Homework 8

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December 19, 2021

1 Solve Poisson Equation

1.1 Question

Solve the Poisson equation with different *rho* and boundary conditions.

$$\nabla^2\phi(x,y) = -\rho(x,y)/\epsilon_0 \tag{1}$$

1.2 Solution

We use Gauss-Seidel Iteration to solve the Poisson equation.

1.3 Psudocode

Algorithm 1 Poisson Equation Solution

Input: x width L_x, y width L_y and step length h,$\rho(x,y)$

Output: Potential distribution $\phi(x,y)$

nx=Lx/h
by=Ly/h
initialize $\phi(x,y)$ with boundary condition
for i in range(iter) do
    for x in range(nx) do
        for y in range(ny) do
            $\phi[x,y] = \frac{1}{4}(\phi[x,y+1]+\phi[x,y-1]+\phi[x+1,y]+\phi[x-1,y]) + \frac{h^2}{4}\rho(x,y)$
        end for
    end for
end for
return $\phi(x,y)$

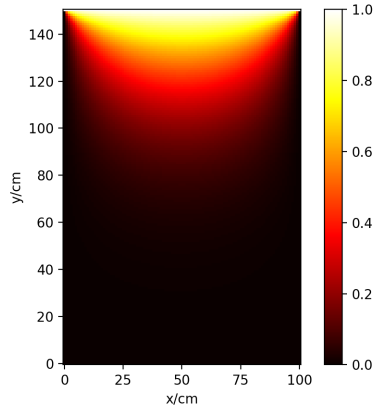

Figure 1: $L_x = 1m, L_y = 1.5m$

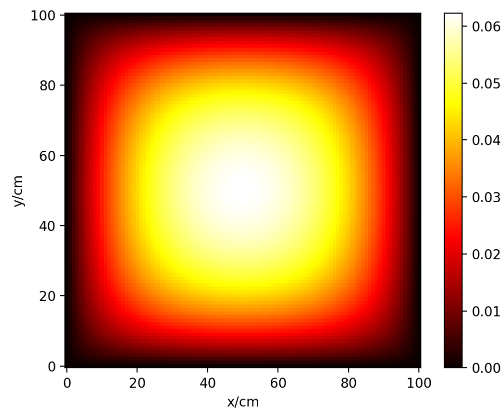

Figure 2: $L_x = 1m, L_y = 1m$

1.4 Results

In Figure 1, we set $\rho(x, y) = 0, \phi(0, y) = \phi(L_x, y) = \phi(x, 0) = 0, \phi(x, L_y) = 1V$.In Figure 2, we set $\rho(x, y)/\epsilon_0 = 1V/m^2, \phi(0, y) = \phi(L_x, y) = \phi(x, 0) = \phi(x, L_y) = 0$.With the increase of the iteration step, the system will eventually reach a full diffusion and get close to the accurate solution.

2 Time-dependent Schrodinger Equation

2.1 Question

Solving the time-dependent Schrodinger Equation with the Crank–Nicolson method with the initial condition

$$\Psi(x,0) = \sqrt{\frac{1}{\pi}} exp[ik_0 x - \frac{(x-\xi_0)^2}{2}] \tag{2}$$

2.2 Solution

When solving the equation with form like

$$-i\frac{\partial \Psi}{\partial t} = -V(x)\Psi(x,t) + \frac{\partial^2 \Psi}{\partial x^2} \tag{3}$$

we discretize the equation and denote $\alpha = \delta t/(\delta x)^2$

$$(-2i\mathbf{I} - \delta t\mathbf{F} + \alpha\mathbf{B})\mathbf{U_j} = (-2i\mathbf{I} + \delta t\mathbf{F} - \alpha\mathbf{B})\mathbf{U_{j-1}} \tag{4}$$

where

$$\mathbf{B} = \begin{bmatrix} 2 & -1 & ... & 0 & 0 \\ -1 & 2 & ... & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & ... & 2 & -1 \\ 0 & 0 & ... & -1 & 2 \end{bmatrix} \tag{5}$$

$$\mathbf{F} = diag(-V_1, -V_2, ..., -V_n) \tag{6}$$

$$\mathbf{U_j} = \begin{bmatrix} \Psi_{1,j} \\ \Psi_{2,j} \\ \Psi_{3,j} \\ \vdots \\ \Psi_{n,j} \end{bmatrix} \tag{7}$$

2.3 Psudocode

Algorithm 2 Schrodinger Equation Solution

Input: number of xs nx, number of ts nt, step length δx and time interval δt

Output: evolution of probability wave $\Psi(x,t)$

1: $\Psi(x,0)$
2: $\alpha = \frac{\delta t}{\delta x^2}$
3: Evaluate $\mathbf{B}$ and $\mathbf{F}$ by (5)(6)
4: **for** i in range(nt) **do**
5: $\quad (-2i\mathbf{I} - \delta t\mathbf{F} + \alpha\mathbf{B})\mathbf{U_j} = (-2i\mathbf{I} + \delta t\mathbf{F} - \alpha\mathbf{B})\mathbf{U_{j-1}}$
6: **end for**
7: **return** $\Psi(x,t)$

2.4 Results

In the program, we set the potential well at $[-3{,}3]$ and its depth 5 and the boundary condition $\Psi(-\infty) = \Psi(\infty) = 0$. From the figure, we can see the wave reflecting back and forth in the potential well and the wave finally relaxes on both sides of the well. You can find more details in the animation in the program.

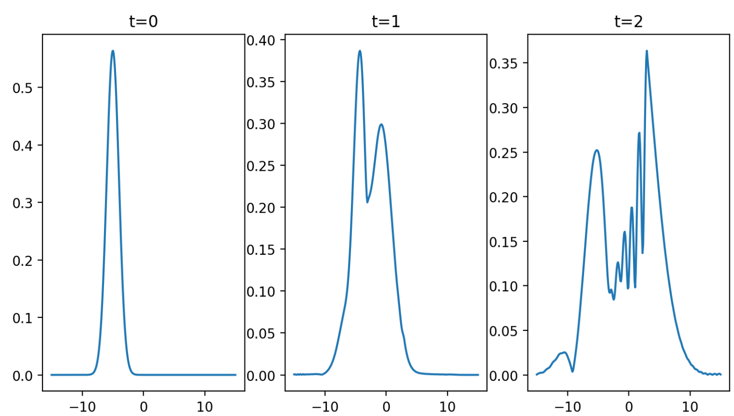

Figure 3: time evolution of wave function

3 Von Neumann stability analysis

3.1 Question

Prove the stability condition of the explicit scheme of the 1D wave equation by performing Von Neumann stability analysis.If $\frac{c\Delta t}{\Delta x} < 1$,the explicit scheme is stable.

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{8}$$

3.2 Solution

$$\frac{\partial^2 u}{\partial t^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta t^2} \frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \tag{9}$$

we denote $\alpha = c\frac{\Delta t}{\Delta x}$,thus,

$$u_{i,j+1} - 2u_{i,j} + u_{i,j-1} = \alpha^2 (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) \tag{10}$$

And we insert that $u_{i,j} = \xi^j e^{IKi\Delta x}$

$$\xi + \frac{1}{\xi} - 2 = -4\alpha^2 sin^2 (\frac{K\Delta x}{2}) \tag{11}$$

We get ξ:

$$\xi = 1 - 2\alpha^2 sin(x)^2 + 2\sqrt{-1 + (1 - 2\alpha^2 sin(x)^2)} \tag{12}$$

$$-\xi = (\sqrt{\alpha^2 sin^2 - 1} \mp \alpha sin)^2 \tag{13}$$

if $\alpha < 1$,then,

$$|\xi| = |\alpha sin \pm i\sqrt{1 - \alpha^2 sin^2}|^2 < 1 \tag{14}$$

So the explicit scheme is stable.