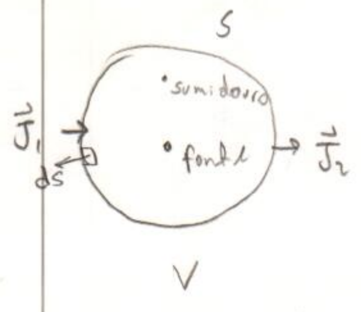
1/19

19/03/2019

Equação de Reação-Difusão

$f \to$ densidade de massa ?



$$\frac{d}{dt}\int_V f(x,t)\,dV = -\int_S \vec{J}\,ds + \int_V S\,dV$$

Pelo Teorema da Divergência:

$$\int_S \vec{J}\cdot ds = \int_V \nabla\cdot\vec{J}\,dV$$

$$\int_V \left(\frac{\partial}{\partial t}f(x,t) + \nabla\cdot\vec{J} - S(x,t)\right) dV = 0$$

$$\frac{\partial}{\partial t}f(x,t) = -\nabla\cdot\vec{J} + S(x,t)$$

Lei de Fick

$$\vec{J} = -D\vec{\nabla} f$$

$$\frac{\partial}{\partial t}f(x,t) = D\nabla^2 f + S(x,t)$$

Adicionando drift:

$$\boxed{\underbrace{\frac{\partial f}{\partial t} = D\nabla^2 f}_{\text{eq. da difusão}} \underbrace{- \vec{v}\cdot\vec{\nabla} f}_{\substack{\text{Termo de deriva} \\ \text{(drift)}}} + \underbrace{S(x,t)}_{\substack{\text{Termo de} \\ \text{fontes ou sumidouros}}}}$$

EXEMPLO SIMPLES:

Equação da Difusão:

$$\frac{\partial f}{\partial t} = D\nabla^2 f \xrightarrow{\text{unidimensional}} \boxed{\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}} \quad (*)$$

Método FTCS

$t = 0, \Delta t, 2\Delta t, \dots, n\Delta t \to t_n$

$x = 0, \Delta x, 2\Delta x, \dots, j\Delta x \to x_j$

$$f(x,t) \to f(x_j, t_n) \equiv f_j^n$$

Cond. Inicial:

$f(0,x)\ \forall\ x \in [0, L]$

Cond. de contorno: (Periódica)

$$f(t,0) = f(t,L)$$

Discretização

$$\frac{\partial f(x,t)}{\partial t} = \frac{f(x,t+\Delta t) - f(x,t)}{\Delta t} = \frac{f_j^{n+1} - f_j^n}{\Delta t}$$

$$\frac{\partial^2 f(x,t)}{\partial x^2} = \frac{\partial}{\partial x}\left[\frac{f(x+\Delta x,t) - f(x,t)}{\Delta x}\right]$$

$$= \frac{1}{\Delta x}\left[\frac{f(x+\Delta x,t) - f(x,t)}{\Delta x} - \frac{(f(x,t) - f(x-\Delta x,t))}{\Delta x}\right]$$

$$= \frac{1}{\Delta x^2}\left[f_{j+1}^n + f_{j-1}^n - 2f_j^n\right]$$

substituindo em (*):

$$\boxed{f_j^{n+1} = f_j^n + \frac{D\Delta t}{\Delta x^2}\left[f_{j+1}^n + f_{j-1}^n - 2f_j^n\right]}$$

↳ Passo de iteração.

função de cópia de listas

copy.deepcopy(L)

21/03/2019

Análise de estabilidade linear do método FCTS ($\Delta x \equiv h$)

Propõe-se solução: $f_j^n = A^n e^{iqjh}$ q: vetor de onda

A) <u>Eq. de difusão:</u> $\frac{\partial f}{\partial t} = D \frac{\partial f}{\partial x^2} \longrightarrow f_j^{n+1} = f_j^n + \frac{D\Delta t}{\Delta x^2}\left(f_{j+1}^n + f_{j-1}^n - 2 f_j^n\right)$

$$A^{n+1} e^{iqjh} = A^n e^{iqjh} + K\left(A^n e^{iqh(j+1)} + A^n e^{iqh(j-1)} - 2A^n e^{iqhj}\right)$$

$$A^{n+1} = A^n + K\left(A^n e^{iqh} + A^n e^{-iqh} - 2A^n\right)$$

$$A^{n+1} = A^n\left(1 + 2K\left(\cos(qh)\right) - 1\right) \longrightarrow \text{Mas } \cos(2a) = \cos^2(a) - \operatorname{sen}^2(a) = 1 - \operatorname{sen}$$

$$= 1 - 2\operatorname{sen}^2(a)$$

$$A^{n+1} = A^n\left(1 - 4K\operatorname{sen}^2\left(\frac{qh}{2}\right)\right)$$

$$\cos(2a) - 1 = -2\operatorname{sen}^2(a)$$

$$\xi \equiv \left|\frac{A^{n+1}}{A^n}\right| < 1 \longrightarrow \text{Na pior hipótese: } \operatorname{sen}^2\frac{qh}{2} = 1$$

$$\xi = 1 - 4K\operatorname{sen}^2\left(\frac{qh}{2}\right)$$

$$\xi = |1 - 4K| < 1 \quad \begin{cases} 1 - 4K < 1 \rightarrow \boxed{K > 0} \\ -1 < 1 - 4K \rightarrow \boxed{K < \frac{1}{2}} \end{cases}$$

B) <u>Equação de deriva:</u> $\frac{\partial f}{\partial t} = -\vec{v}\,\vec{\nabla} f$

$$\frac{\partial f}{\partial t} = -v_x \frac{\partial f}{\partial x}$$

Aplicando o método FTCS:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = -\frac{v_x}{2}\left[\frac{f_{j+1}^n - f_j^n}{\Delta x} + \frac{f_j^n - f_{j-1}^n}{\Delta x}\right]$$

$$f_j^{n+1} = f_j^n - \frac{v_x \Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right)$$

Método de Lax

Substituir f_j^n por $\frac{1}{2}\left(f_{j+1}^n - f_{j-1}^n\right)$

$$f_j^{n+1} = \frac{1}{2}\left(f_{j+1}^n + f_{j-1}^n\right) - \frac{v\Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right)$$

* Testar estabilidade do método de Lax na eq. da deriva

28/03/2019

Procedimentos Explícito, implícito e Crank-Nicholson

$$\frac{\partial f(\vec{r},t)}{\partial t} = L_{\vec{r}}\, f(\vec{r},t) + s(\vec{r},t)$$

$L_{\vec{r}} \rightarrow \vec{v}_0 \cdot \vec{\nabla}$, ∇^2, $-s_0$ ← operador

Explícito: $f^{n+1}(\vec{r}) - f^{n}(\vec{r}) = \Delta t \left[L_{\vec{r}} f^{n}(\vec{r}) + s(\vec{r}) \right]$

Implícito: $f^{n+1}(\vec{r}) - f^{n}(\vec{r}) = \Delta t \left[L_{\vec{r}} f^{n+1}(\vec{r}) + s(\vec{r}) \right]$

$$f^{n+1}(\vec{r}) - f^{n}(\vec{r}) = \frac{\Delta t}{2} \left[L_{\vec{r}} \left(f^{n+1}(\vec{r}) + f^{n}(\vec{r}) \right) + 2\, s(\vec{r}) \right]$$

$$f^{n+1}(\vec{r}) \left(1 - \frac{\Delta t}{2} L_{\vec{r}}\right) = f^{n}(\vec{r}) \left(1 + \frac{\Delta t}{2} L_{\vec{r}}\right) + \Delta t\, s(\vec{r})$$

$$\boxed{f^{n+1}(\vec{r}) = \frac{\overbrace{\left(1 + \frac{\Delta t}{2} L_{\vec{r}}\right)}^{\overleftrightarrow{M}}}{\underbrace{\left(1 - \frac{\Delta t}{2} L_{\vec{r}}\right)}_{\overleftrightarrow{E}}} f^{n}(\vec{r}) + \frac{\Delta t}{\underbrace{\left(1 - \frac{\Delta t}{2} L_{\vec{r}}\right)}_{\overleftrightarrow{E}}} s(\vec{r})}$$

Escrevendo na forma matricial:

$\left(\overleftrightarrow{M} = \overleftrightarrow{I} + \frac{\Delta t}{2} \overleftrightarrow{L}_r\right)$, $\left(\overleftrightarrow{E} = \overleftrightarrow{I} - \frac{\Delta t}{2} \overleftrightarrow{L}_r\right)$

$$\boxed{f^{n+1} = E^{-1}\left(M f^{n} + \Delta t\, s\right)}$$ ← Crank-Nicholson

Condições de contorno: $M_{1,L}$, $M_{L,1}$, $E_{1,L}$, $E_{L,1}$

Deriva por Crank-Nicholson

$$L_x = -v \frac{\partial}{\partial x} \quad ; \quad \frac{\partial f}{\partial t} = -v \frac{\partial f}{\partial x}$$

(fazendo a média das derivadas)

$$L_x f = \frac{-v}{2\Delta x}\left[f_{j+1} - f_{j-1}\right]$$

$$\left[L_x\right]_{kj} = \frac{-v}{2\Delta x}\left(\delta_{k,j+1} - \delta_{k,j-1}\right) \qquad C \equiv \frac{-v\Delta t}{4\Delta x}$$

$$\overleftrightarrow{M} = \overleftrightarrow{I} + \frac{\Delta t}{2}\overleftrightarrow{L}_x$$

Elementos da matriz: $M_{kj} = \delta_{kj} + c\left(\delta_{k,j+1} - \delta_{k,j-1}\right)$

$$M = \begin{pmatrix} 1 & c & 0 & 0 & 0 & \cdots & -c \\ -c & 1 & c & 0 & 0 & \cdots & 0 \\ 0 & -c & 1 & c & 0 & 0 \cdots & 0 \\ & \vdots & & \ddots & & & \\ & & & & \ddots & & 0 \\ c & 0 & 0 & 0 & \cdots & -c & 1 \end{pmatrix}$$

δ_{ab} são elementos da matriz identidade

$$E = \begin{pmatrix} 1 & -c & 0 & 0 & 0 & \cdots & c \\ c & 1 & -c & 0 & 0 & \cdots & 0 \\ 0 & c & 1 & -c & 0 & \cdots & 0 \\ & & \vdots & & \ddots & & \\ -c & 0 & 0 & \cdots & & c & 1 \end{pmatrix}$$

Difusão e deriva por Crank-Nicholson

02/04/2019

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} - v\frac{\partial f}{\partial x} \equiv \mathcal{L}_r f$$

$$\boxed{f^{n+1} = \underbrace{\left(1 - \frac{dt}{2}\mathcal{L}_r\right)^{-1}}_{E}\underbrace{\left(1 + \frac{dt}{2}\mathcal{L}_r\right)}_{M} f^n}$$

↳ Método de Cronk-Nicholson

$$\delta_{jk} = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases}$$

$$\mathcal{L}_r f = \left[D\frac{\partial^2}{\partial x^2} - v\frac{\partial}{\partial x}\right] f$$

$$\mathcal{L}_r f^n = \frac{D}{\Delta x^2}\left(f^n_{i+1} + f^n_{i-1} - 2f_i\right) - \frac{v}{2\Delta x}\left(f_{i+1} - f_{i-1}\right)$$

$$= \frac{D}{\Delta x^2}\begin{pmatrix} -2 & 1 & 0 & \cdots & 1 \\ 1 & -2 & 1 & \cdots & 0 \\ & & \ddots & & \\ 1 & 0 & \cdots & 1 & -2 \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_L \end{pmatrix} - \frac{V}{2\Delta x}\begin{pmatrix} 0 & 1 & 0 & \cdots & -1 \\ -1 & 0 & 1 & \cdots & 0 \\ 0 & -1 & 0 & 1 \cdots & 0 \\ & & \ddots & & \\ 1 & 0 & \cdots & -1 & 0 \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_L \end{pmatrix}$$

Escrevendo na forma de deltas de Kroenicker

$$\mathcal{L}_r f = \frac{D}{\Delta x^2}\left(\delta_{i+1,j} + \delta_{i-1,j} - 2\delta_{i,j}\right) - \frac{V}{2\Delta x}\left(\delta_{i-1,j} - \delta_{i+1,j}\right)$$

$$E_{ij} = \delta_{ij}\underbrace{\left(1 + \frac{D\Delta t}{\Delta x^2}\right)}_{a} - \delta_{i+1,j}\underbrace{\left(\frac{V\Delta t}{4\Delta x} + \frac{D\Delta t}{2\Delta x^2}\right)}_{b} + \delta_{i-1,j}\underbrace{\left(\frac{V\Delta t}{4\Delta x} - \frac{D\Delta t}{2\Delta x^2}\right)}_{c}$$

$$M_{ij} = \delta_{i,j}\underbrace{\left(1 - \frac{D\Delta t}{\Delta x^2}\right)}_{d} + \delta_{i+1,j}\left(\frac{V\Delta t}{4\Delta x} + \frac{D\Delta t}{2\Delta x^2}\right) - \delta_{i-1,j}\left(\frac{V\Delta t}{4\Delta x} - \frac{D\Delta t}{2\Delta x^2}\right)$$

$$M = \begin{pmatrix} a & -b & 0 & \cdots & 0 & +c \\ +c & a & -b & \cdots & 0 & 0 \\ & & \ddots & & & \\ -b & 0 & \cdots & & +c & a \end{pmatrix} ; \quad E = \begin{pmatrix} d & +b & 0 & \cdots & 0 & -c \\ -c & d & +b & \cdots & 0 & 0 \\ & & \ddots & & & \\ +b & 0 & \cdots & & -c & d \end{pmatrix}$$

$$f^{n+1} = \left(1 - \frac{\Delta t}{2} \mathcal{L}_r\right)^{-1} \left(1 + \frac{\Delta t \mathcal{L}_r}{2}\right) f \qquad \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

$$\mathcal{L}_r f^n = \frac{D}{\Delta x^2}\left(f^n_{i+1} + f^n_{i-1} - 2 f^n_i\right) - \frac{V}{2\Delta x}\left(f^n_{i+1} - f^n_{i-1}\right)$$

$$\mathcal{L}_r f^n_i = \left[\left[\frac{D}{\Delta x^2} - \frac{V}{2\Delta x}\right] \delta_{i+1,j} + \left[\frac{D}{\Delta x^2} + \frac{V}{2\Delta x}\right] \delta_{i-1,j} - \frac{2D}{\Delta x^2} \delta_{i,j}\right] f^n_i$$

$$E = \left(1 - \frac{\Delta t}{2} \mathcal{L}_r\right)$$

$$E = \underbrace{\left[\frac{V\Delta t}{4\Delta x} - \frac{D\Delta t}{2\Delta x^2}\right]}_{-c} \delta_{i+1,j} - \underbrace{\left[\frac{D\Delta t}{2\Delta x^2} + \frac{V\Delta t}{4\Delta x}\right]}_{b} \delta_{i-1,j} + \underbrace{\left[1 + \frac{D\Delta t}{\Delta x^2}\right]}_{a} \delta_{i,j}$$

$$M = \left(1 + \frac{\Delta t}{2} \mathcal{L}_r\right)$$

$$M = \underbrace{\left[\frac{D\Delta t}{2\Delta x^2} - \frac{V\Delta t}{4\Delta x}\right]}_{c} \delta_{i+1,j} + \underbrace{\left[\frac{D\Delta t}{2\Delta x^2} + \frac{V\Delta t}{4\Delta x}\right]}_{b} \delta_{i-1,j} + \underbrace{\left[1 - \frac{D\Delta t}{\Delta x^2}\right]}_{d} \delta_{i,j}$$

$$E \begin{pmatrix} a & -b & 0 & \cdots & -c \\ -c & a & -b & \cdots & 0 \\ & & \ddots & & \\ -b & 0 & \cdots & -c & a \end{pmatrix} ; \quad M = \begin{pmatrix} d & b & 0 & \cdots & c \\ c & d & b & \cdots & 0 \\ & & \ddots & & \\ b & 0 & \cdots & c & d \end{pmatrix}.$$

Teste de estabilidade

$$\frac{f^{n+1} - f^n_i}{\Delta t} = \frac{D}{2\Delta x^2}\left(f^{n+1}_{i+1} + f^{n+1}_{i-1} - 2 f^{n+1}_i\right) + \frac{D}{2\Delta x^2}\left(f^n_{i+1} + f^n_{i-1} - 2 f^n_i\right)$$

11/04/2019

Equação de Onda Eletromagnética e o Fóton

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} \quad ; \quad E = E_0 \cos(kx - \omega t) \quad ; \quad k^2 = \frac{\omega^2}{c^2} \rightarrow \omega = kc$$

Da quantização: $E = h\nu = \hbar\omega$; $p = \hbar k$

$$\Rightarrow \boxed{E = pc}$$

Eq. de Schrödinger

$$E = \frac{p^2}{2m} + V \quad ; \quad p^2 = \hbar^2 k^2$$

$$E = \frac{\hbar^2 k^2}{2m} + V \rightarrow \hbar\omega = \frac{\hbar^2 k^2}{2m} + V$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (A)$$

$$\Psi = A e^{i(kx - \omega t)}$$

$$\frac{\partial \Psi}{\partial t} = -i\omega A e^{i(kx-\omega t)}$$

$$\frac{\partial \Psi}{\partial x} = ik A e^{i(kx-\omega t)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A e^{i(kx-\omega t)}$$

Substituindo em (A):

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V$$

$$H\Psi = -i\frac{\partial \Psi}{\partial t} \quad ; \quad \underbrace{\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{(x)}}_{\text{operador Hamiltoniano}}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x) = i\hbar\frac{\partial \Psi}{\partial t}$$

$$\mathcal{L}_r = -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{(x)}\right)$$

Aplicando para o Método de Crank-Nicholson:

$$\psi^{n+1} = \underbrace{\left(1 + \frac{i\,dt}{2\hbar} H\right)}_{E}^{-1} \underbrace{\left(1 - \frac{i\,dt}{2\hbar} H\right)}_{M} \psi^{n}$$

$E^{*} = M$

Ex: Partícula livre $(V(x) = 0)$

Discretizando H e Ψ como na eq. da difusão:

$$H_{ij}\Psi_j = \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & & \ddots & & & \\ 1 & 0 & 0 & 0 & \cdots 1 & -2 \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{pmatrix}$$

?

$(\hbar = 1 \,,\; m = 1)$

Exemplo:

$$\Psi_k = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \exp\left\{ i k_0 x - (x_k - x_0)^2 / 2\sigma^2 \right\}$$

16/04/2019

Eq. de Schrödinger com potencial $V(x) \neq 0$

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$$

$(m=1)$

$$\Psi^{n+1} = \underbrace{\left(1 + \frac{i\Delta t}{2\hbar}H\right)^{-1}}_{E}\underbrace{\left(1 - \frac{i\Delta t}{2\hbar}H\right)}_{M = E^*}\Psi^n$$

$(\hbar = 1)$

Relembrando método de Crank-Nicholson:

$$\frac{\partial f}{\partial t} = \mathcal{L} f$$

Discretizando: média das derivadas

$$\frac{f^{n+1} + f^n}{\Delta t} = \frac{1}{2}\left(\mathcal{L} f^{n+1} + \mathcal{L} f^n\right)$$

$$f^{n+1} = \left(1 - \frac{\Delta t}{2}\mathcal{L}\right)^{-1}\left(1 + \frac{\Delta t}{2}\mathcal{L}\right)f^n$$

Derivada segunda espacial:

$$-\frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2} \rightarrow -\frac{1}{2}\left(\Psi_{i+1} + \Psi_{i-1} - 2\Psi_i\right)$$

Com $V(x) \neq 0$ a matriz que representa o operador Hamiltoniano fica

$$\hat{H}\Psi = -\frac{1}{2}\begin{pmatrix} -2 & 1 & 0 & \cdots & 1 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & & & 0 \\ 1 & 0 & \cdots & 1 & -2 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_L \end{pmatrix} + \begin{pmatrix} V(x_1) & 0 & 0 & \cdots \\ 0 & V(x_2) & 0 & 0 \\ 0 & 0 & V(x_2) & \\ & & \ddots & \\ 0 & & & V(x_L) \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_L \end{pmatrix}$$

o potencial só adiciona na diagonal então.

$$a = \frac{\Delta t}{4i} \quad ; \quad b = 1 + 2a(1 + V(x))$$

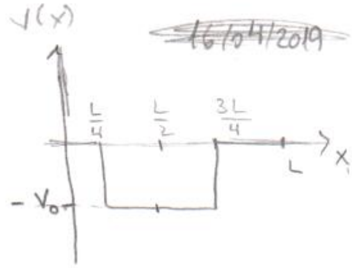
$$E = \left(\mathbb{I} + \frac{i\Delta t}{2}\hat{H}\right) = \begin{pmatrix} b & -a & 0 & \cdots & -a \\ -a & b & -a & \cdots & 0 \\ 0 & -a & b & \cdots & 0 \\ & \vdots & \ddots & \cdots & \\ & \vdots & & & 0 \\ -a & 0 & 0 & & b \end{pmatrix}$$

Iteração temporal ficará:

$$\boxed{\Psi^{n+1} = E^{-1}E^*\Psi^n}$$

~~16/04/2019~~

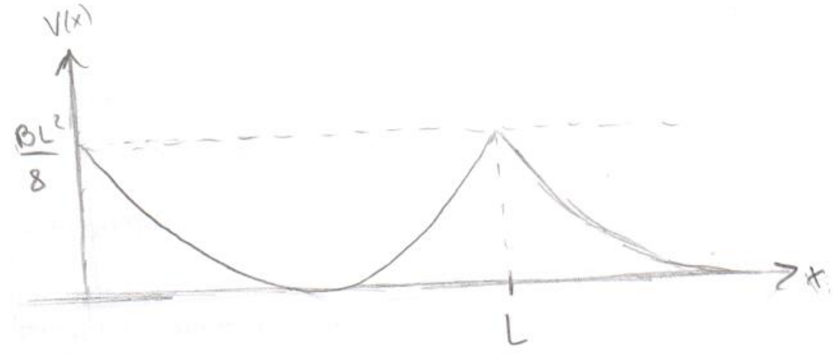
Exercícios:



① Poço quadrado:

$$V(x_i) = \begin{cases} -V_0 & \text{se } |x_i - \frac{L}{2}| < \frac{L}{4} \\ 0 & \text{se } |x_i - \frac{L}{2}| > \frac{L}{4} \end{cases}$$

② Oscilador harmônico:



$$V(x_i) = \frac{B}{2}\left(x_i - \frac{L}{2}\right)^2$$

①a) O que acontece para $\frac{\hbar^2 k_0^2}{2m} \ll V_0$?

b) E para $\frac{\hbar^2 k_0^2}{2m} \approx V_0$?

$$\Psi(x) = A e^{-i\hbar k_0 x} e^{-(x-\frac{L}{2})^2/2\sigma^2}$$

△ Truque para evitar números grandes nas computações de exponenciais:

$$V(x_i) = \frac{B}{2} V_0 \frac{\left(x_i - \frac{L}{2}\right)^2}{\left(\frac{L}{2}\right)^2}$$

Testar conservação de energia:

$$\frac{\langle p^2 \rangle}{2m} = \frac{-\hbar^2}{2m} \int_{-\infty}^{+\infty} \psi^* \frac{\partial^2}{\partial x^2} \psi \, dx$$

Calcular coeficientes de transmissão e reflexão

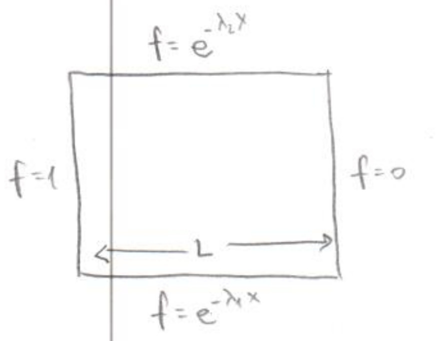
23/04/2019

PROVA (09/05)

Métodos de Relaxação em Duas Dimensões

$$\begin{cases} E = -\nabla U \\ \nabla \cdot E = 0 \end{cases} \rightarrow \nabla^2 U = 0$$

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$$



$$\frac{\partial f}{\partial t} = a\left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}\right) \rightarrow$$

Usando método FCTS:

$$f^{n+1}_{i,j} = f^n_{i,j} + \frac{a\Delta t}{\Delta x^2}\left(f^n_{i+1,j} + f^n_{i-1,j} + f^n_{i,j-1} + f^n_{i,j+1} - 4 f^n_{i,j}\right)$$

$$f^{n+1}_{i,j} \approx f^n_{i,j} \Rightarrow$$ Problema resolvido!

Algoritmo de Jacobi

Critério de estabilidade do FCTS:

$$\frac{a\Delta t}{\Delta x^2} + \frac{a\Delta t}{\Delta y^2} \leq \frac{1}{2} \xrightarrow[\Delta x = \Delta y]{} \frac{a\Delta t}{\Delta x^2} \leq \frac{1}{4}$$

Considerando a igualdade:

$$\boxed{f^{n+1}_{i,j} = \frac{1}{4}\left(f^n_{i+1,j} + f^n_{i-1,j} + f^n_{i,j+1} + f^n_{i,j-1}\right)}$$

Exemplo de método explícito

Algoritmo de Gauss-Seidel

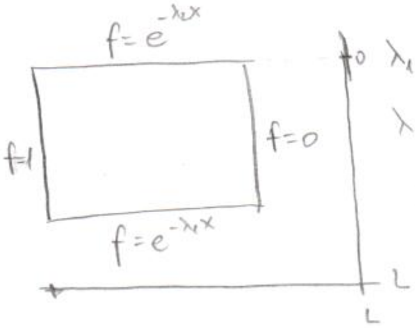
$$\boxed{f^{n+1}_{i,j} = \frac{1}{4}\left(f^n_{i+1,j} + f^{n+1}_{i-1,j} + f^n_{i,j+1} + f^{n+1}_{i,j-1}\right)}$$

Algoritmo de Super-Relaxação

$$\boxed{f^{n+1}_{i,j} = -\alpha f^n_{i,j} + \frac{1+\alpha}{4}\left(f^n_{i+1,j} + f^{n+1}_{i-1,j} + f^n_{i,j+1} + f^{n+1}_{i,j-1}\right)}$$

Exercício: Dada a equação

$\nabla^2 f = 0$ e o contorno



$\lambda_1 = 0.1$

$\lambda_2 = 0.3$

$L = 50$

$tol = 10^{-4}$

Determine o valor de f em cada ponto do espaço.

Compare os tempos de convergência dos 3 métodos.

Exercício

Mostrar que o FCTS aplicado à eq. de Deriva é instável.

Supondo solução na forma $f_j^n = A^n e^{iqjh}$

$$f_j^{n+1} = f_j^n - \frac{V_x \Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right)$$

$$A^{n+1} e^{iqjh} = A^n e^{iqjh} - \frac{V_x \Delta t}{2\Delta x}\left(A^n e^{iqh(j+1)} - A^n e^{iqh(j-1)}\right)$$

$$A^{n+1} = A^n - \frac{V_x \Delta t}{2\Delta x}\left(A^n e^{iqh} - A^n e^{-iqh}\right) \qquad \frac{V_x \Delta t}{2\Delta x} = K$$

$$A^{n+1} = A^n\left(1 + 2i\,sen(qh)\right)$$

$$\left|\frac{A^{n+1}}{A^n}\right|^2 = \left(1 - 2i\,sen(qh)\right)\left(1 + 2i\,sen(qh)\right)$$

$$\left|\frac{A^{n+1}}{A^n}\right|^2 = 1 + 4\,sen^2(qh) \rightarrow$$ instável pois $\left|\frac{A^{n+1}}{A^n}\right| \geq 1$ para qualquer h ou vetor de onda (q).

No limite que $h \to 0$, o método seria estável?

Transformada de Fourier da eq. de Schrödinger

30/04/2019

$$f(x) = \sum_{i=0}^{N-1} \hat{f}_k e^{ikx} \quad ; \quad k_i = \frac{2\pi i}{L} \quad ; \quad i = 0, N-1$$

$$\hat{f}_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)\, e^{-ikx}\, dx$$

$$\sum_k e^{ik(x-x')} = 2\pi\, \delta(x-x')$$

$$\int_{-\pi}^{\pi} dx\, e^{ix(k-k')} = 2\pi\, \delta_{k,k'}$$

$$-i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\, \Psi$$

$$\Psi(x,t) = \sum_k \hat{\varphi}_k(t)\, e^{ikx} \quad ; \quad V(x) = \sum_k V_k(x)\, e^{ikx}$$

$$i\hbar \sum_k e^{ikx} \frac{\partial \hat{\varphi}_k(t)}{\partial t} = \frac{-\hbar^2}{2m} \sum_k (-k^2)\, \hat{\varphi}_k(t)\, e^{ikx} + \sum_{k'} V_{k'}(x)\, e^{ik'x} \sum_k \hat{\varphi}_k(t)\, e^{ikx}$$

$* \int dx\, e^{-iqx}$ (semelhante ao truque de Fourier)

$$i\hbar \sum_k \frac{\partial \varphi_k(t)}{\partial t} \underbrace{\int_{-\pi}^{\pi} dx\, e^{ix(k-q)}}_{2\pi \delta_{k,q}} = \frac{-\hbar^2}{2m} \sum_k (-k^2)\, \hat{\varphi}_k(t) \underbrace{\int dx\, e^{ix(k-q)}}_{2\pi \delta_{k,q}} + \sum_{k,k'} \hat{\varphi}_k V_{k'} \underbrace{\int dx\, e^{ix(k+k'-q)}}_{2\pi \delta_{k,k',q}}$$

$$\boxed{i\hbar \frac{\partial \hat{\varphi}_k}{\partial t} = +\frac{\hbar^2 q^2}{2m} \frac{\partial^2 \hat{\varphi}_k}{\partial x^2} + \sum_k \hat{\varphi}_k\, \hat{v}_{q-k}}$$

↳ Euler-explicito

$$\hat{\varphi}_q^{n+1} = \hat{\varphi}_q^n + \frac{\hbar^2 q^2 \Delta t}{2m} \hat{\varphi}_q^n + \sum_{k=0} \hat{\varphi}_q\, v_{k-q}\, \Delta t$$

02/05/2019

Solução exata da partícula livre no espaço-k

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \xrightarrow[\text{Transformada de Fourier}]{} i\hbar \frac{\partial \hat{\varphi}(t)}{\partial t} = \frac{-\hbar^2}{2m}\hat{\varphi}(t)$$

$$\frac{d\hat{\varphi}}{\hat{\varphi}} = -\frac{i\hbar k^2}{2m}dt \rightarrow \hat{\varphi}(t) = \varphi_0 e^{-\frac{i\hbar k^2}{2m}t}$$

1) Solução exata da partícula livre no espaço-k

2) Solução com integração numérica da partícula livre (no espaço-k)

2.a) Método de Euler Explícito

2.b) Método RK2

07/05/2019

- Simetria conveniente para problema de eq. de Schrödinger pelo método espectral

$$\hat{f}_k = \sum e^{+ikx} f(x)$$

$$\hat{f}^*_{-k} = \hat{f}_k \quad \text{se} \quad f(x) \text{ for real}$$

Método espectral p/ eq. de Schrödinger com potencial não-nulo 07/05/2019

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$$

$$\hat{\varphi}_k^{n+1} = i\frac{k^2}{2}\varphi^n \Delta t + \varphi^n$$

$$\downarrow$$

$$\Psi^{n+1}_{(x)} = \Psi^{n+1}_{(x)} + V(x)\Psi^{n+1}(x)\Delta t$$

RESUMO

Método FTCS

↳ A parte temporal é assimétrica: $\frac{\partial f}{\partial t} \approx \frac{f(x,t+dt) - f(x,t)}{\Delta t}$

↳ A parte espacial é simétrica: $\frac{\partial f}{\partial x} \approx \frac{f(x+dx,t) - f(x-dx,t)}{2\Delta x}$

Assim temos: $\frac{\partial^2 f}{\partial x^2} \approx \frac{f(x+dx,t) + f(x-dx,t) - 2f(x,t)}{\Delta x^2}$

$$f_j^{n+1} = f_j^n + \frac{D\Delta t}{\Delta x^2}\left(f_{j+1}^n + f_{j+1}^n - 2f_j^n\right)$$

(difusão)

↳ condicionalmente estável: $\boxed{\frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}}$

$$f_j^{n+1} = f_j^n - \frac{v\Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right)$$

(deriva) ⟵ Instável → $|G|^2 = 1 + 4\,\text{sen}^2(q\Delta x) \geq 1$

Método de Lax

- Parte do FTCS, mas elimina dependência no ponto central ao substituir: $f_j^n = \frac{1}{2}\left(f_{j+1}^n + f_{j-1}^n\right)$.

$$f_j^{n+1} = \frac{1}{2}\left(1 - \frac{v\Delta t}{\Delta x}\right) f_{j+1}^n + \frac{1}{2}\left(1 + \frac{v\Delta t}{\Delta x}\right) f_{j-1}^n$$

(deriva)

→ condicionalmente estável: $\boxed{\frac{v\,dt}{2\,dx} = \frac{1}{2}}$

Método de Crank-Nicholson

- Assume que $\frac{\partial f}{\partial t} = \mathcal{L}_r f + s(x)$, onde $f = f(x,t)$ e $\mathcal{L}_r$ é um operador que só depende de x e suas derivadas.

Crank-Nicholson faz uma média sobre a aplicação de $\mathcal{L}_r$ com Euler explícito e implícito:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = \frac{1}{2}\left[\mathcal{L}_r f_j^n + \mathcal{L} f_j^{n+1}\right] + s(x)$$

Mantém a média espacial centrada:

$$\frac{df}{dx} = \frac{f_{j+1}^n - f_{j-1}^n}{2\Delta x}$$