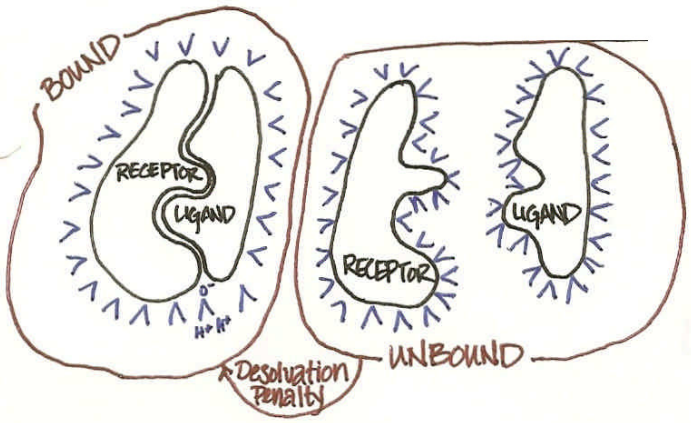
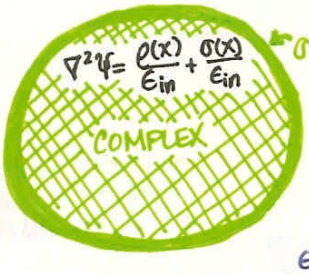


MODELING



$\nabla^2\psi = 0$

$\epsilon_r = \frac{\epsilon_{out}}{\epsilon_{in}}$

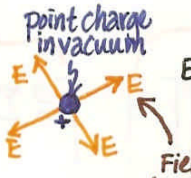
Choose $\sigma(x)$ so that:

$\frac{\partial\psi}{\partial n}_{inside} = \epsilon_r \frac{\partial\psi}{\partial n}_{outside}$ [original]

$\frac{\partial\psi}{\partial n}_{inside} - \frac{\partial\psi}{\partial n}_{outside} = -4\pi\frac{\sigma(x)}{\epsilon_{in}}$ [fictitous problem]

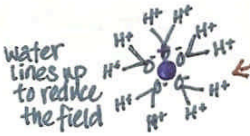
CONTINUUM MODEL

Outside water:



$E = \nabla_x\left(\frac{q}{\epsilon_0|x-x'|}\right)$

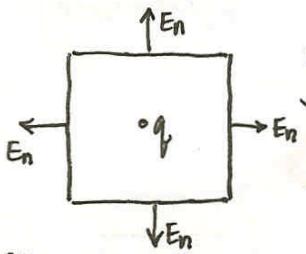
in water:



Field produced by pt charge in water is less than that in a vacuum

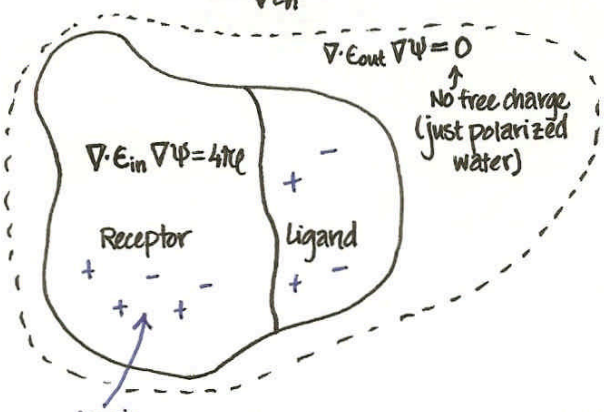
$E = \nabla_x\left(\frac{q}{\epsilon_r\epsilon_0|x-x'|}\right)$

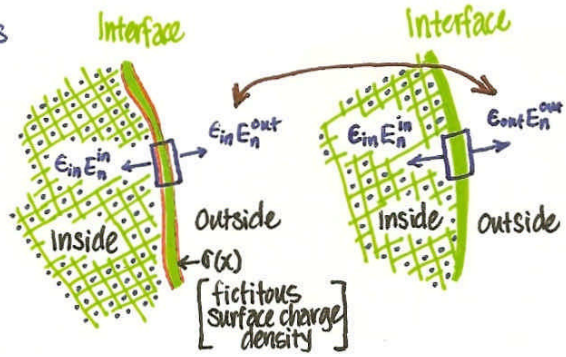
relative epsilon $\epsilon_r \sim 40\text{-}80 > 1$



$\int_{surface} E\cdot dn = \int_{V_d} 4\pi\frac{\rho(x)}{\epsilon}dx$

$\nabla\cdot E = 4\pi\frac{\rho}{\epsilon}$





$\epsilon_r = \frac{\epsilon_{out}}{\epsilon_{in}}$

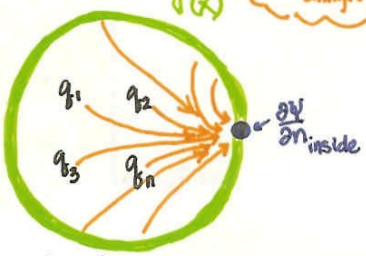
Choose $\sigma(x)$ so that:

$\frac{\partial\psi}{\partial n}_{inside} = \epsilon_r \frac{\partial\psi}{\partial n}_{outside}$ [original]

$\frac{\partial\psi}{\partial n}_{inside} - \frac{\partial\psi}{\partial n}_{outside} = -4\pi\frac{\sigma(x)}{\epsilon_{in}}$ [fictitous problem]

$\frac{\epsilon_{in}}{4\pi\epsilon_r}(1-\epsilon_r)\frac{\partial\psi(\vec{x}_{ci})}{\partial n}_{inside} = \sigma(\vec{x}_{ci})$ — $\vec{x}_{ci}$: center of the i^{th} panel

$\frac{\partial}{\partial n}\left(\sum_{\text{Atomic charges}} + \sum_{\text{Panels}}\right)$



Interaction between atomic charges is changed by surrounding water

$\psi(x)_{Panel_i} = \int_{Panel_i}\frac{\sigma_i}{\epsilon_0|x-x'|}ds'$

$\psi(x) = \underbrace{\sum_{\text{atomic charges}}^{M}\frac{q_i}{\epsilon_{in}|\vec{x}-\vec{x}_i|}}_{\psi_A} + \underbrace{\sum_{\text{panel charges}}^{N}\int_{Panel_i}\frac{\sigma_i}{\epsilon_{in}|\vec{x}-\vec{x}_i|}}_{\psi_P}$

Panel net charge $\sigma_i \cdot$ Panel

Better image on next page