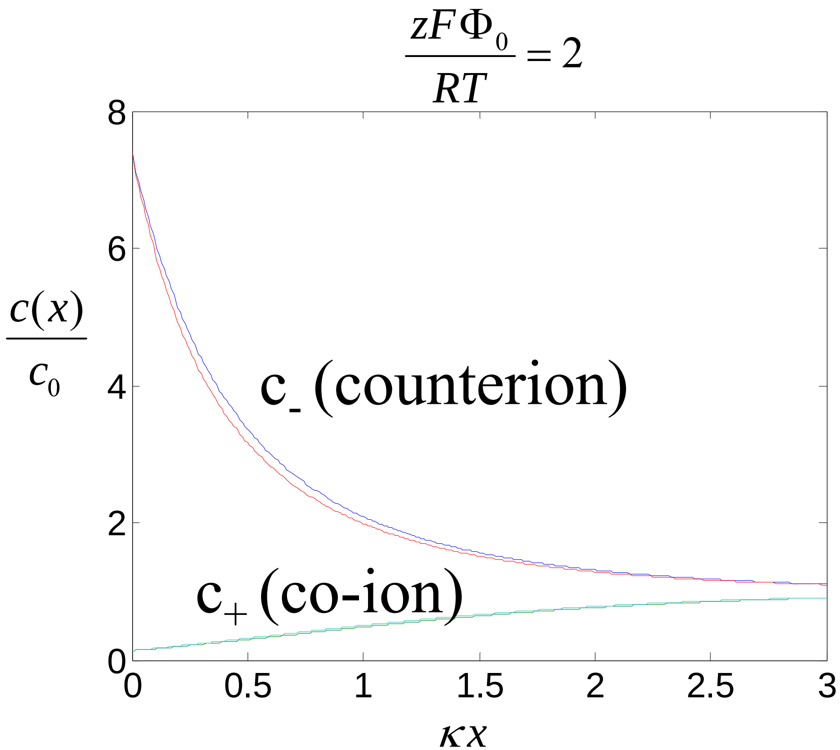


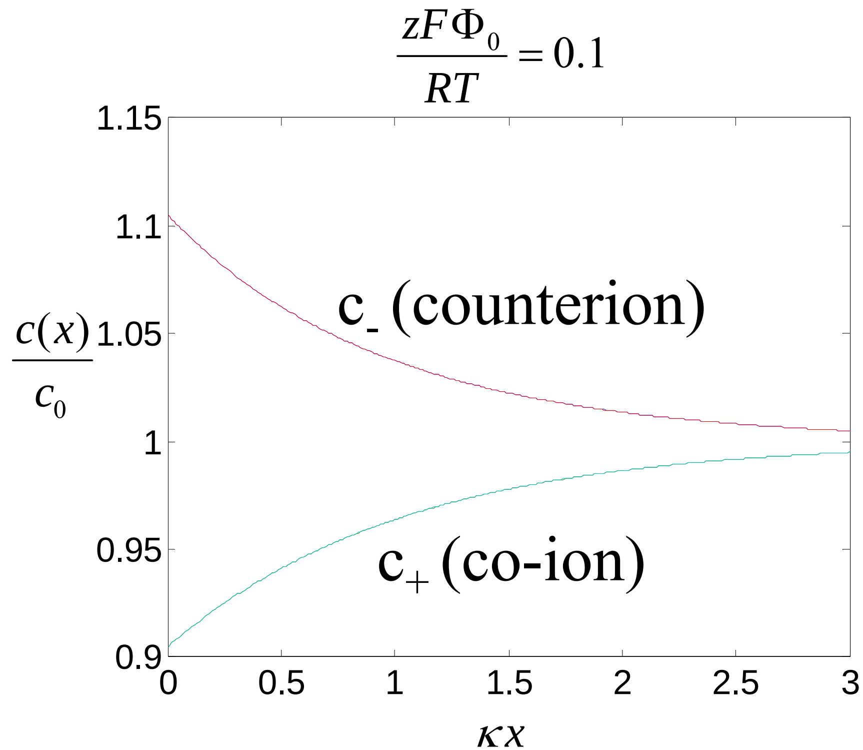
Exact solution

$$\Phi(x) = \frac{2RT}{zF} \ln\left[\frac{1 + \mathrm{e}^{-\kappa x}\tanh\left(\dfrac{zF\Phi_0}{4RT}\right)}{1 - \mathrm{e}^{-\kappa x}\tanh\left(\dfrac{zF\Phi_0}{4RT}\right)}\right], \quad \kappa = \left(\frac{2z^2F^2c_0}{\varepsilon RT}\right)^{1/2}$$

Debye-Huckel approximation

$$\Phi(x) = \Phi_0 e^{-\kappa x} \qquad \text{When} \qquad zF\Phi_0 << RT$$



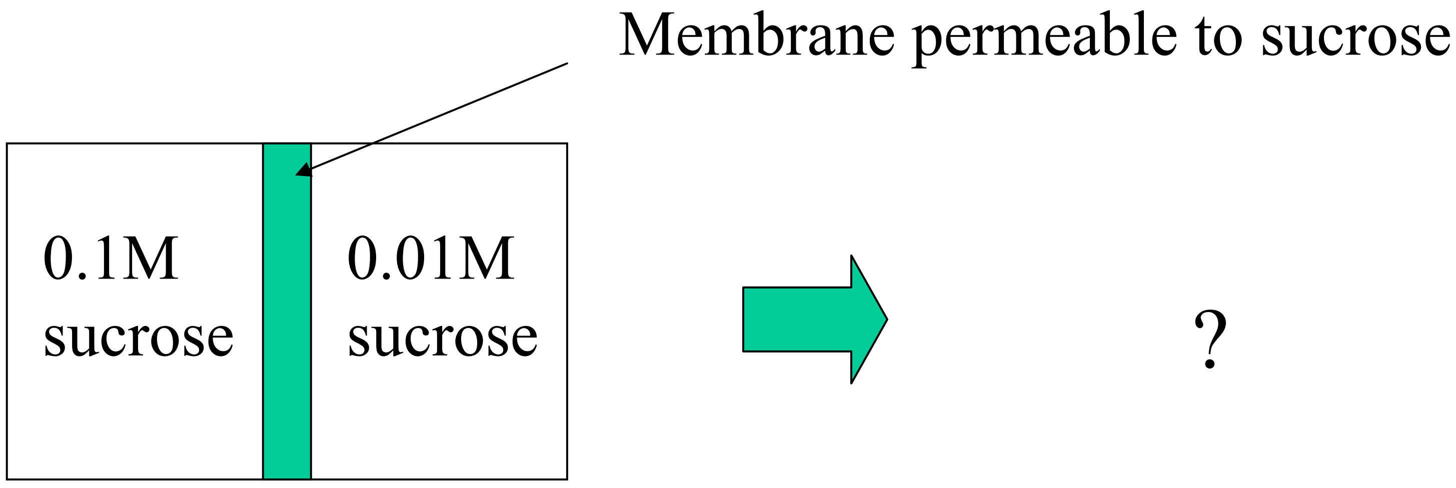


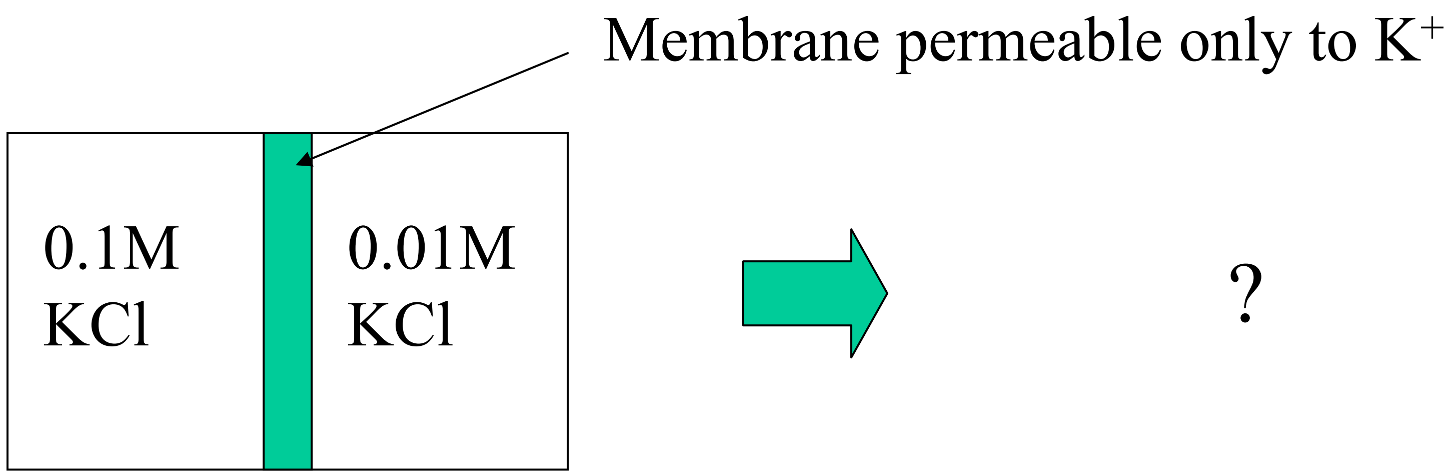
When $zF\Phi_0 << RT \quad (ze\Phi_0 << kT)$

thermal energy >> electrical potential energy
(diffusion dominates.)

When $zF\Phi_0 >> RT \quad (ze\Phi_0 >> kT)$

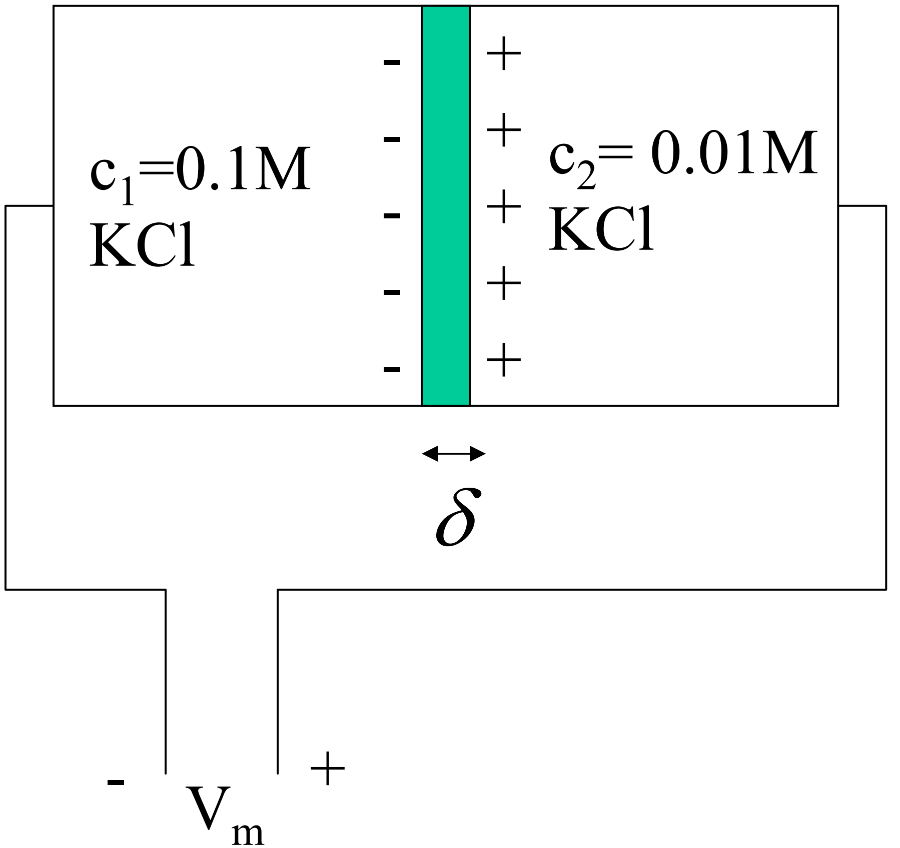
thermal energy << electrical potential energy
(drift dominates. significant charge accumulation)


Membrane permeable to sucrose
0.1M sucrose
0.01M sucrose
?


Membrane permeable only to K+
0.1M KCl
0.01M KCl
?

Nernst Equilibrium Potential

Membrane permeable only to K^+



c: K+ concentration

$$-D\frac{dc}{dx} + E \cdot u \cdot c = 0 \qquad E = -\frac{d\Phi}{dx}$$

$$-D\frac{dc}{c} = u \cdot \frac{d\Phi}{dx}dx$$

$$-D\int_{x=0}^{x=\delta} \frac{dc}{c} = u \cdot \int_{x=0}^{x=\delta} \frac{d\Phi}{dx}dx$$

$$-D\ln\left(\frac{c_2}{c_1}\right) = u\left[\Phi(x=\delta) - \Phi(x=0)\right]$$

$$\Delta\Phi_{12} = \Phi_1 - \Phi_2 = \frac{D}{u}\ln\left(\frac{c_2}{c_1}\right) = \frac{RT}{zF}\ln\left(\frac{c_2}{c_1}\right)$$

Nernst Equilibrium potential

Diffusion of charged particles -> generate electric field -> stops diffusion of ions

Quasi-Electrostatics

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

$$\frac{1}{\mu}\nabla\times\vec{B} = \vec{J}_e + \varepsilon\frac{\partial\vec{E}}{\partial t}$$

0

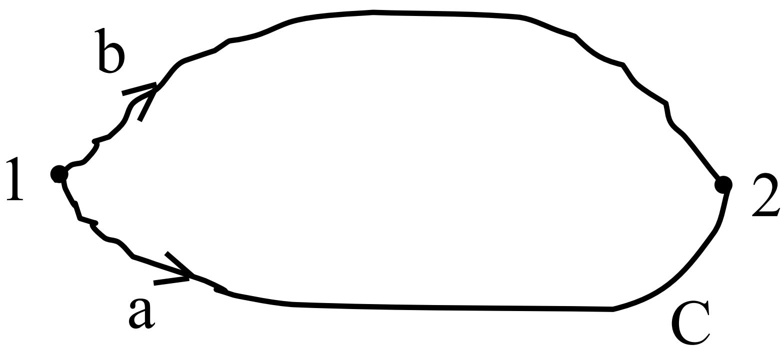
$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

0

$$\nabla\cdot\vec{B} = 0$$

$$\nabla\times\vec{E} = 0 \quad\Rightarrow\quad \oint_S\left(\nabla\times\vec{E}\right)\cdot d\vec{s} = \oint_C \vec{E}\cdot d\vec{l} = 0$$

$$\int_{1(a)}^{2}\vec{E}\cdot d\vec{l} - \int_{1(b)}^{2}\vec{E}\cdot d\vec{l} = 0$$



Electrostatic force : conservative

Potential function Φ can be defined.

$$\Phi(2)-\Phi(1) = -\int_{1}^{2}\vec{E}\cdot d\vec{l}$$

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

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

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

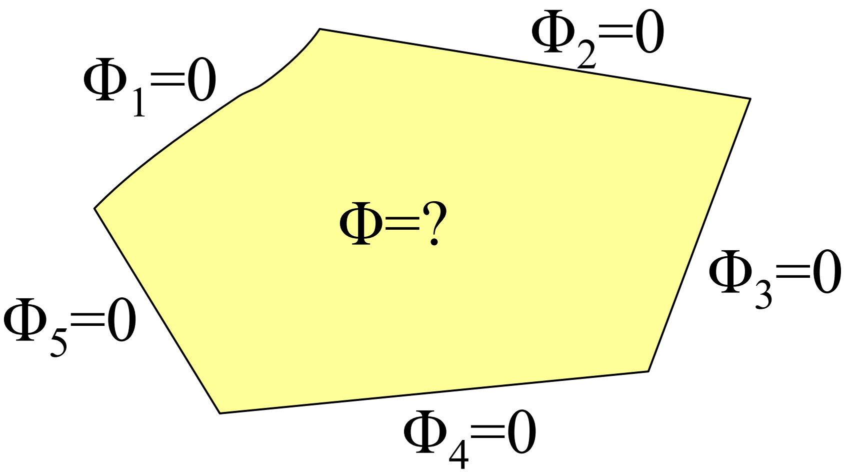
It all comes down to solving….. $\nabla^2\Phi = 0 \quad (Laplace's\ Equation)$

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

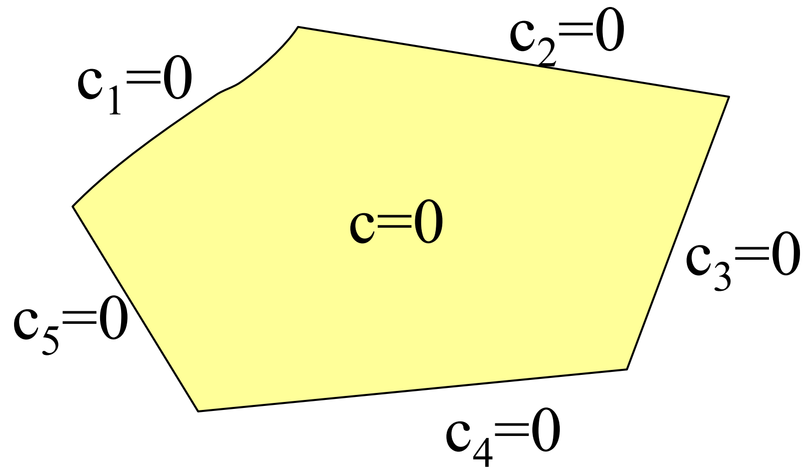
$\vec{q} = -k\nabla T$ (Fourier's law for heat conduction)

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

Electrostatics

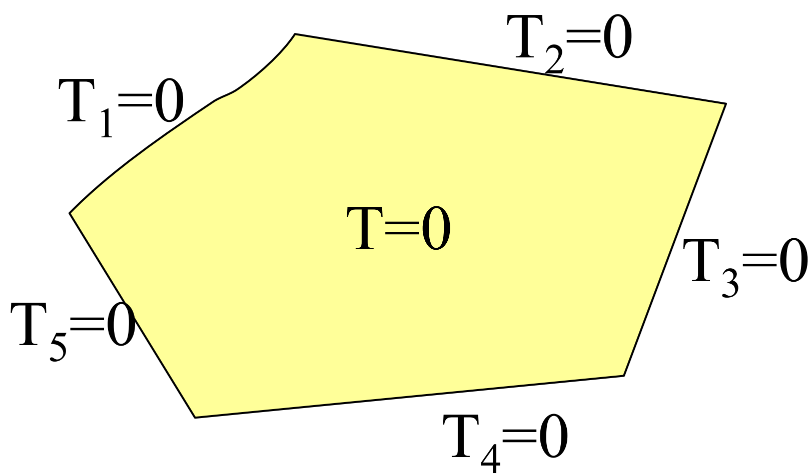


Steady state diffusion $\nabla^2 c = 0$



Thermal conduction

$$\nabla^2 T = 0$$



Uniqueness of Solution

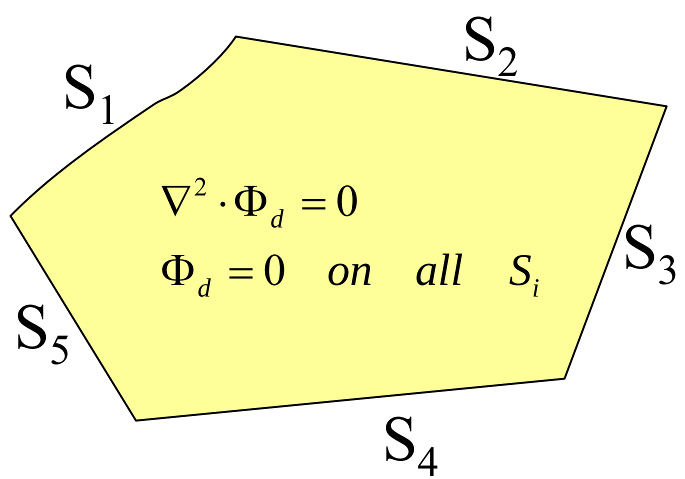
Let's assume two different solutions, Φ_a and Φ_b

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

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

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.)

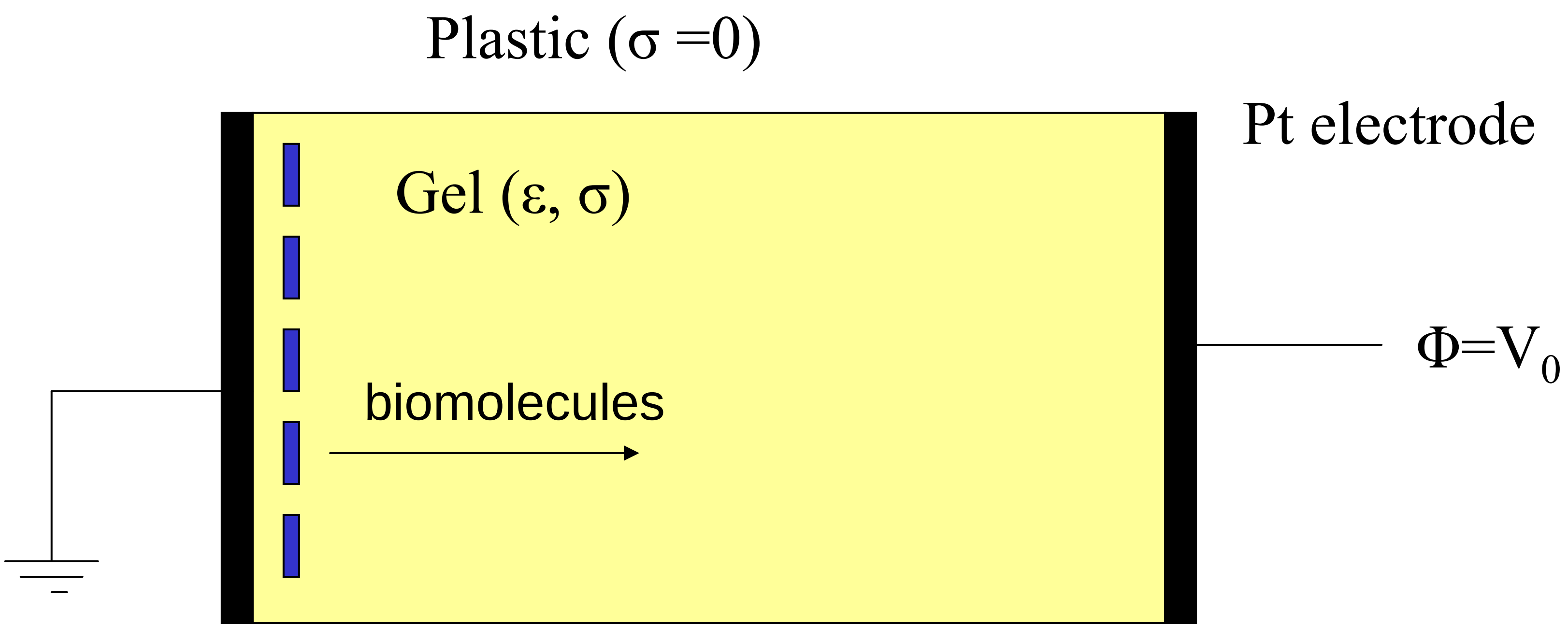


Answer:

$$\Phi_d = 0$$ for everywhere

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

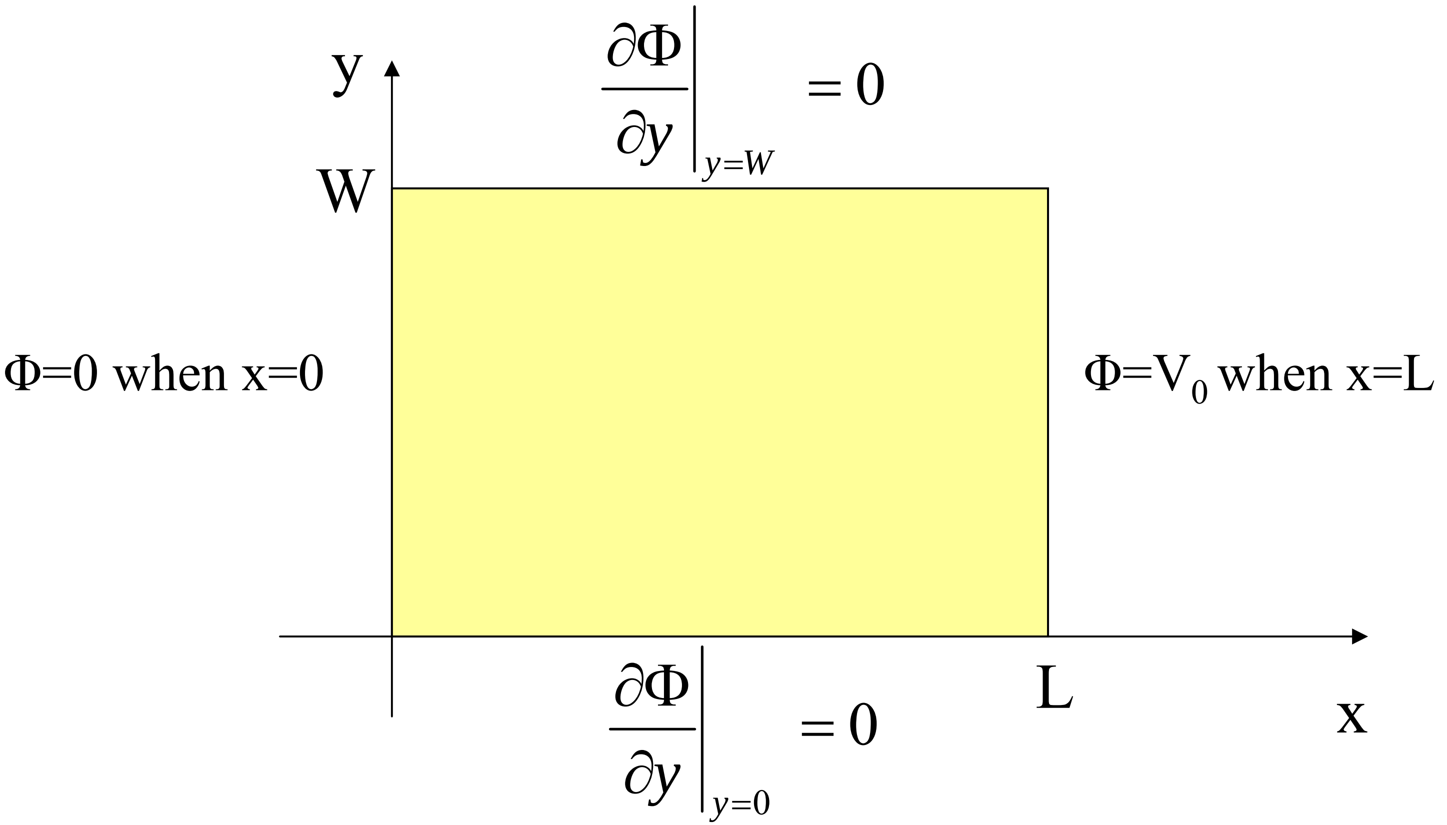
Gel Electrophoresis



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

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

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



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

$$\vec{J} = J_x \hat{x}$$

➡ $$J_y = \sigma E_y = 0 = \left.\frac{\partial \Phi}{\partial y}\right|_{y=0\ or\ W}$$

J=0 (insulator)

Boundary Conditions (For EQS approximation)

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

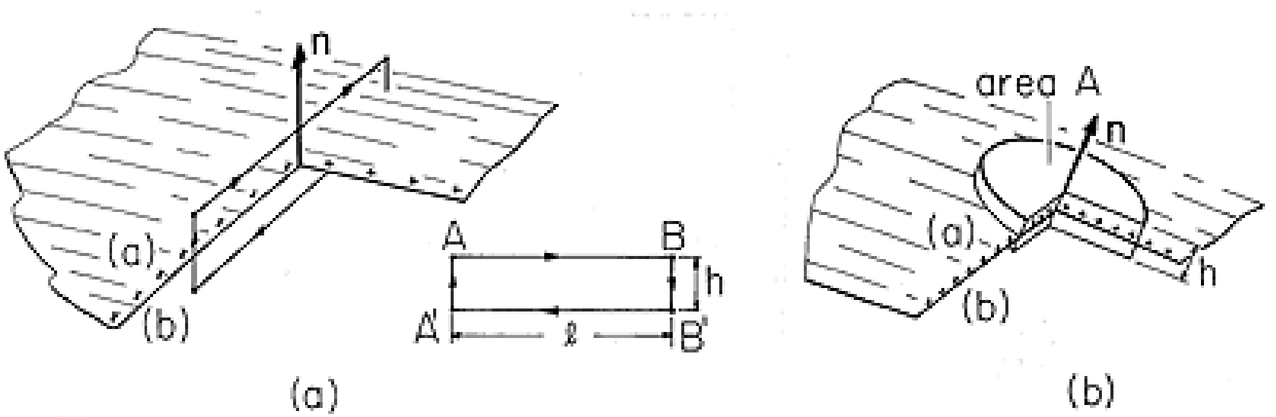
$$\hat{n}\cdot(\varepsilon_1\vec{E}_1-\varepsilon_2\vec{E}_2)=\sigma_s$$

$$\nabla\times\vec{E}=0$$

$$\hat{n}\times\vec{E}_1=\hat{n}\times\vec{E}_2 \quad \left(\vec{E}_1\Big|_{\text{tangential}}=\vec{E}_2\Big|_{\text{tangential}}\right)$$

$$\nabla\cdot\vec{J}=-\frac{\partial\rho}{\partial t}$$

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

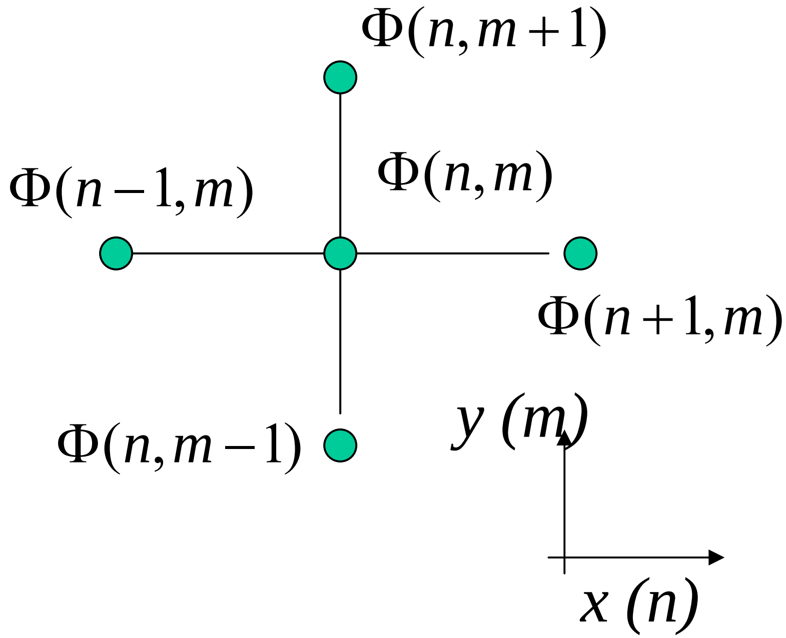


From H&M

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

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

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



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

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

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

$$= \Phi(n+1, m) + \Phi(n-1, m) - 2\Phi(n, m)$$

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

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

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