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## Problem 2

CFL condition:  $\frac{v \Delta t}{\Delta x} \leq 1$  sol of form  $f(t, x) = \xi^t e^{ikx}$

$$f(t + \Delta t, x) - f(t - \Delta t, x) = -v \frac{f(t, x + \Delta x) - f(t, x - \Delta x)}{\Delta x}$$

$$\xi^{t+\Delta t} e^{ikx} - \xi^{t-\Delta t} e^{ikx} = -v \frac{\xi^t e^{ik(x+\Delta x)} - \xi^t e^{ik(x-\Delta x)}}{\Delta x}$$

$$\xi^{t+\Delta t} e^{ikx} - \xi^{t-\Delta t} e^{ikx} = -\frac{v \Delta t}{\Delta x} \left( \xi^t e^{ik(x+\Delta x)} - \xi^t e^{ik(x-\Delta x)} \right)$$

$$\xi^{\Delta t} - \xi^{-\Delta t} = -\frac{v \Delta t}{\Delta x} (e^{ik\Delta x} - e^{-ik\Delta x})$$

$$\xi^{2\Delta t} - 1 = -\frac{v \Delta t}{\Delta x} \xi^{\Delta t} 2i \sin(k\Delta x)$$

$$\xi^{2\Delta t} + 2i \frac{v \Delta t}{\Delta x} \sin(k\Delta x) \xi^{\Delta t} - 1 = 0 \quad (\text{let } \Delta t = 1)$$

$$\xi = -\frac{i v \Delta t \sin(k\Delta x)}{\Delta x} \pm \sqrt{1 - \left( \frac{v \Delta t \sin(k\Delta x)}{\Delta x} \right)^2}$$

if  $|\xi| = 1$ , energy stable

if  $\frac{v \Delta t}{\Delta x} > 1$  then  $\sqrt{1 - \left( \frac{v \Delta t \sin(k\Delta x)}{\Delta x} \right)^2}$  complex and  $|\xi| > 1$

if  $\frac{v \Delta t}{\Delta x} \leq 1$  then  $\sqrt{1 - \left( \frac{v \Delta t \sin(k\Delta x)}{\Delta x} \right)^2}$  real

$$|\xi|^2 = \left( \frac{v \Delta t \sin(k\Delta x)}{\Delta x} \right)^2 + 1 - \left( \frac{v \Delta t \sin(k\Delta x)}{\Delta x} \right)^2$$

$$|\xi| = 1$$

$$\therefore \frac{v \Delta t}{\Delta x} \leq 1 \text{ necessary!}$$

2.

a)  $V = -\frac{1}{4\pi\epsilon_0} \rho_{\text{in}}(r) \quad \nabla^2 V = \rho \quad \rho = V - \bar{V}_{\text{in}} \text{ is bands}$

Convolve  $\rho$  with  $\frac{1}{r}$  to get  $V$

Solving  $Av = b$   $\begin{cases} \neq 0 \text{ surface} \\ 0 \text{ elsewhere} \end{cases}$

Conjugate gradient

Way of approximately solving  $Ax = b$

Search directions:  $P_n$

$P_n^T A P_n \propto \delta_{nn}$   $P_n$  are orthogonal to each other

Say  $Ax = b \quad \begin{cases} x = \sum \alpha_n P_n \\ b = \sum \alpha_n A P_n \end{cases}$

$$P_n^T A x = P_n^T b$$

$$= P_n^T A P_n \alpha_n = 0 \text{ unless } n' = n$$

$$= \alpha_n \delta_{nn'}$$

$Ax = b \Rightarrow$  remap to minimize  $\frac{x^T A x - x^T b}{2}$

$$V_{\text{in bands}} = P_{\text{bands}} @ g(r) \quad g(r) = \text{green's function}$$

$$V_{\text{in bands}} = \text{IFFT}(\hat{g}(u) \cdot \text{FFT}(\rho))$$

$$U_b = \text{FFT} \cdot \hat{g} \cdot \text{FT} \cdot \rho \Rightarrow \text{FFT} \cdot \hat{g} \cdot \text{FT} = A$$

$$U_b = A P_b$$

get a  $m$  and plot  $m$