Homework 7

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Diffusion Equation solve

The diffusion equation can be written as follows:

$$\frac{\delta\psi}{\delta t} = \frac{\delta^2\psi}{\delta x^2} \tag{1}$$

with boundary conditions,

$$\psi(0,t) = \psi(2,t) = 0 \tag{2}$$

, and initial conditions,

$$\psi(x, t = 0) = x, 0 \leq x \leq 1 \tag{3}$$

$$= -x + 2, 1 \leq x \leq 2 \tag{4}$$

It can be solved using three methods Which are discussed below.

0.0.1 Explicit Method

The explicit method solves the diffusion equation using the forward time centered space (FTCS). The explicit scheme can be implemented as

$$\psi^{n+1} = (1 - H\Delta t)\psi^n \tag{5}$$

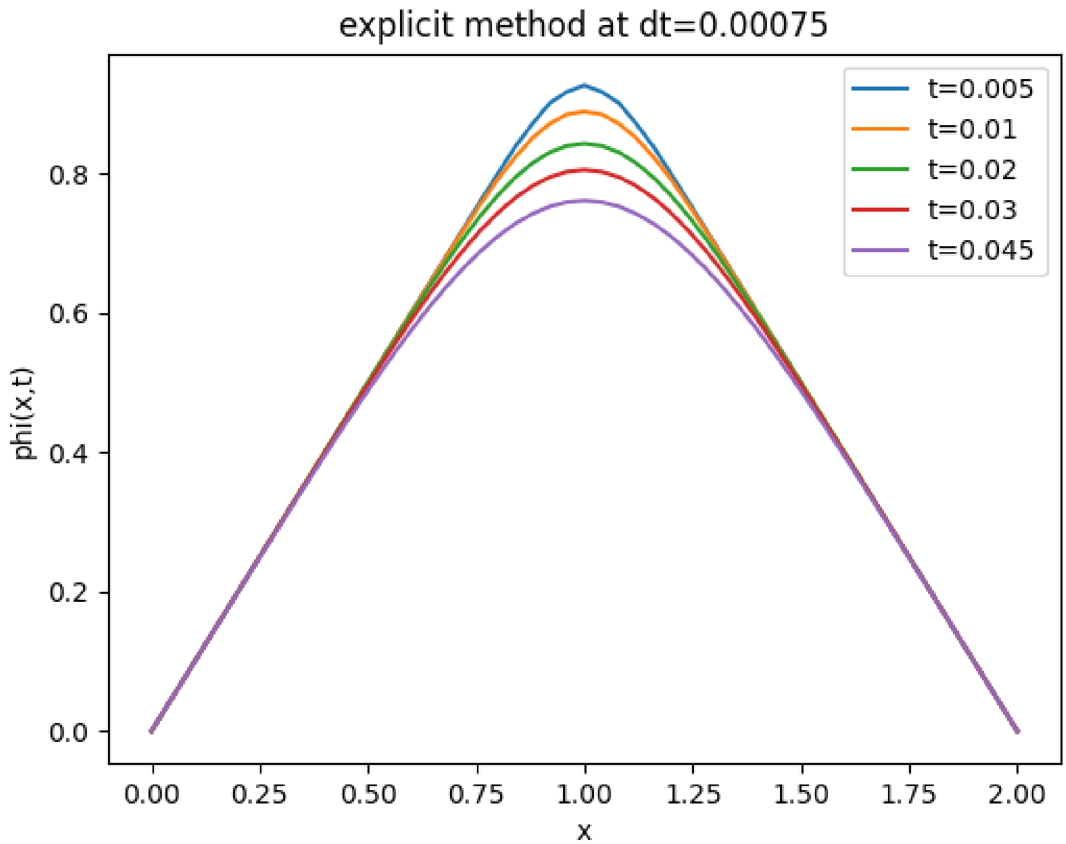

Figure 1: Numerical solution at timestep dt=0.00075

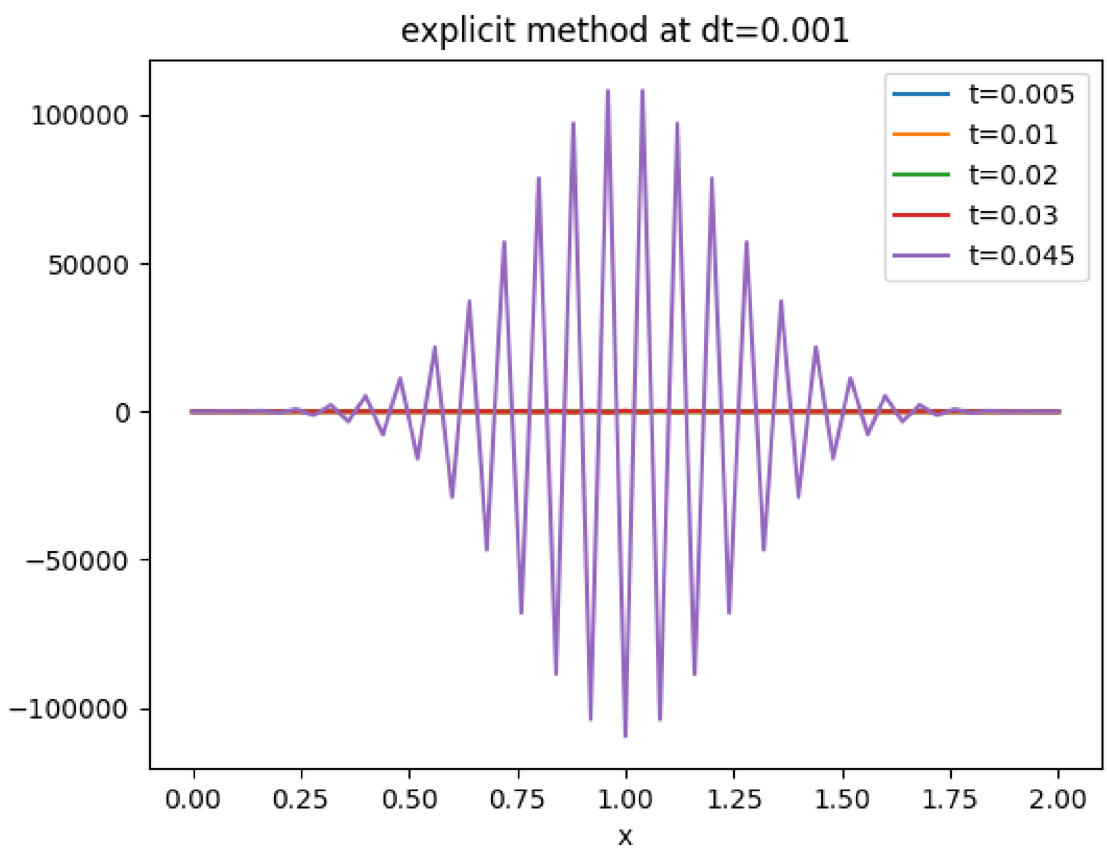

Figure 2: Numerical solution at timestep dt=0.001

where the H can be expressed as

$$(H\psi)_i = -(\psi_{i+1} + \psi_{i-1} - 2\psi_i)/h^2, h = \text{lattice spacing} \tag{6}$$

For timestep, $\Delta t = 0.00075$, the explicit method gives a good solution comparable to the analytical solution. But, if we increase the timestep, the explicit method becomes unstable which can be verified by the Von Neumann Stability Analysis. We can see the unstable solution from Figure 2.

0.0.2 Implicit Method

The implicit method can be implemented as

$$\psi^{n+1} = \frac{1}{(1 + H\Delta t)}\psi^n \tag{7}$$

This is formulated using the backward central difference formula in the derivation. If we turn this problem in a set of linear equations, then we can write the problem as $Ax = b$. For each time step the problem can be written as :

$$\begin{bmatrix} 1+2\lambda & -\lambda & 0 \\ -\lambda & 1+21 & -1 \\ 0 & -\lambda & 1+21 \end{bmatrix} \begin{bmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \end{bmatrix} = \begin{bmatrix} T_{1,0} \\ T_{2,0} \\ T_{3,0} \end{bmatrix} + \lambda \begin{bmatrix} T_{0,0} \\ 0 \\ T_{4,0} \end{bmatrix} \tag{8}$$

where $\lambda = \frac{\Delta t}{h^2}$ and T is the solution matrix. Then we loop over all the time steps to get the solution matrix. The implicit method is unconditionally stable. The analytical solution of the wavefunction can be written as:

$$\Psi(x,t) = 8\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2\pi^2} \exp\left[-\frac{(2n+1)^2\pi^2 t]}{4}\right] \sin(n/2) \tag{9}$$

$$n = 1, 2 \ldots \tag{10}$$

The difference between analytical and numerical solutions can be seen in Figure 4.

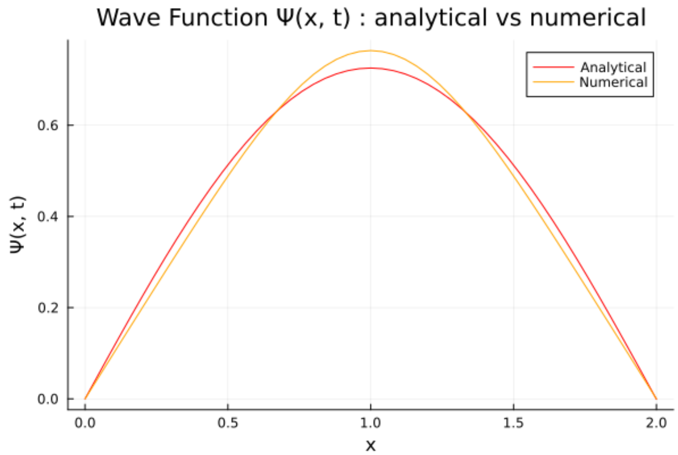

Figure 4: $\psi(x,t)$ analytical vs numerical solution computed using implicit method

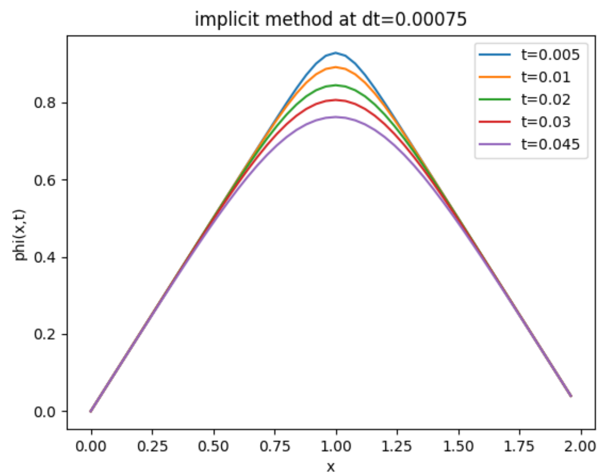

Figure 5: Numerical solution at timestep dt=0.00075 for implicit method

0.0.3 Sophisticated Method: Crank Nicolson Method

The Crank-Nicolson method can be implemented as

$$\psi^{n+1} = \frac{(1 - \frac{1}{2}H\Delta t)}{(1 + \frac{1}{2}H\Delta t)}\psi^n \tag{11}$$

Similarly, for each time step the problem can be written as :

$$\begin{bmatrix} 2(1+\lambda) & -\lambda & 0 \\ -\lambda & 2(1+\lambda) & -\lambda \\ 0 & -\lambda & 2(1+\lambda \end{bmatrix} \begin{bmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \end{bmatrix} = \begin{bmatrix} 2(1-\lambda) & \lambda & 0 \\ \lambda & 2(1-\lambda) & 0 \\ 0 & \lambda & 2(1-\lambda) \end{bmatrix} \begin{bmatrix} T_{1,0} \\ T_{2,0} \\ T_{3,0} \end{bmatrix} + \lambda \begin{bmatrix} T_{0,0} + T_{0,1} \\ 0 \\ T_{4,0} + T_{4,1} \end{bmatrix} \tag{12}$$

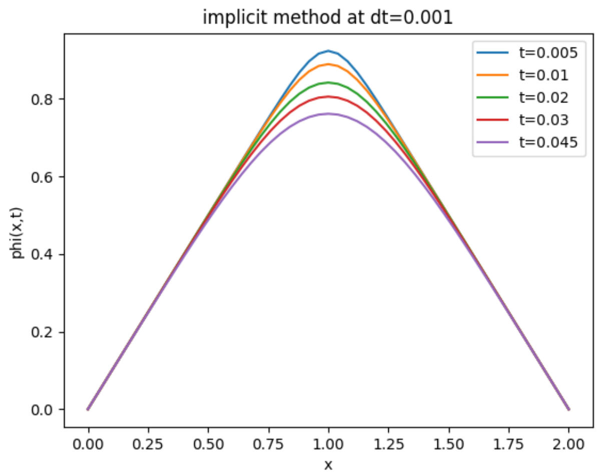

Figure 6: Numerical solution at timestep dt=0.001 for implicit method

Similar to the implicit method, we can solve this problem. The difference between analytical and numerical solutions can be seen in Figure 7.

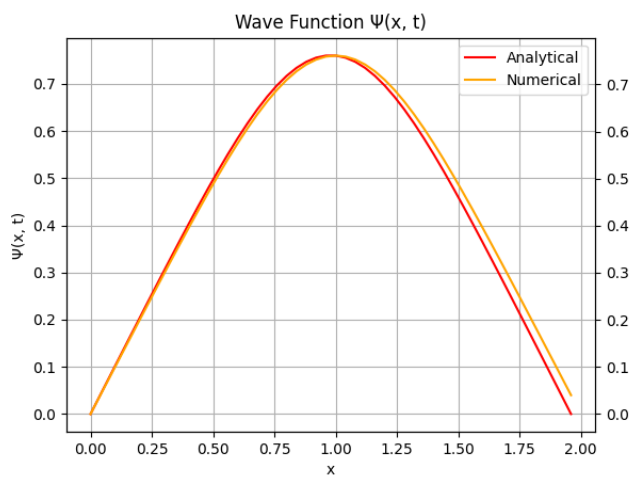

Figure 7: $\psi(x,t)$ analytical vs numerical solution computed using Crank-Nicolson method

The timestep size does not make any difference in the numerical solution of the implicit and sophisticated method.

0.1 Numerical Implicit Method vs Numerical Crank Nicolson Method

Both the Implicit Method vs Crank Nicolson Method can get good numerical results in comparison to the analytical result. I have not computed the error between these methods. From the graph, it's not conclusive which one is better.

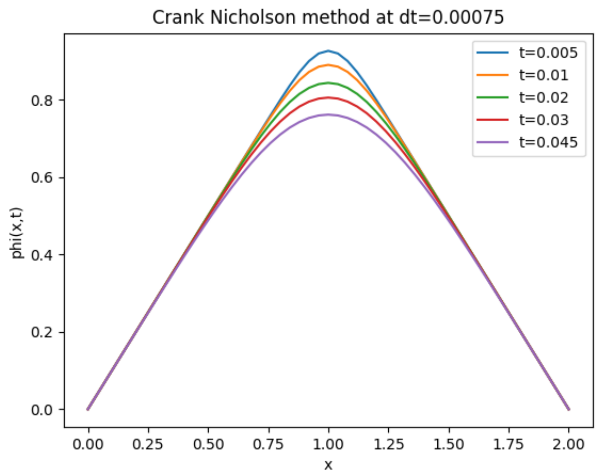

Figure 8: Numerical solution at timestep dt=0.00075 for Crank-Nicolson method

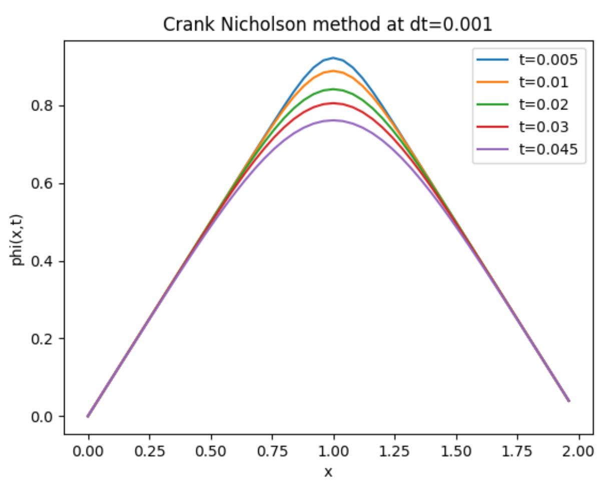

Figure 9: Numerical solution at timestep dt=0.001 for Crank-Nicolson method

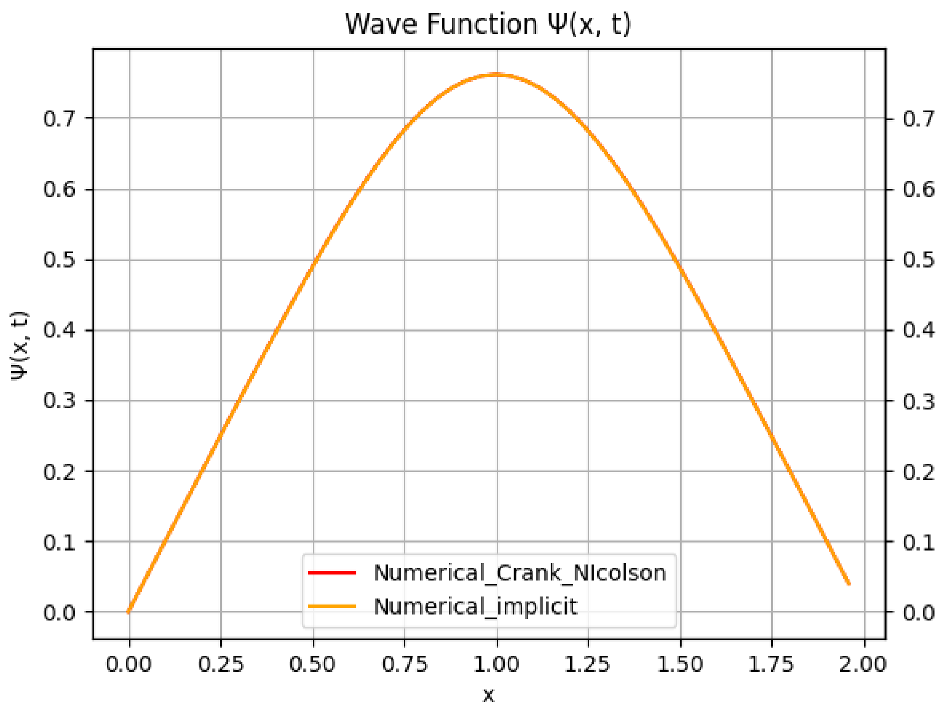

Figure 10: Numerical Implicit Method vs Numerical Crank Nicolson Method