LECTURE 8: CONTINUUM ELECTROSTATICS MODELING II

TUESDAY 7 MARCH 2006

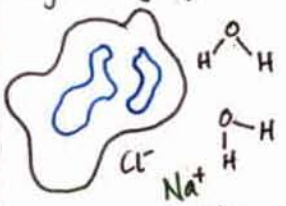
TWO CASES:

Periodic case "crystal"

Ewald Sums

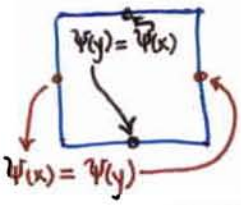
$\nabla^2\psi = \frac{4\pi\rho}{\epsilon}$

Surrounded by water (salt)



$\psi(r) = \int \frac{\rho(\vec{r}')}{\epsilon|\vec{r}-\vec{r}'|}\,dr$

PERIODIC CASE:



Periodic Boundary Conditions on Potential

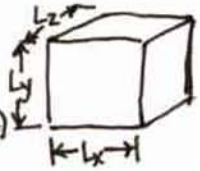
Fourier Series Coeffs for potential

$$\sum_{m_x,m_y,m_z=-\infty}^{\infty} \underline{U}(m_x,m_y,m_z)\, e^{j2\pi\left(\frac{m_x}{L_x}x+\frac{m_y}{L_y}y+\frac{m_z}{L_z}z\right)}$$

(indices; periodic function)

Fourier Series Coefficients for Potential

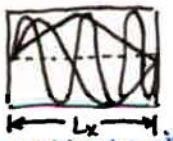
$$\underline{U}(m_x,m_y,m_z) = \frac{4\pi}{(2\pi)^2\vec{m}^2}\cdot\underline{\sigma}(m_x,m_y,m_z)$$



(∇^2 doesn't mix frequency) F.S. for charge

$[m_x\ m_y\ m_z]$

$$\sigma(\vec{r}) = \sum \underline{\sigma}(\vec{m})\cdot e^{j2\pi\vec{m}\cdot\vec{r}}$$



→ multiply by $e^{-j2\pi\vec{m}\cdot\vec{r}}$ & integrate

$$\underline{\sigma}(\vec{m}) = \frac{1}{L_xL_yL_z}\int_V \sigma(\vec{r})e^{j2\pi(\vec{m}\cdot\vec{r})}dV'$$

$$\hat{\sigma}(\vec{r}) = \sum q_i\delta(\vec{r}-\vec{r}_i')$$

$$\underline{\sigma}(\vec{m}) = \frac{1}{V}\sum_{i=1}^{N} q_i e^{j2\pi\vec{m}\cdot\vec{r}_i}$$

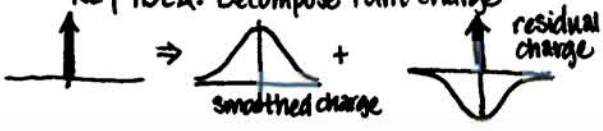
FROM MATCHING:

$$\underline{U}(\vec{m}) = \frac{1}{\pi V}\sum q_i\frac{e^{j2\pi\vec{m}\cdot\vec{r}_i}}{(\vec{m}\cdot\vec{m})}$$

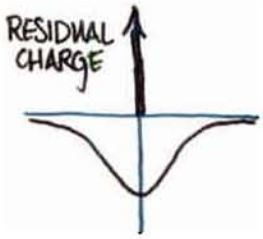
$|m|^2$

$\underline{U}(\vec{m}) \propto \frac{1}{|m|^2}$ ⇒ SLOW DECAY

KEY IDEA: Decompose Point Charge



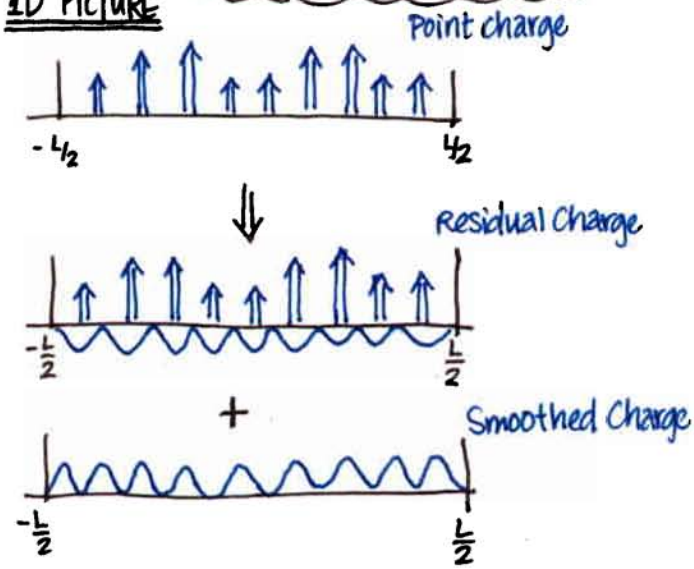
Fourier series of potential due to smoothed σ
- decays exponentially fast in Fourier space
- few Fourier Coef's can be truncated



Potential dies exponentially fast in physical space
- can be truncated

NOTE: Not charge neutral

1D PICTURE

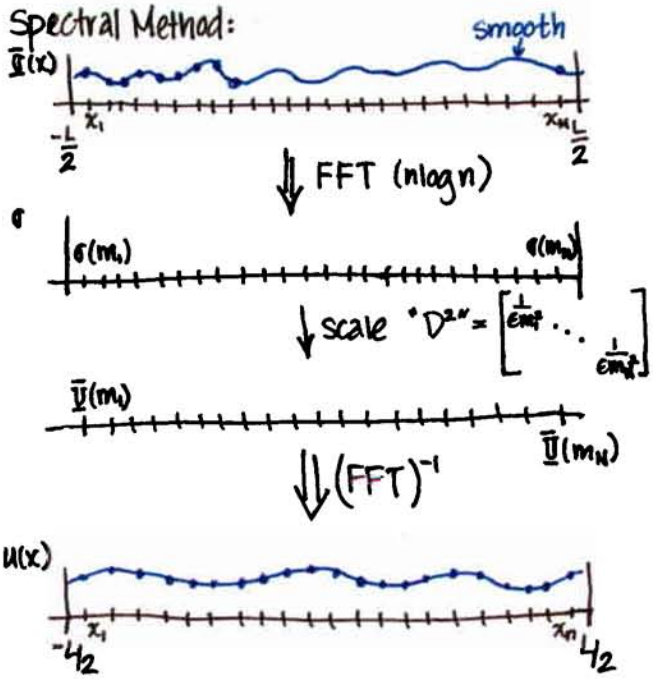


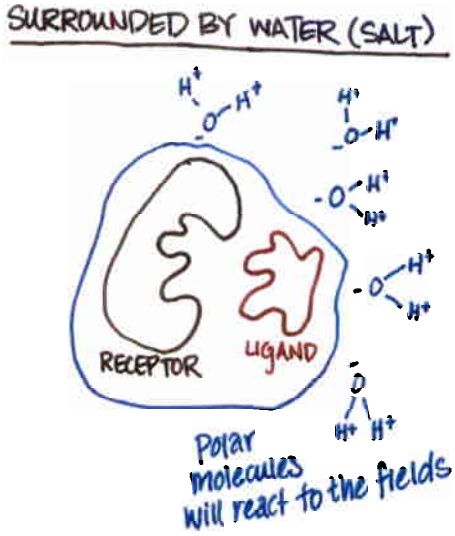
1.) Potential due to ρ residual affects nearby points only ($O(N)$ ops constant # pots per residual charge)

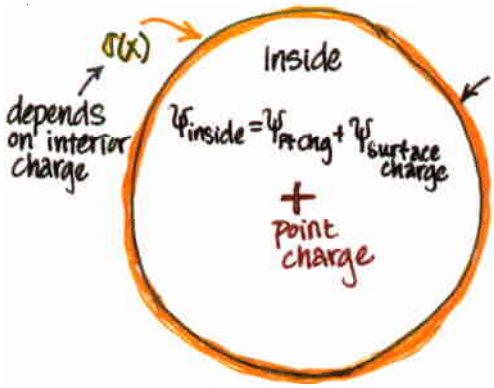
2.) Use Spectral Method to compute: $\nabla^2 u_{smooth} = \frac{4\pi\rho_{smooth}}{\epsilon}$

3.) Add results

Spectral Method:







ψ due to σ(x) matches (inside) water concentration

Original Problem: