PHY604 Lecture 18

October 28, 2025

Today’s lecture:
PDEs

- Stability analysis of PDEs
- Implicit schemes

Stability analysis of PDEs

- Empirically, we found that stability was a significant problem for PDEs
- In most cases, the stability was conditional on the timestep
  - Often related to the spatial discretization
- It is useful to be able to test for stability before running the calculation

Stability analysis of the advection equation

- Consider the advection equation discussed previously:

$$\frac{\partial a}{\partial t} = -c\frac{\partial a}{\partial x}$$

  - FTCS was always unstable
  - Other methods were unstable for timesteps that were too large compared to the spatial discretization *h*

- Let's consider a trial solution of the form:

$$a(x,t) = A(t)e^{ikx}$$

Complex amplitude

von Neumann stability analysis

- In discretized form: $a_j^n = A^n e^{ikjh}$

- Advancing the solution by one step:

$$a_j^{n+1} = A^{n+1} e^{ikjh} = \xi A^n e^{ikjh}$$

- ξ is the amplification factor

- von Neumann stability analysis: Insert this trial solution into the numerical scheme and solve for amplification factor given h and τ
  - Unstable if $|\xi| > 1$

Stability of FTCS for advection equation

- FTCS scheme: $$a_i^{n+1} = a_i^n - \frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n)$$

- Insert trial solutions: $a_j^n = A^n e^{ikjh}$ $\qquad$ $a_j^{n+1} = \xi A^n e^{ikjh}$

$$\begin{aligned}
\xi A^n e^{ikjh} &= A^n e^{ikjh} - \frac{c\tau}{2h}\left[A^n e^{ik(j+1)h} - A^n e^{ik(j-1)h}\right] \\
&= A^n e^{ikjh}\left[1 - \frac{c\tau}{2h}\left(e^{ikh} - e^{-ikh}\right)\right] \\
&= A^n e^{ikjh}\left[1 - i\frac{c\tau}{h}\sin(kh)\right]
\end{aligned}$$

- Therefore:

$$|\xi| = \left|1 - i\frac{c\tau}{h}\sin(kh)\right|$$

FTCS is not stable for advection equation

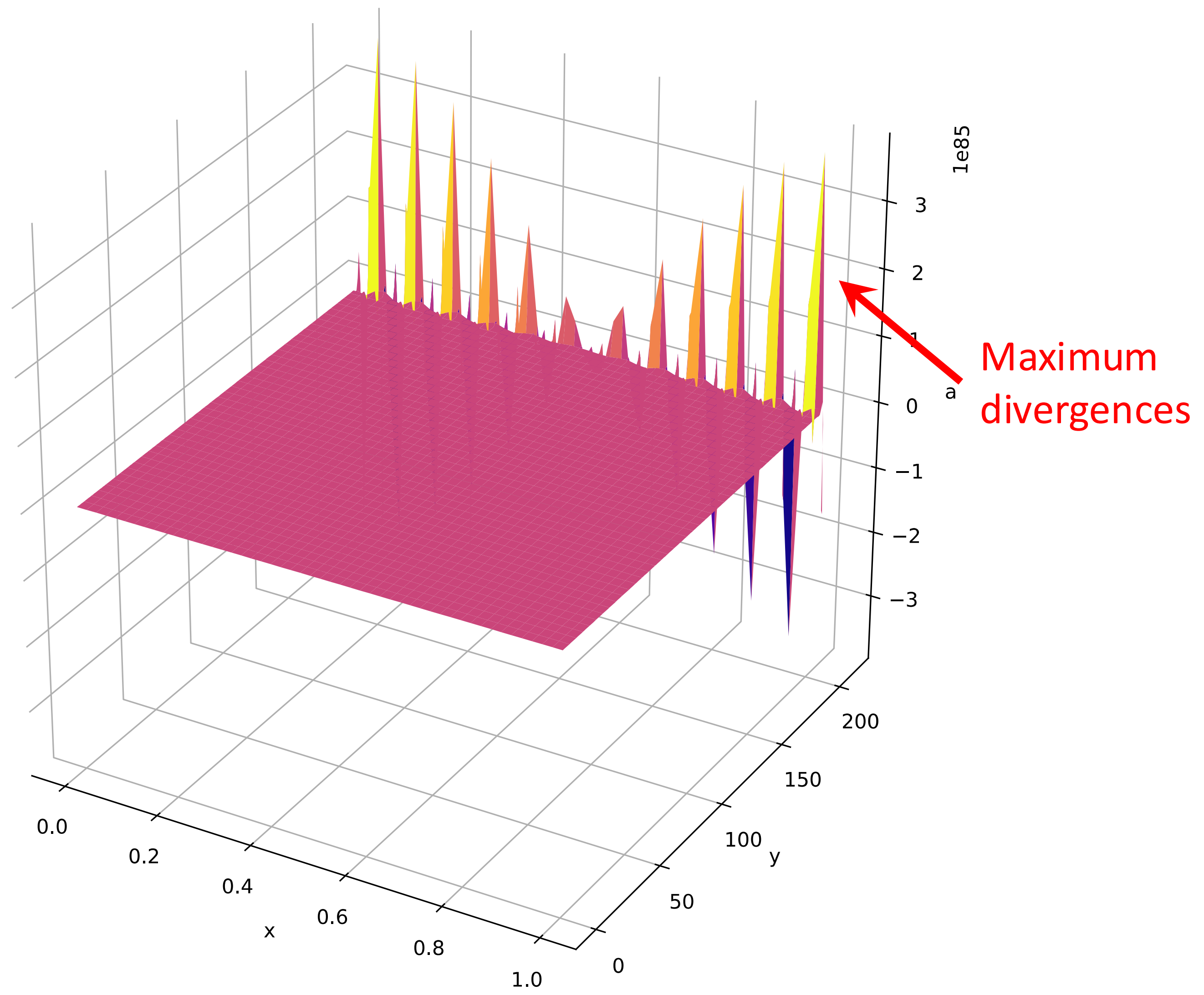
- We have that: $|\xi| = \left|1 - i\frac{c\tau}{h}\sin(kh)\right| = \sqrt{1 + \left(\frac{c\tau}{h}\right)^2 \sin(kh)^2}$

- So, the solution in general grows with each timestep, and therefore unstable
- Degree to which it is unstable depends on the "mode" *k*
- Fastest growing mode is when: $\sin^2(k_{\max}h) = 1$

- Or: $k_{\max} = \frac{\pi}{2h}$

- Since $k=2\pi/\lambda$: $\lambda_{\max} = 4h$

Divergent modes for FTCS on advection equation



von Neumann stability of the Lax scheme

- Apply the same analysis to the Lax method:

$$a_i^{n+1} = \frac{1}{2}(a_{i+1}^n + a_{i-1}^n) - \frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n)$$

- Plugging in our trial solution:

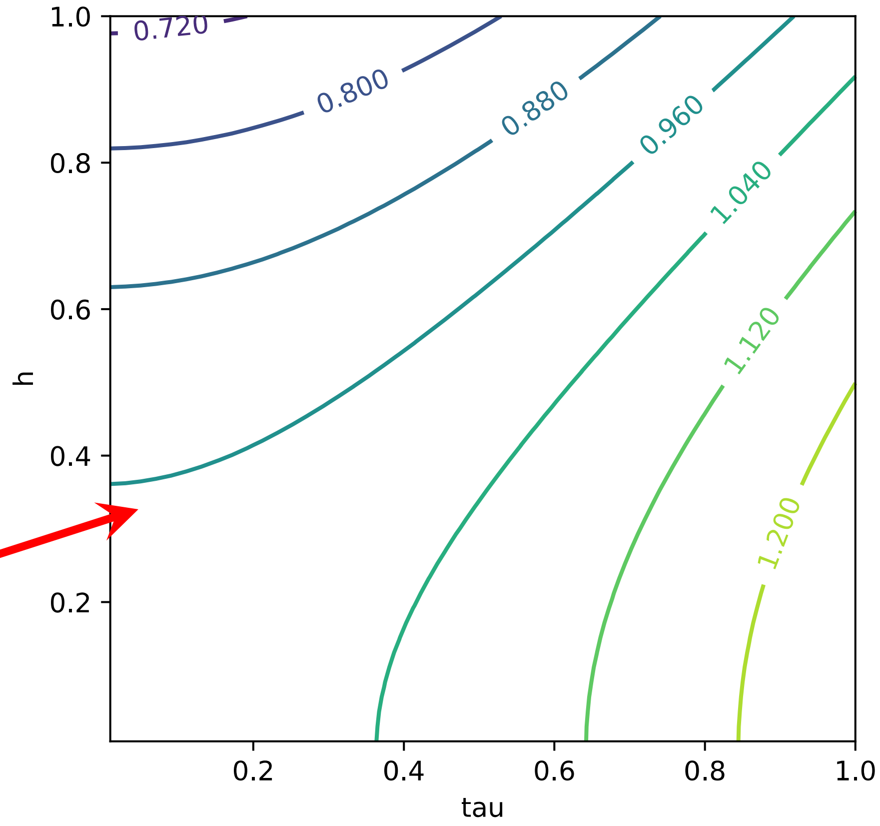
$$\xi A^n e^{ikjh} = \frac{1}{2}\left[A^n e^{ik(j+1)h} + A^n e^{ik(j-1)h}\right] - \frac{c\tau}{2h}\left[A^n e^{ik(j+1)h} - A^n e^{ik(j-1)h}\right]$$
$$= A^n e^{ikjh}\left[\frac{1}{2}\left(e^{ikh} + e^{ikh}\right) - \frac{c\tau}{2h}\left(e^{ikh} - e^{-ikh}\right)\right]$$

- So: $$\xi = \cos(kh) - i\frac{c\tau}{h}\sin(kh)$$

Stability of the Lax scheme

- So, we have: $$|\xi| = \sqrt{\cos^2(kh) + \left(\frac{c\tau}{h}\right)^2 \sin^2(kh)}$$
- Example: take $k=\pi/4$, $c=1$:
- In general: $\left|\frac{c\tau}{h}\right| \leq 1$
- Same as the Courant-Friedrichs-Lewy stability criterion

τ must be less than or equal to h



Matrix stability analysis

- von Neumann approach is a simple and popular way to investigate the stability of solution scheme
- However, does not take into account the influence of boundary conditions
- Recall our discussion of relaxation methods in terms of iteratively solving linear equations
- Matrix stability analysis: Analyze the linear problem to see how stable the PDE solution will be

FTCS for diffusion equation

- Consider the FTCS method for the 1D diffusion equation:

$$T_j^{n+1} = T_j^n + \frac{\tau}{2t_\sigma}(T_{j+1}^n + T_{j-1}^n - 2T_j^n)$$

- Where: $t_\sigma = h^2/2\kappa$
- For Dirichlet boundary conditions we can write FTCS as:

$$\begin{aligned}\mathbf{T}^{n+1} &= \mathbf{T}^n + \frac{\tau}{2t_\sigma}\mathbf{D}\mathbf{T}^n \\ &= \left(\mathbf{I} + \frac{\tau}{2t_\sigma}\mathbf{D}\right)\mathbf{T}^n \\ &= \mathbf{A}\mathbf{T}^n\end{aligned}$$

Matrix form of the diffusion equation

$$\mathbf{T}^{n+1} = \left(\mathbf{I} + \frac{\tau}{2t_\sigma}\mathbf{D}\right)\mathbf{T}^n$$

Zero rows so boundary points don't change

$$\mathbf{T}^n = \begin{bmatrix} T_0^n \\ T_1^n \\ T_2^n \\ T_3^n \\ \vdots \\ T_{N-1}^n \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix}$$

Decomposing in eigenvectors

- To determine the stability of the problem $\mathbf{T}^{n+1}=\mathbf{A}\mathbf{T}^{n}$ consider the eigenvalue problem for the matrix **A**:

$$\mathbf{A}\mathbf{v}_k = \lambda_k \mathbf{v}_k$$

- Assuming eigenvectors form a complete basis, initial conditions may be written as:

$$\mathbf{T}^1 = \sum_{k=0}^{N-1} c_k \mathbf{v}_k$$

- Then we can get **T** at a later time by repeatedly applying **A**:

$$\mathbf{T}^{n+1} = \mathbf{A}\mathbf{T}^n = \mathbf{A}(\mathbf{A}\mathbf{T}^{n-1}) = \mathbf{A}^2(\mathbf{A}\mathbf{T}^{n-2}) = \cdots = \mathbf{A}^n\mathbf{T}^1$$

- Using our eigenvector decomposition

$$\mathbf{T}^{n+1} = \sum_{k=0}^{N-1} c_k \mathbf{A}^n \mathbf{v}_k = \sum_{k=0}^{N-1} c_k (\lambda_k)^n \mathbf{v}_k$$

Stability condition on eigenvalues

$$\mathbf{T}^{n+1} = \sum_{k=0}^{N-1} c_k (\lambda_k)^n \mathbf{v}_k$$

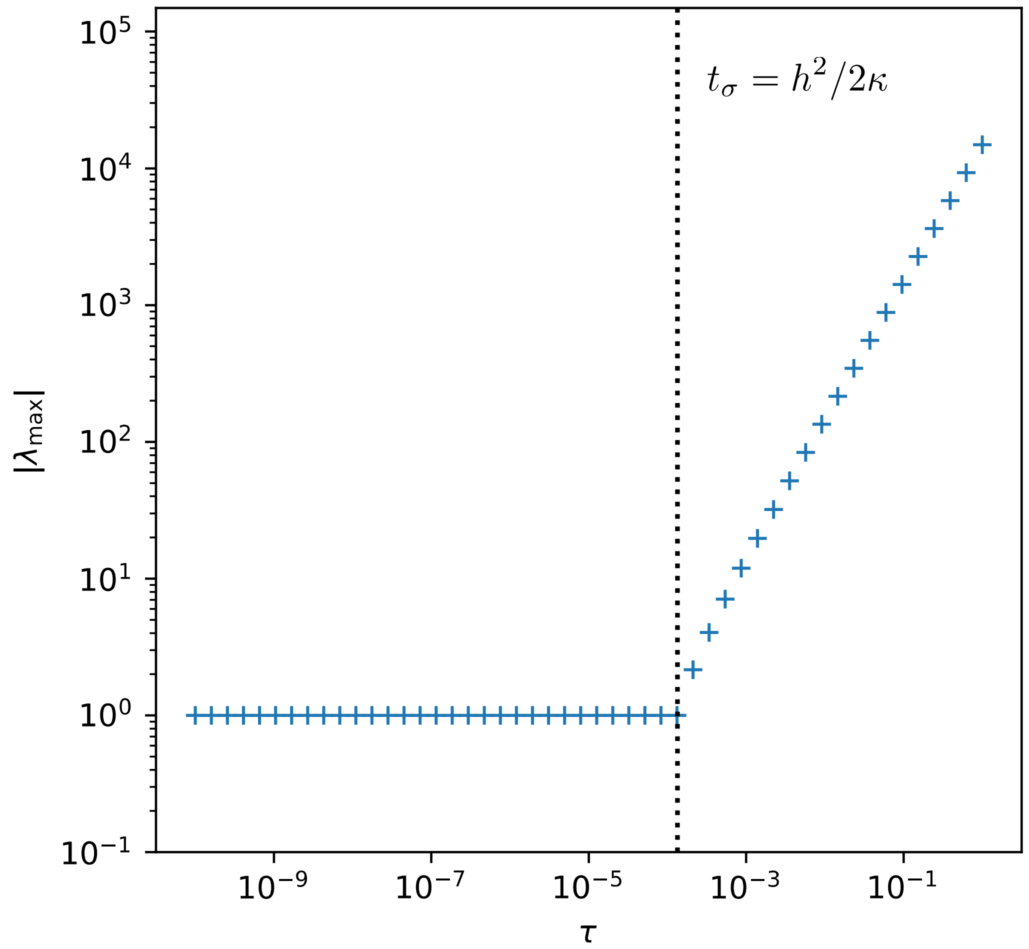
- We see that we will have divergence if we have any eigenvalues that are: $|\lambda_k| > 1$
- Spectral radius of **A**: Magnitude of the largest eigenvalue

$$\rho(\mathbf{A}) = |\lambda_{\max}|$$

- Scheme is matrix stable if the spectral radius is less than or equal to unity

Stability of FTCS for diffusion equation with timestep

- 61 spatial grid points with unit length, $\kappa = 1$:



Some comments on stability analysis

- The two stability analyses discussed here are only suitable for linear PDEs
- Can use for nonlinear PDEs by linearizing around a reference state
- Often can use physical intuition to estimate stability criteria, as we did originally for CFL condition
- Note that we have not tested numerical schemes for unwanted dissipation (e.g., in the Lax method) or changes to dispersion
    - Can be studied with extensions of von Neumann analysis

Today’s lecture:
PDEs

- Stability analysis of PDEs
- Implicit schemes

Example for implicit schemes: Schrödinger equation

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

- Or:

$$i\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi$$

- Formal solution:

$$\psi(x,t) = \exp\left[-\frac{i}{\hbar}\mathcal{H}t\right]\psi(x,0)$$

Discretizing the Schrödinger equation

- FTCS for the Schrödinger equation:

$$i\hbar\frac{\psi_j^{n+1} - \psi_j^n}{\tau} = -\frac{\hbar^2}{2m}\frac{\psi_{j+1}^n + \psi_{j-1}^n - 2\psi_j^n}{h^2} + V_j\psi_j^n$$

- Since the Hamiltonian is a linear operator:

$$i\hbar\frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \sum_{k=0}^{N-1} H_{jk}\psi_k^n$$

- Where:

$$H_{jk} = -\frac{\hbar^2}{2m}\frac{\delta_{j+1,k} + \delta_{j-1,k} - 2\delta_{jk}}{h^2} + V_j\delta_{jk}$$

FTCS steps for Schrödinger equation

- Final FTCS scheme in matrix notation:

$$\Psi^{n+1} = \left(\mathbf{I} - \frac{i\tau}{\hbar}\mathbf{H} \right) \Psi^n$$

- First term in Taylor expansion of the formal solution for one time step:

$$\psi(x,t) = \exp\left[-\frac{i}{\hbar}\mathcal{H}t \right] \psi(x,0)$$

Implicit schemes for the Schrödinger equation

- We have seen that the FTCS is numerically unstable for time steps that are too large
- Alternative approach: Apply the Hamiltonian to the future value of ψ

$$i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \sum_{k=0}^{N-1} H_{jk} \psi_k^{n+1}$$

- Or:

$$\Psi^{n+1} = \Psi^n - \frac{i\tau}{\hbar} \mathbf{H} \Psi^{n+1}$$

- Solving for Ψ^{n+1}:

$$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\tau}{\hbar} \mathbf{H} \right)^{-1} \Psi^n$$

Implicit FTCS scheme

- Implicit FTCS:

$$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\tau}{\hbar}\mathbf{H}\right)^{-1} \Psi^n$$

- Compare with explicit FTCS:

$$\Psi^{n+1} = \left(\mathbf{I} - \frac{i\tau}{\hbar}\mathbf{H}\right) \Psi^n$$

- Equivalent as τ goes to 0 since for small ε:

$$\frac{1}{1+\epsilon} \to (1-\epsilon)$$

- Con: Implicit method requires evaluation of matrix inverse, which can be costly
- Pro: Unconditionally stable!

More accurate approximations: Crank-Nicholson

- As we saw before, numerically stable does not mean accurate
- More accurate scheme: Crank-Nicholson
  - Average of implicit and explicit FTCS:

$$i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \frac{1}{2} \sum_{k=0}^{N-1} H_{jk} (\psi_k^n + \psi_k^{n+1})$$

  - In matrix form:

$$\Psi^{n+1} = \Psi^n - \frac{i\tau}{2\hbar} \mathbf{H} (\Psi^n + \Psi^{n+1})$$

- Isolating the *n*+1 term:

$$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\tau}{2\hbar} \mathbf{H} \right)^{-1} \left(\mathbf{I} - \frac{i\tau}{2\hbar} \mathbf{H} \right) \Psi^n$$

Properties of Crank-Nicolson

$$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right)^{-1} \left(\mathbf{I} - \frac{i\tau}{2\hbar}\mathbf{H}\right) \Psi^{n}$$

- Unconditionally stable
- Centered in both space and time
- “Páde” approximationfor exponential is
  - See (https://en.wikipedia.org/wiki/Pad%C3%A9_approximant)

$$e^{-z} \simeq \frac{1 - z/2}{1 + z/2}$$

- CN can be interpreted as Páde for the formal solution
- Preserves the unitarity of e^{-z}

Example: Numerical solution of the Schrödinger equation

- Initial conditions: Gaussian wave packet
  - Localized around x_0
  - Width of σ_0
  - Average momentum of: $p_0 = \hbar k_0$

$$\psi(x, t=0) = \frac{1}{\sqrt{\sigma_0\sqrt{\pi}}} \exp\left(ik_0 x\right) \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right]$$

- Which is normalized so that:

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

- Also, has the special property that uncertainty produce $\Delta x \Delta p$ is minimized $(\hbar/2)$

Propagation of wave packet in free space

- Wavefunction evolves like:

$$x \to x - \frac{p_0 t}{2m}, \qquad \sigma_0^2 \to \alpha^2 \equiv \sigma_0^2 + \frac{i\hbar t}{m}$$

- So we have:

$$\psi(x,t) = \frac{1}{\sqrt{\sigma_0\sqrt{\pi}}}\frac{\sigma_0}{\alpha}\exp\left[ik_0\left(x - \frac{p_0 t}{2m}\right)\right]\exp\left[-\frac{(x - x_0 - \frac{p_0 t}{2m})^2}{2\alpha^2}\right]$$

- And for the probability density:

Remains a Gaussian in time

$$P(x,t) = |\psi(x,t)|^2 = \frac{\sigma_0}{|\alpha|^2\sqrt{\pi}}\exp\left[-\left(\frac{\sigma_0}{|\alpha|}\right)^4\frac{(x - x_0 - \frac{p_0 t}{m})^2}{\sigma_0^2}\right]$$

Propagation of wave packet in free space

- By symmetry, max of Gaussian equals its expectation value:

$$\langle x \rangle = \int_{-\infty}^{\infty} x P(x,t) dx$$

- In time, it moves as: $\langle x \rangle = x_0 + \frac{p_0 t}{m}$

- And the wave packet spreads as:

$$\sigma(t) = \sigma_0 \sqrt{1 + \frac{\hbar^2 t^2}{m^2 \sigma_0^4}}$$

DEMO

- CN_schro.ipynb
- Start with N=30, t=1, r=3
  - Looks ok, but only move halfway
- Change t=0.1, r=30
  - Still only moves halfway
- Change t=1, N=80, r=3
  - Much better!
- Change N=150

DEMO

- Interactive plot for probability density

Why does the rough spatial discretization give errors?

- The reason is a poor representation of the initial conditions

- Rough discretization suppresses the higher wave number modes
  - Difficult to represent those modes on a coarse grid

- Because of this suppression, the discretized version has a lower momentum than $\psi(x,t)$

Can we avoid the taking the inverse of the matrix?

- As usual, we can trade taking the matrix inverse for solving a linear system of equations:

$$\begin{aligned}\Psi^{n+1} &= \left(\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right)^{-1} \left(\mathbf{I} - \frac{i\tau}{2\hbar}\mathbf{H}\right) \Psi^n \\ &= \left(\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right)^{-1} \left[2\mathbf{I} - \left(\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right)\right] \Psi^n \\ &= \left[2\left(\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right)^{-1} - \mathbf{I}\right] \Psi^n\end{aligned}$$

- Or:

$$\Psi^{n+1} = \mathbf{Q}^{-1}\Psi^n - \Psi^n, \quad \mathbf{Q} = \frac{1}{2}\left[\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right]$$

Crank-Nicolson for tridiagonal matrices

$$\Psi^{n+1} = \mathbf{Q}^{-1}\Psi^n - \Psi^n, \quad \mathbf{Q} = \frac{1}{2}\left[\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right]$$

- Now we can solve for the next timestep by solving the linear system:

$$\mathbf{Q}\chi = \Psi^n$$

- And then:

$$\Psi^{n+1} = \chi - \Psi^n$$

- Recall that for banded matrices, solving linear systems via, e.g., Gaussian elimination, is particularly efficient

DEMO

- CN_schro_no_inv.ipynb

Some comments in implicit schemes

- Recall that the killer app of implicit methods was that they are unconditionally stable

- Major downside is that for higher-dimensional problems, matrices become very large and difficult to manipulate
    - Can use approaches to separately perform implicit steps in different dimensions

After class tasks

- Homework 4 is posted, due Nov. 5, 2025

- Readings
  - Garcia Chapters 8 and 9
  - MIke Zingale's notes on computational hydrodynamics