

# PHY604 Lecture 17

October 21, 2021

# Review: Relaxation methods for Laplace eq.

- Methods based on this physical intuition are called relaxation methods
- We can use the FTCS method that we have used previously for the diffusion equation

- Start with the 2D “diffusion” equation:

$$\frac{\partial \Phi}{\partial t} = \mu \left( \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right)$$

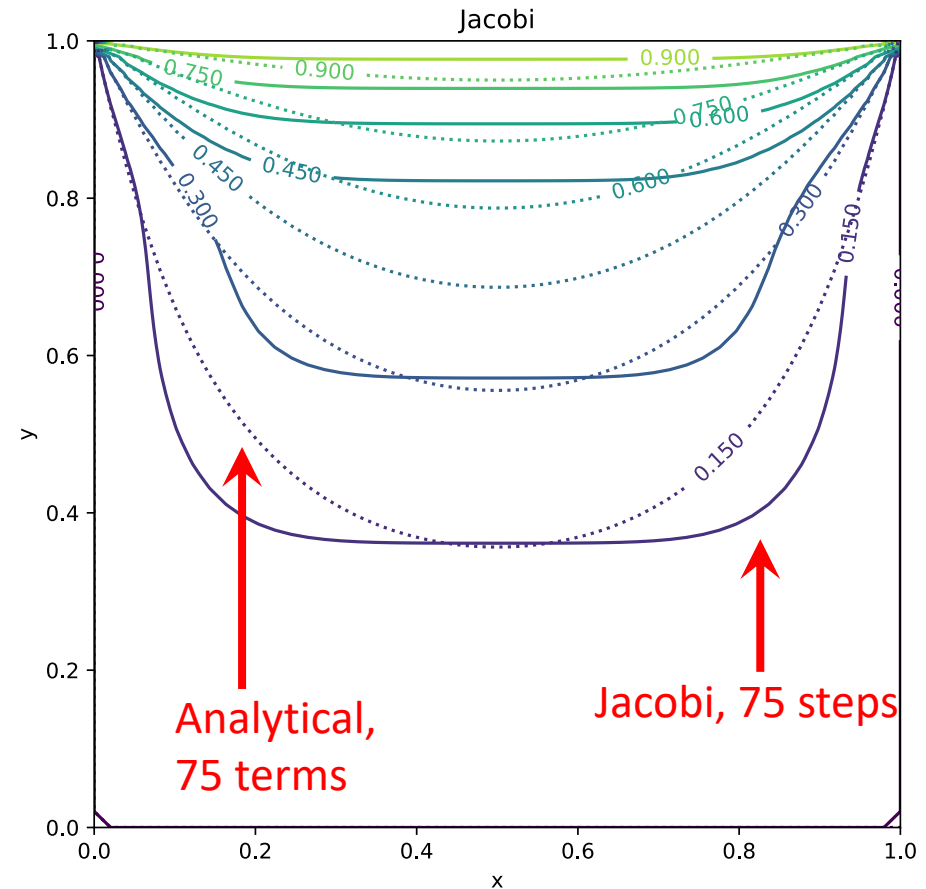
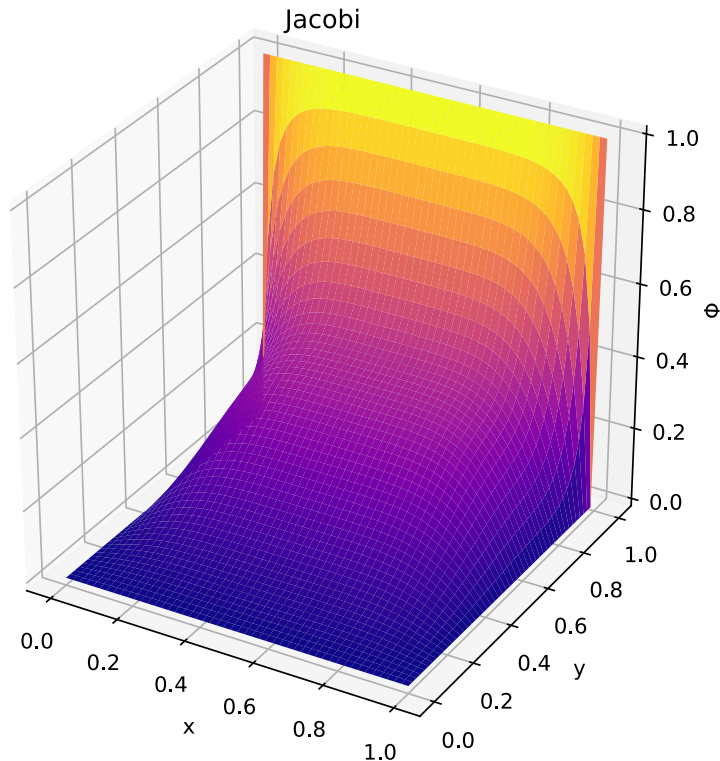
- Discretize:

$$\begin{aligned} \Phi_{i,j}^{n+1} = & \Phi_{i,j}^n + \frac{\mu\tau}{h_x^2} (\Phi_{i+1,j}^n + \Phi_{i-1,j}^n - 2\Phi_{i,j}^n) \\ & + \frac{\mu\tau}{h_y^2} (\Phi_{i,j+1}^n + \Phi_{i,j-1}^n - 2\Phi_{i,j}^n) \end{aligned}$$

- $n$  here is not really time, more an improved guess for the solution

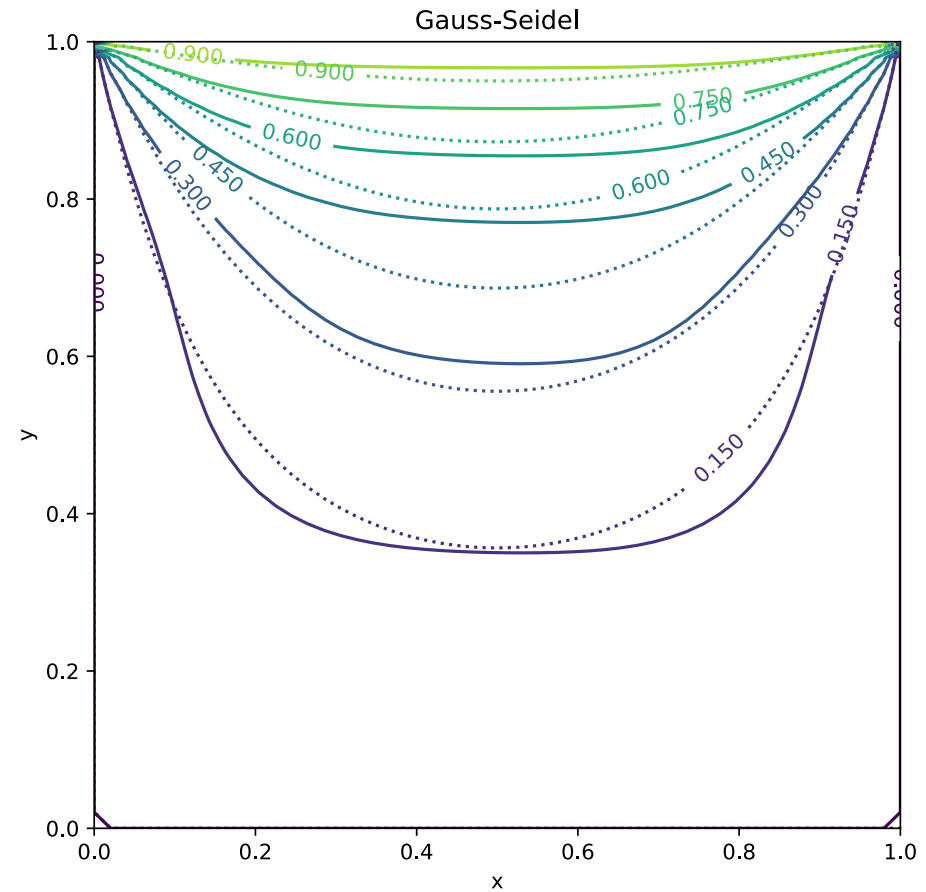
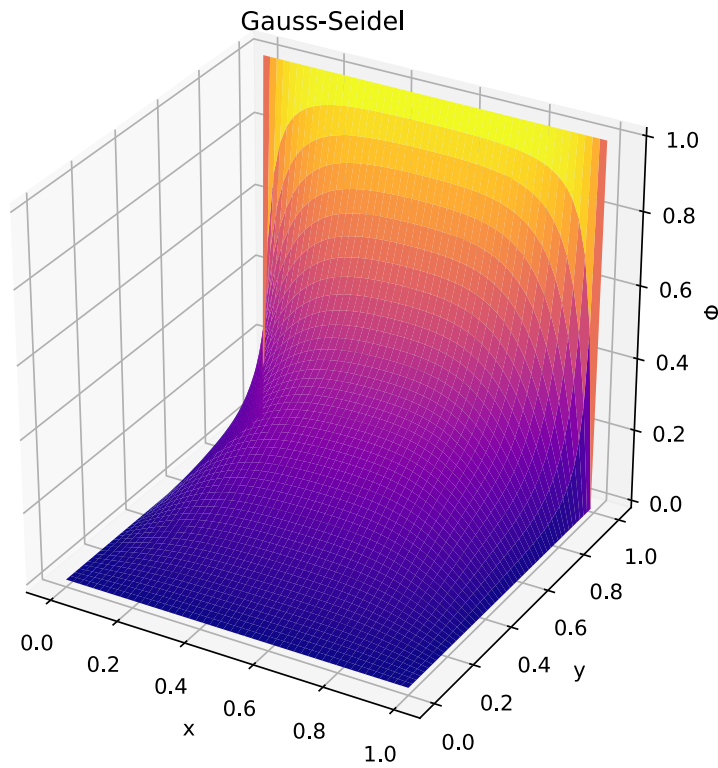
# Review: Jacobi method for Laplace equation

$$\Phi_{i,j}^{n+1} = \frac{1}{4} (\Phi_{i+1,j}^n + \Phi_{i-1,j}^n + \Phi_{i,j+1}^n + \Phi_{i,j-1}^n)$$



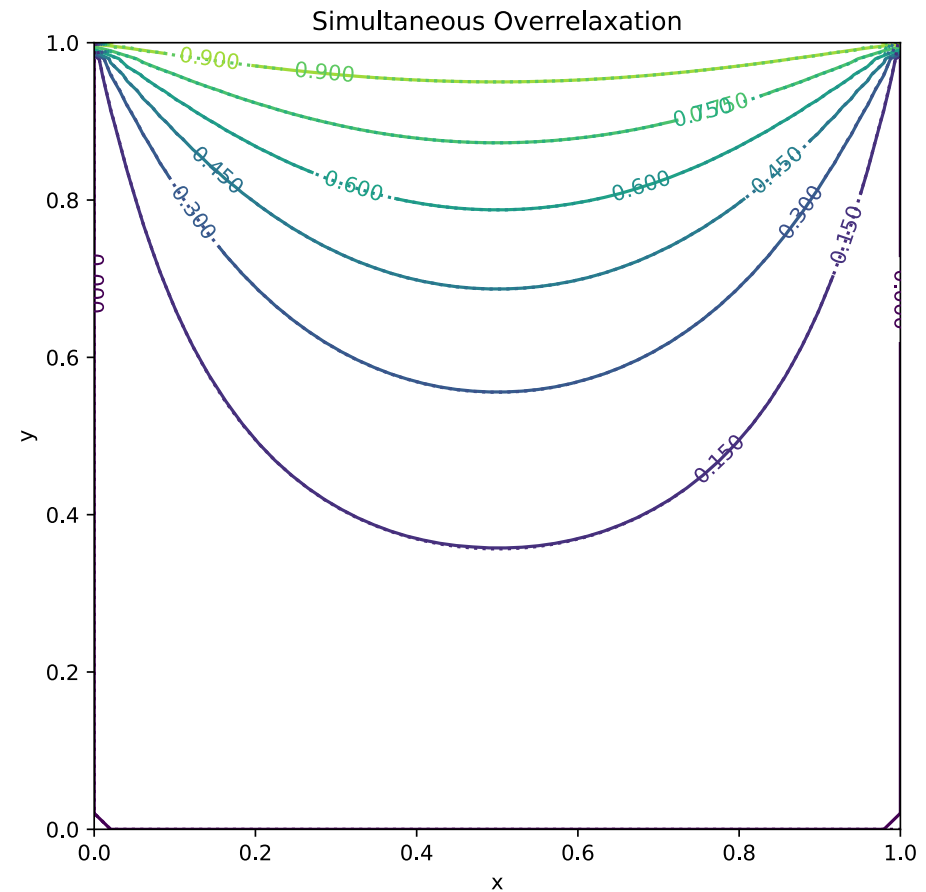
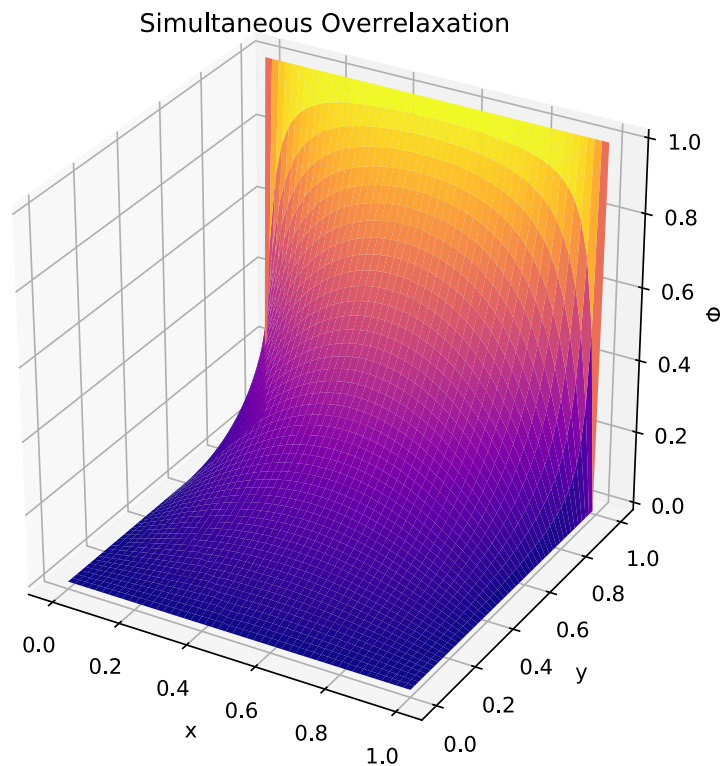
# Review: Gauss-Seidel for Laplace eq.

$$\Phi_{i,j}^{n+1} = \frac{1}{4} (\Phi_{i+1,j}^n + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^n + \Phi_{i,j-1}^{n+1})$$



# Review: Simultaneous overrelaxation

$$\Phi_{i,j}^{n+1} = (1 - \omega)\Phi_{i,j}^n + \frac{\omega}{4}(\Phi_{i+1,j}^n + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^n + \Phi_{i,j-1}^{n+1})$$



# Review: Approximate solution by spectral decomposition

$$\Phi(x, y) = \Phi_a(x, y) + T(x, y)$$

- To simplify the approximate solution, we take orthogonal trial functions:

$$\int_0^L dx \int_0^L dy f_k(x, y) f_{k'}(x, y) = A_k \delta_{k, k'}$$

- Insert into the Poisson equation:

$$\nabla^2 \left[ \sum_k a_k f_k(x, y) \right] + \frac{1}{\epsilon_0} \rho(x, y) = R(x, y)$$

- Where the residual  $R$  is:

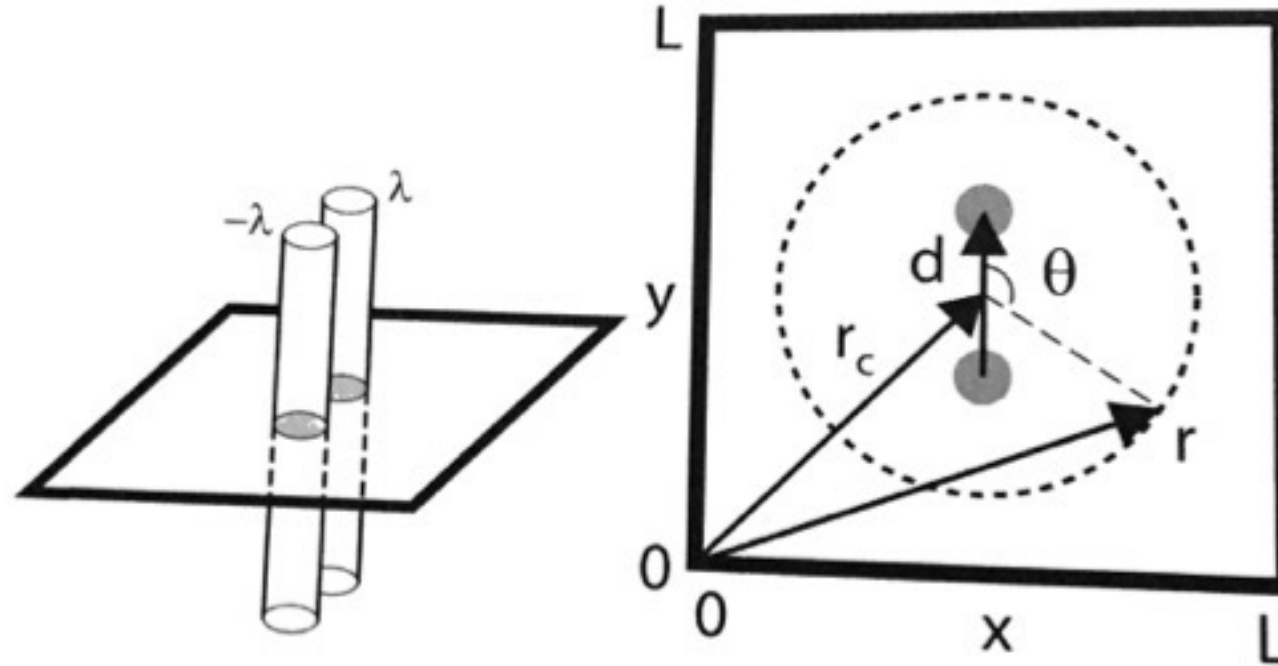
$$R(x, y) = -\nabla^2 T(x, y)$$

# Review: Final solution with Galerkin method

$$\Phi_a(x, y) = \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} a_{m,n} \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

$$a_{m,n} = \frac{4}{\pi^2 \epsilon_0 (m^2 + n^2) (1 + \delta_{m,0}) (1 + \delta_{n,0})} \int_0^L dx \int_0^L dy \rho(x, y) \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

# Ex: charge distribution of 2D dipoles (Garcia Sec. 8.2)



$$\rho(\mathbf{r}) = \lambda[\delta(\mathbf{r} - \mathbf{r}_+) - \delta(\mathbf{r} - \mathbf{r}_-)]$$

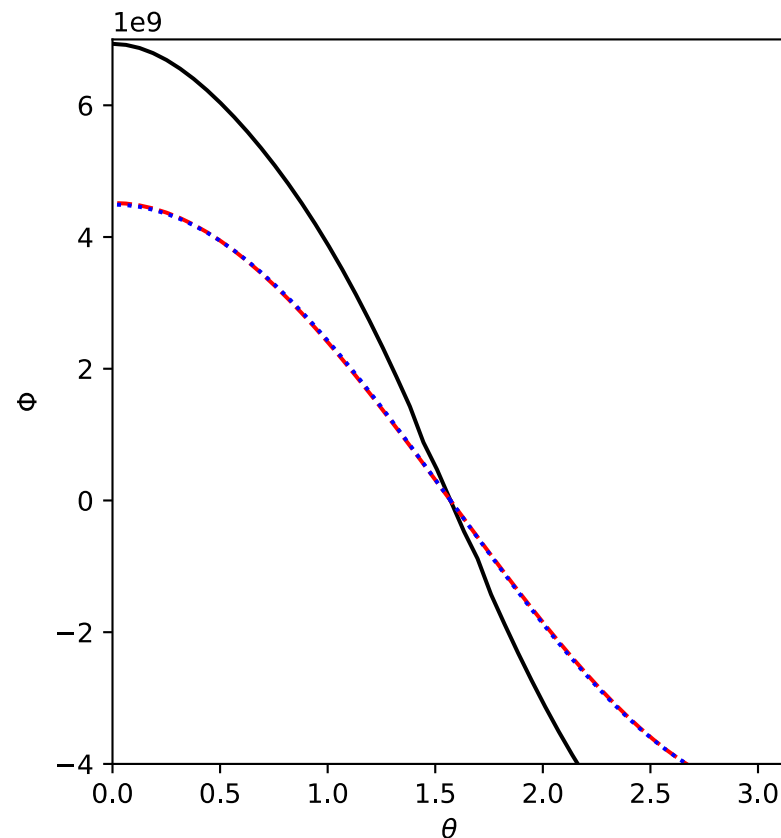
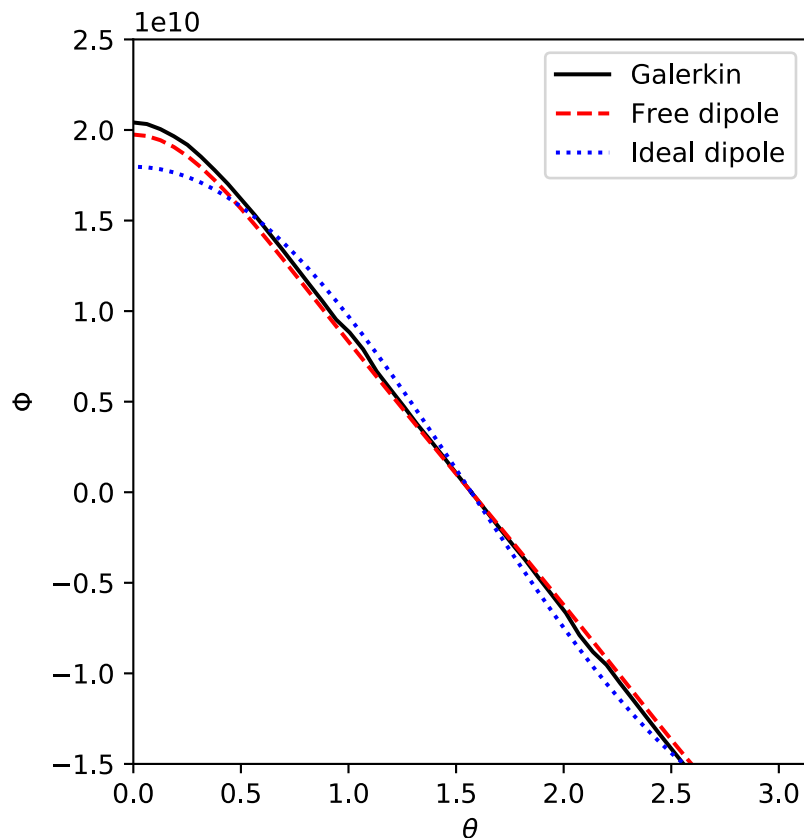
- Where:

$$\mathbf{r}_{\pm} = \mathbf{r}_c \pm \frac{1}{2}\mathbf{d}$$



# Review: Galerkin solution to the dipole potential

- Compare to free dipole:  $\Phi^{\text{free}}(\mathbf{r}) = -\frac{\lambda}{2\pi\epsilon_0} [\ln |\mathbf{r} - \mathbf{r}_+| - \ln |\mathbf{r} - \mathbf{r}_-|]$
- Or “ideal” dipole potential (far away):  $\Phi^{\text{ideal}}(\mathbf{r}) = \frac{\lambda}{2\pi\epsilon_0} \frac{|\mathbf{d}|}{|\mathbf{r} - \mathbf{r}_c|} \cos \theta$



# Today's lecture:

## Spectral methods and stability

- Spectral methods: Multiple Fourier transform method
- Stability analysis of PDEs
- Implicit schemes for PDEs

# Multiple Fourier transform method

- The Galerkin method involved taking a cosine DFT:

$$a_{m,n} = \frac{4}{\pi^2 \epsilon_0 (m^2 + n^2) (1 + \delta_{m,0}) (1 + \delta_{n,0})} \int_0^L dx \int_0^L dy \rho(x, y) \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

- And then the inverse:

$$\Phi_a(x, y) = \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} a_{m,n} \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

- Let's do this instead with FFTs
  - Cosine transformation good for Neumann boundary conditions
  - Sine transformation good for Dirichlet boundary conditions (with  $\Phi=0$ )
  - Standard FFT is good for periodic boundary conditions

# Fourier transform of the Poisson equation

- We first discretize in 2D:

$$\frac{1}{h^2} [\Phi_{j+1,k} + \Phi_{j-1,k} - 2\Phi_{j,k}] + \frac{1}{h^2} [\Phi_{j,k+1} + \Phi_{j,k-1} - 2\Phi_{j,k}] = -\frac{1}{\epsilon_0} \rho_{j,k}$$

- Now define the 2D Fourier transform of the potential and charge density:

$$F_{m,n} = \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \Phi_{j,k} \exp\left(-\frac{i2\pi jm}{N}\right) \exp\left(-\frac{i2\pi kn}{N}\right), \quad R_{m,n} = \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \rho_{j,k} \exp\left(-\frac{i2\pi jm}{N}\right) \exp\left(-\frac{i2\pi kn}{N}\right)$$

- With reverse transform:

$$\Phi_{j,k} = \frac{1}{N^2} \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} F_{m,n} \exp\left(\frac{i2\pi jm}{N}\right) \exp\left(\frac{i2\pi kn}{N}\right), \quad \rho_{j,k} = \frac{1}{N^2} \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} R_{m,n} \exp\left(\frac{i2\pi jm}{N}\right) \exp\left(\frac{i2\pi kn}{N}\right)$$

# Fourier transform of the Poisson equation

- So, for the transformed Poisson equation:

$$\left[ \exp\left(\frac{-i2\pi m}{N}\right) + \exp\left(\frac{i2\pi m}{N}\right) + \exp\left(\frac{-i2\pi n}{N}\right) + \exp\left(\frac{i2\pi n}{N}\right) - 4 \right] F_{m,n} = -\frac{h^2}{\epsilon_0} R_{m,n}$$

- Solving for the **F** matrix:

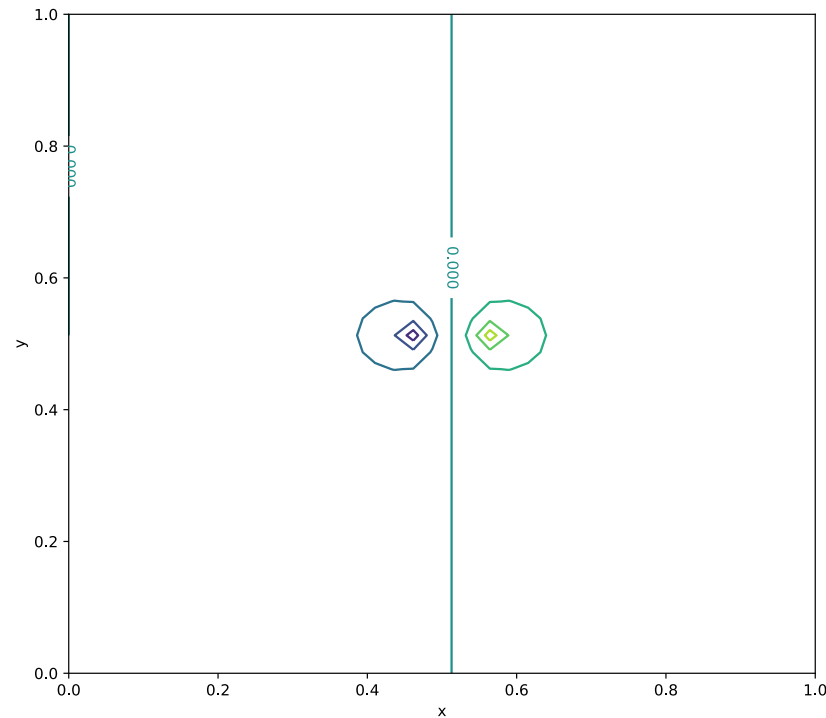
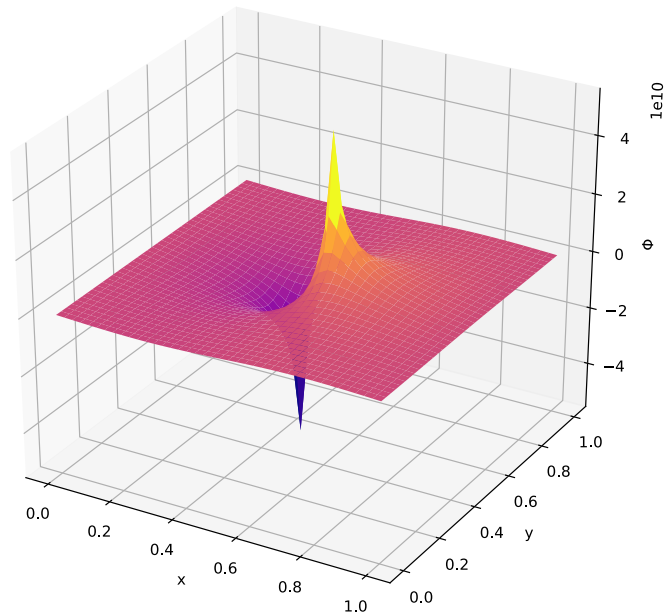
$$F_{m,n} = -\frac{h^2}{2\epsilon_0(\cos(2\pi m/N) + \cos(2\pi n/N) - 2)} R_{m,n}$$

- To get the potential, we just need to take the inverse FFT:

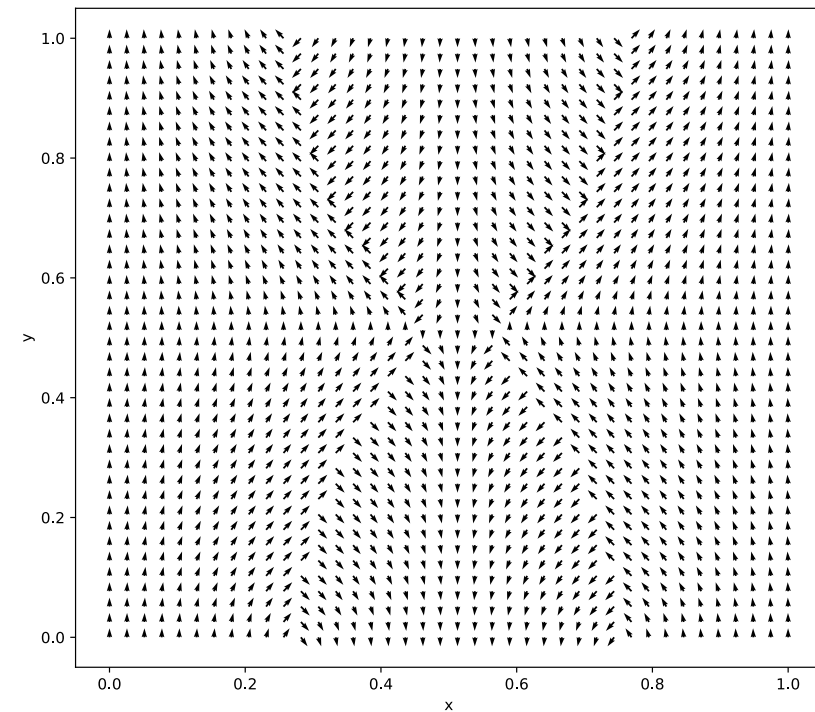
$$\Phi_{j,k} = \frac{1}{N^2} \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} F_{m,n} \exp\left(\frac{i2\pi jm}{N}\right) \exp\left(\frac{i2\pi kn}{N}\right)$$

# Ex: charge distribution of 2D dipole (Garcia Sec. 8.2)

Potential:



Field direction:



# Today's lecture:

## Spectral methods and stability

- Spectral methods: Multiple Fourier transform method
- Stability analysis of PDEs
- Implicit schemes for PDEs

# 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:

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

- $\xi$  is the **amplification factor**
- **von Neumann stability analysis**: Insert this trial solution into the numerical scheme and solve for amplification factor given  $h$  and  $\tau$ 
  - 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: 
$$a_j^n = A^n e^{ikjh} \quad a_j^{n+1} = \xi A^n e^{ikjh}$$

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

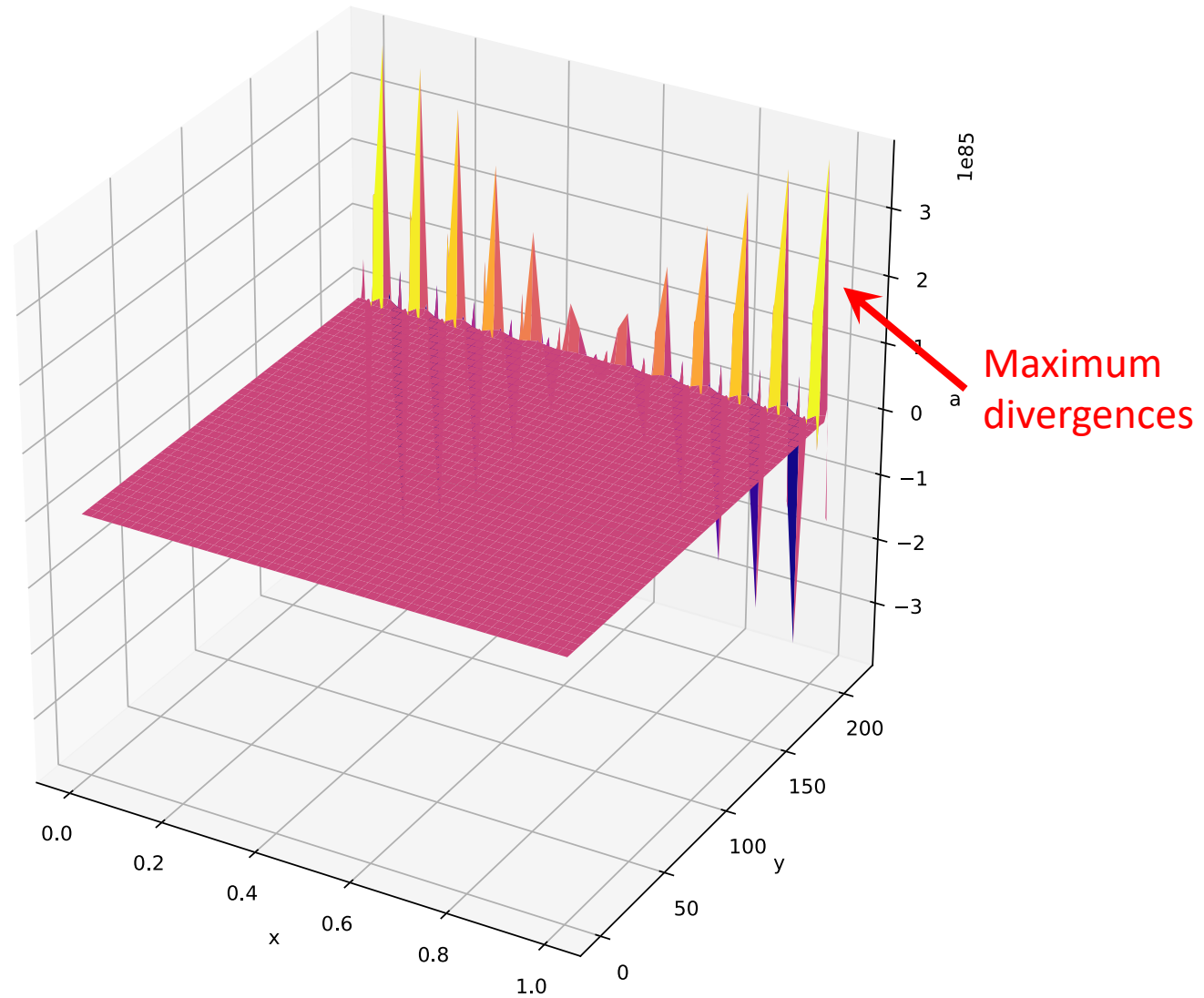
- Therefore:

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

# FTCS is not stable for advection equation

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

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

- So:

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

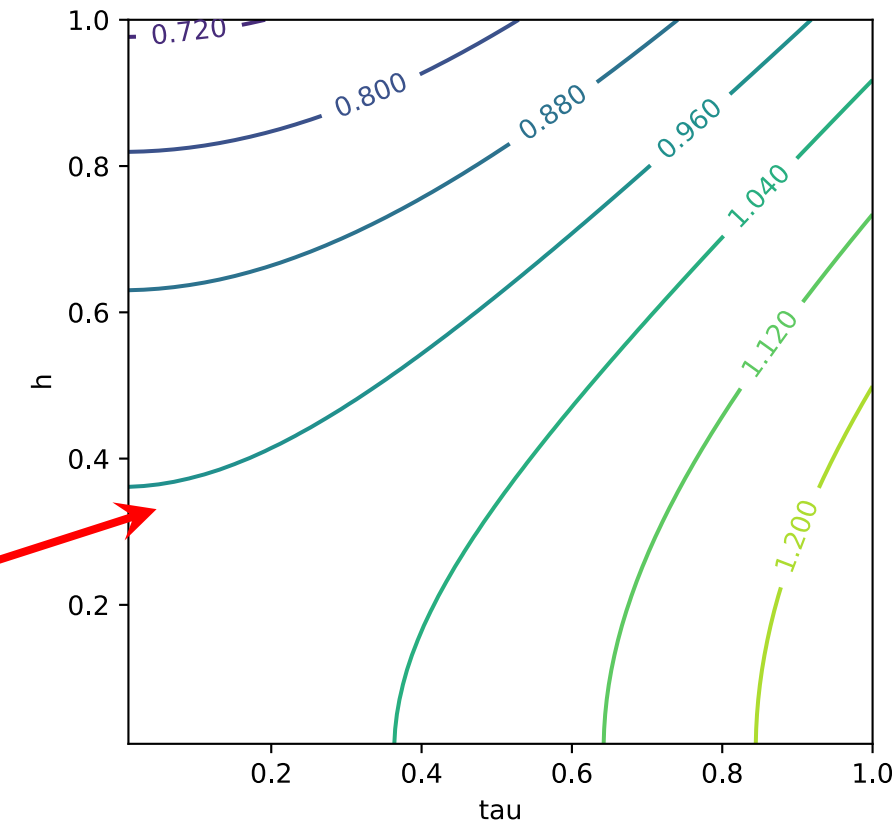
# Stability of the Lax scheme

- 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



# 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:

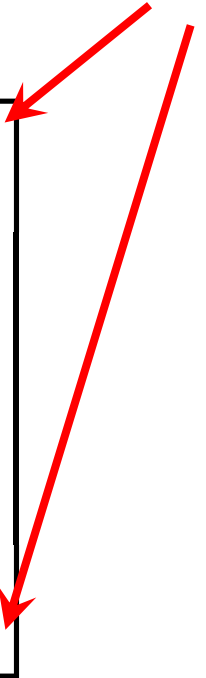
$$\begin{aligned} \mathbf{T}^{n+1} &= \mathbf{T}^n + \frac{\tau}{2t_\sigma} \mathbf{D} \mathbf{T}^n \\ &= \left( \mathbf{I} + \frac{\tau}{2t_\sigma} \mathbf{D} \right) \mathbf{T}^n \\ &= \mathbf{A} \mathbf{T}^n \end{aligned}$$

# Matrix form of the diffusion equation

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

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

Zero rows so boundary points don't change



# 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  $\mathbf{A}$ :

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

- 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  $\mathbf{T}$  at a later time by repeatedly applying  $\mathbf{A}$ :

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

- 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

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

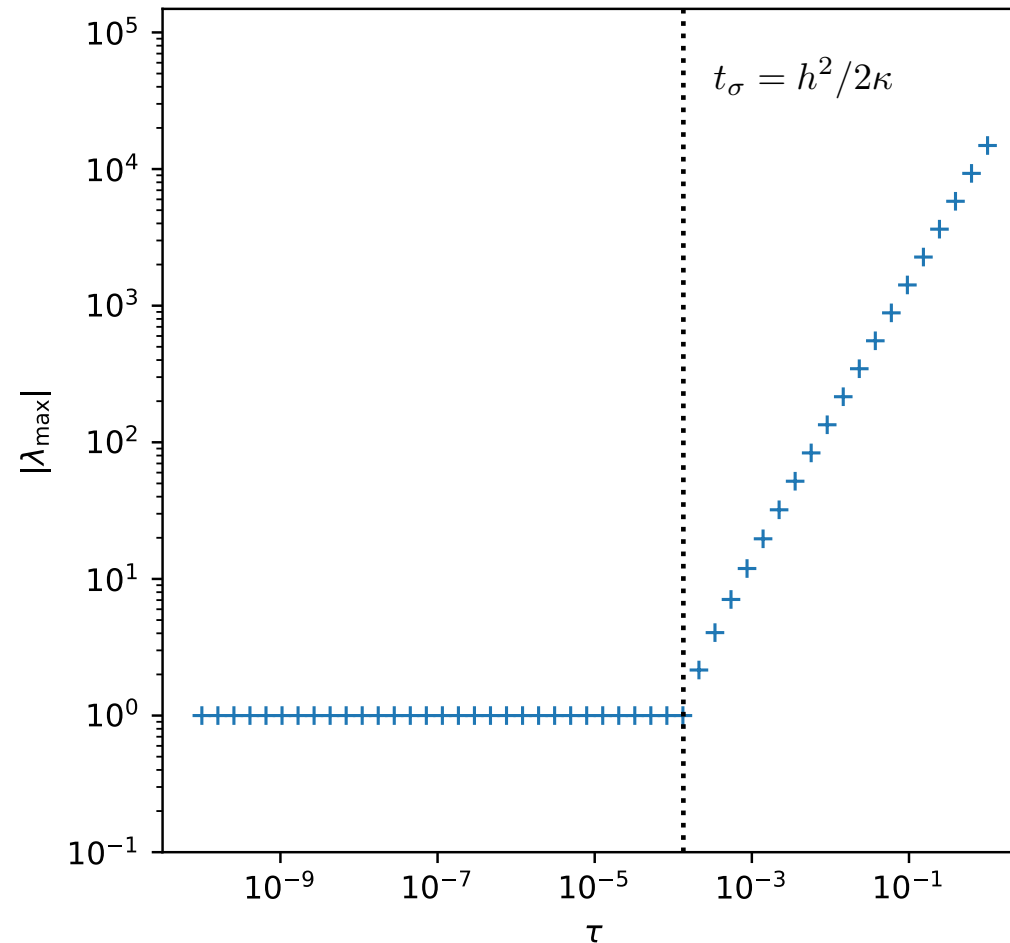
- We see that we will have divergence if we have any eigenvalues that are:  $|\lambda_k| > 1$
- **Spectral radius of  $\mathbf{A}$** : Magnitude of the largest eigenvalue

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

- 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: Spectral methods and stability

- Spectral methods: Multiple Fourier transform method
- Stability analysis of PDEs
- **Implicit schemes for PDEs**

# 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  $\psi$

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

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

- Solving for  $\Psi^{n+1}$ :

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

# 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  $\tau$  goes to 0 since for small  $\epsilon$ :

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

- 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” approximation for exponential is
  - See ([https://en.wikipedia.org/wiki/Pade%27s\\_approximant](https://en.wikipedia.org/wiki/Pade%27s_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  $\sigma_0$
  - Average momentum of:  $p_0 = \hbar k_0$

$$\psi(x, t = 0) = \frac{1}{\sqrt{\sigma_0} \sqrt{\pi}} \exp(i k_0 x) \exp\left[-\frac{(x - x_0)^2}{2\sigma_0^2}\right]$$

- Which is normalized so that:

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

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

# Propagation of wave packet in free space

- Wavefunction evolves like:


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

- So we have:

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

- And for the probability density:

Remains a Gaussian in  
time


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



# 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:

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

# 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

# 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 Oct. 28, 2021
- Readings
  - Garcia Chapters 8 and 9