

Extra problems

1. Solve the Laplacian Equation in 2D

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad 0 < x, y < 1$$

with the boundary conditions $u(0, y) = 0$; $u(1, y) = 0$; $u(x, 0) = \sin(\pi x)$; $u(x, 1) = 0$. Compare the Explicit, Implicit, and Crank-Nicolson methods with proper choice of Δx and Δy . Which one is better? For the Crank-Nicolson method, plot the solution in a 3D graph.

2. Consider the case of 1D Harmonic oscillator (quantum). The corresponding Schrödinger equation is given by

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

where $V(x) = \frac{kx^2}{2}$. Solve the above equation numerically using the boundary conditions, $\Psi(\pm\infty, t) = 0$. The initial condition is given by $\Psi(x, 0) = \frac{1}{\sqrt{2\sqrt{\pi}}} 2x e^{-\frac{x^2}{2}}$. For the simulations, choose the x range in $[-5, 5]$, t from 0 to 5, and set $\hbar = m = k = 1$ for simplicity. Also, choose $\Delta x = 0.01$ and $\Delta t = 0.1\Delta x^2$. Plot the real part of the wave function in 3D and the corresponding probability density $\rho(x, t) = \Psi(x, t)\Psi^*(x, t)$ for the discrete values of $t = 0, 1, 2, 4, 5$.

3. The two-dimensional Schrödinger equation for the case of a particle in a box, where the potential $V(x, y) = 0$ between $x \in [0, 1]$ and $y \in [0, 1]$ and infinite otherwise, is given by

$$i\hbar \frac{\partial \Psi(x, y, t)}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi(x, y, t)}{\partial x^2} + \frac{\partial^2 \Psi(x, y, t)}{\partial y^2} \right] + V(x, y) \Psi(x, y, t).$$

$\Psi(x, y, t) = 0$ on all the faces of the boundary. The initial condition is given by $\Psi(x, y, t = 0) = 2 \sin(n_x \pi x) \sin(n_y \pi y)$, where n_x and n_y are

integers. Solve the above equation numerically for $n_x = n_y = 3$ and find the wave function $\Psi(x, y, t)$. You may set $\hbar = m = 1$ for simplicity. Choose $\Delta x = \Delta y = 0.01$ and $\Delta t = 0.1\Delta x^2$. Plot the real part of the wave function in 3D for $t = 0, 2, 4$ and the corresponding probability density $\rho(x, y, t) = \Psi(x, y, t)\Psi^*(x, y, t)$ for the same t values.

Note that the analytical solution is given by $\Psi(x, y, t) = 2e^{-iE_n t} \sin(n_x \pi x) \sin(n_y \pi y)$, where $E_n = \frac{\pi^2}{2}(n_x^2 + n_y^2)$.