PHY604 Lecture 17

October 23, 2025

Today's lecture:
PDEs

- Elliptical PDEs: Spectral methods

- Stability analysis of PDEs

A different way to represent the potential

- Consider again the Poisson equation:

$$\nabla^2 \Phi(\mathbf{r}) = -\frac{1}{\epsilon_0}\rho(\mathbf{r})$$

- For simplicity, square geometry: $0 \leq x \leq L, \quad 0 \leq y \leq L$
- Relaxation methods discretize space and solve for $\Phi_{i,j}$
- We constructed out analytical solution as in infinite sum of trigonometric functions
- Let's build an approximate solution as a finite sum:

$$\Phi(x,y) = a_1 f_1(x,y) + a_2 f_2(x,y) + \cdots + a_K f_K(x,y) + T(x,y)$$

$$= \sum_{k=1}^{K} a_k f_k(x,y) + T(x,y)$$

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

Approximate solution

Approx. solution

Error

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

- 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:

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

Obtain coefficients with Galerkin method

- Next step is to obtain coefficients a_k
- Galerkin method imposes the condition that the residual is orthogonal to all of the trial functions:

$$\int_0^L dx \int_0^L dy f_k(x,y) R(x,y) = 0$$

- Choice of trial functions motivated by geometry and boundary conditions
- Let's take Neumann boundary conditions:

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x=0} = \left.\frac{\partial \Phi}{\partial x}\right|_{x=L} = \left.\frac{\partial \Phi}{\partial y}\right|_{y=0} = \left.\frac{\partial \Phi}{\partial y}\right|_{y=L} = 0$$

- Normal component of electric field zero at the boundaries

Trial functions for our geometry and BCs

- Natural set of trial functions:

$$f_{m,n}(x,y) = \cos\left[\frac{m\pi x}{L}\right]\cos\left[\frac{n\pi y}{L}\right]$$

- Can confirm that these functions are orthogonal:

$$\int_0^L dx \int_0^L dy f_{m,n}(x,y) f_{m',n'}(x,y) = \frac{L^2}{4}(1+\delta_{m,0})(1+\delta_{n,0})\delta_{m,m'}\delta_{n,n'}$$

- Inserting into Poisson equation

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

- Gives:

$$-\sum_{m=0}^{M-1}\sum_{n=0}^{M-1} a_{m,n}\frac{\pi^2(m^2+n^2)}{L^2} f_{m,n}(x,y) + \frac{1}{\epsilon_0}\rho(x,y) = R(x,y)$$

Now we need so solve for coefficients

- Apply to both sides of the equation:

$$\int_0^L dx \int_0^L dy f_{m',n'}(x,y)$$

- And use “Galerkin condition”:

$$\int_0^L dx \int_0^L dy f_k(x,y) R(x,y) = 0$$

- Which gives:

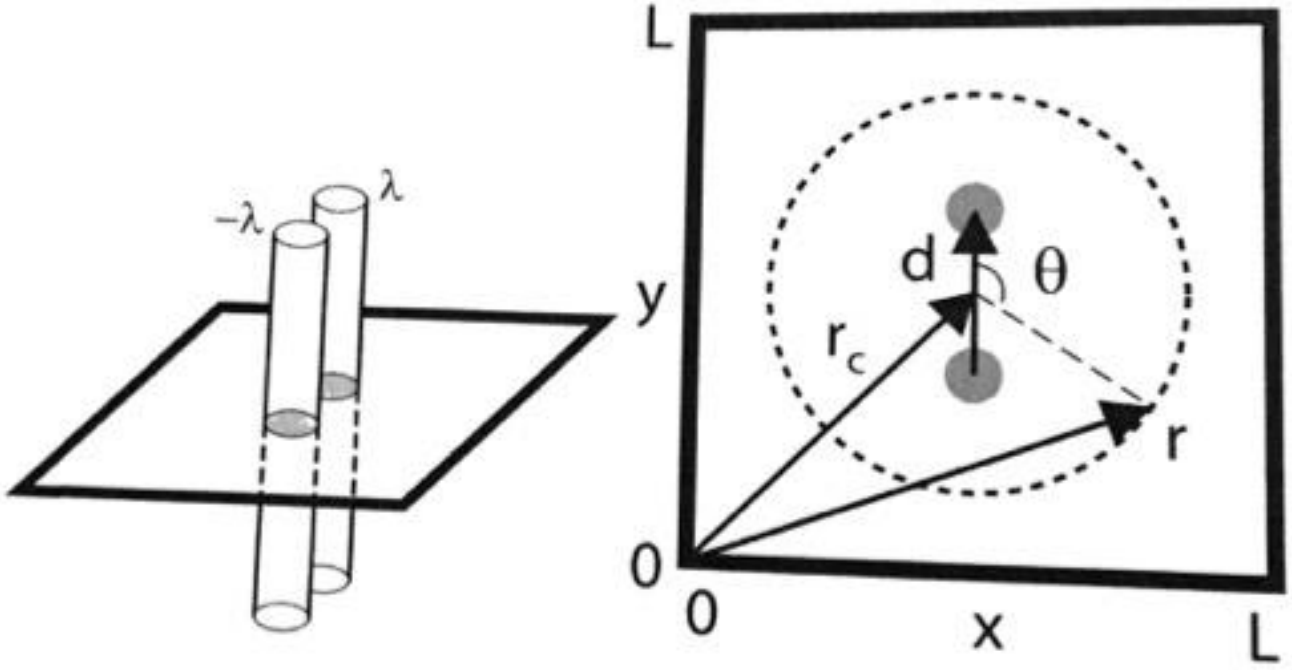
$$a_{m,n} = \frac{4}{\pi^2 \epsilon_0 (m^2+n^2)(1+\delta_{m,0})(1+\delta_{n,0})} \int_0^L dx \int_0^L dy \rho(x,y) \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

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)



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

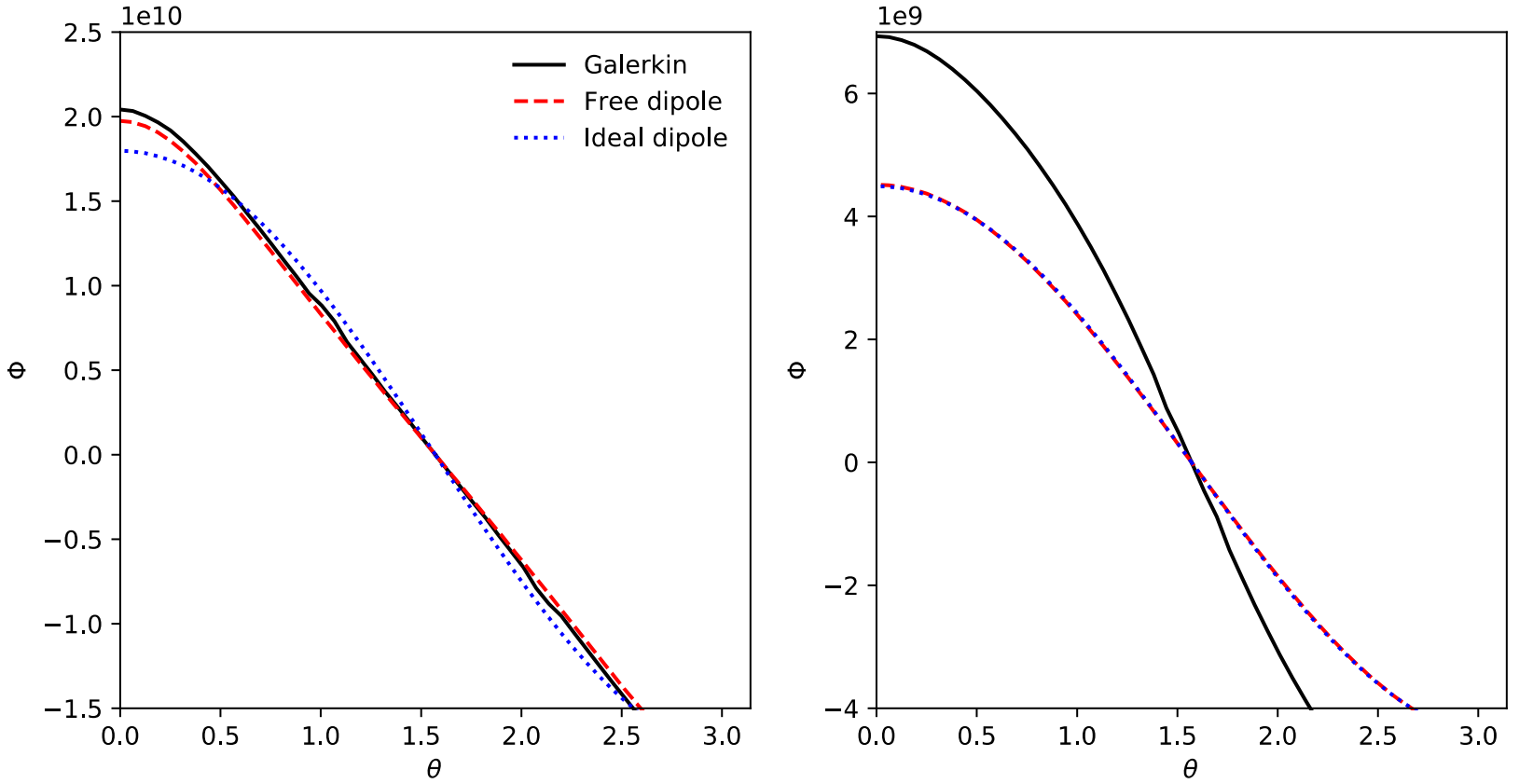
- Where:

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

Galerkin solution to the dipole potential

- Compare to free dipole: $\Phi^{\mathrm{free}}(\mathbf{r}) = -\dfrac{\lambda}{2\pi\epsilon_0}\left[\ln|\mathbf{r}-\mathbf{r}_+| - \ln|\mathbf{r}-\mathbf{r}_-|\right]$

- Or "ideal" dipole potential (far away): $\Phi^{\mathrm{ideal}}(\mathbf{r}) = \dfrac{\lambda}{2\pi\epsilon_0}\dfrac{|\mathbf{d}|}{|\mathbf{r}-\mathbf{r}_c|}\cos\theta$



Comments on the Galerkin method

- Can choose any trial functions that are orthogonal and obey the boundary conditions
  - In contrast to the separation of variables, where we first found general solutions to PDE, the imposed boundary conditions

- Should be interpreted as a spectral transform approach, i.e., representing the solution as a Fourier series
  - In our example, it was a cosine series because of our boundary conditions

- Did not use a spatial grid
  - Convenient if only need the answer at specific points
  - Inefficient if we want to map the potential over the whole range, because of the computation of the prefactors, especially for a more complex potential

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 Φ=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:

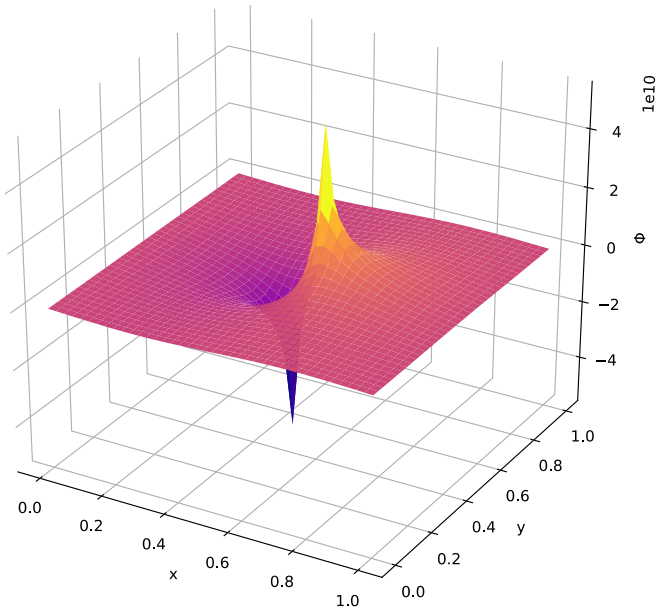
$$\Phi_{j,k}=\frac{1}{N^2}\sum_{m=0}^{N-1}\sum_{n=0}^{N-1}F_{m,n}\exp\left(\frac{i2\pi jm}{N}\right)\exp\left(\frac{i2\pi kn}{N}\right)$$

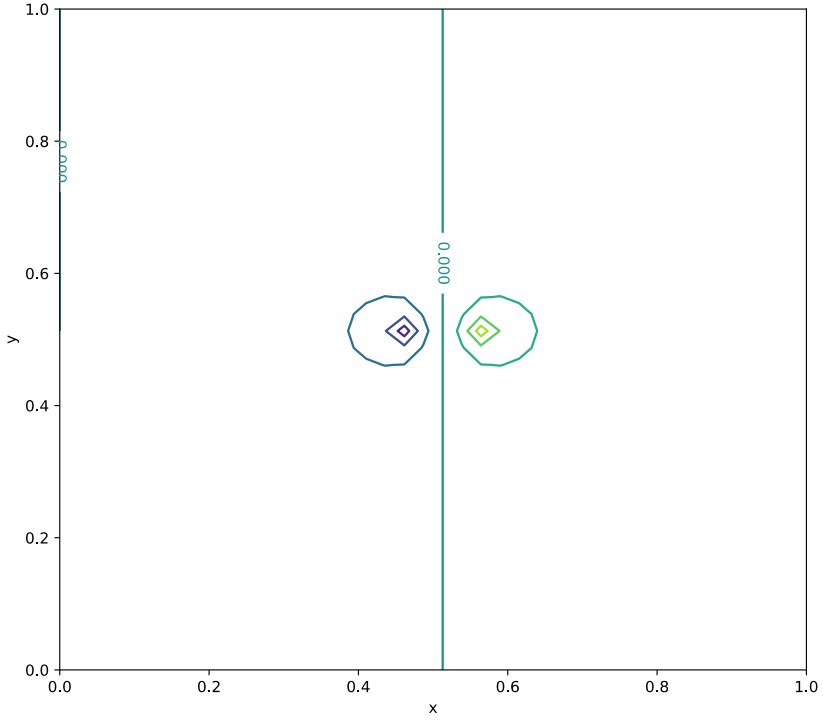
DEMO

- spectral_dipole.ipynb

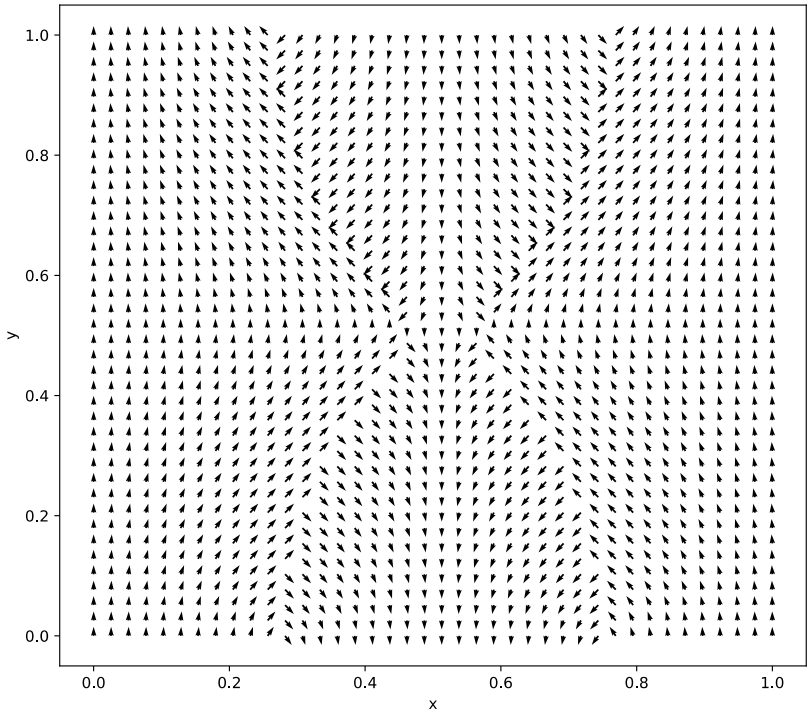
Ex: charge distribution of 2D dipole (Garcia Sec. 8.2)

Potential:





Field direction:



Today's lecture:
PDEs

- Elliptical PDEs: Spectral methods

- Stability analysis of 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:

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

- 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:

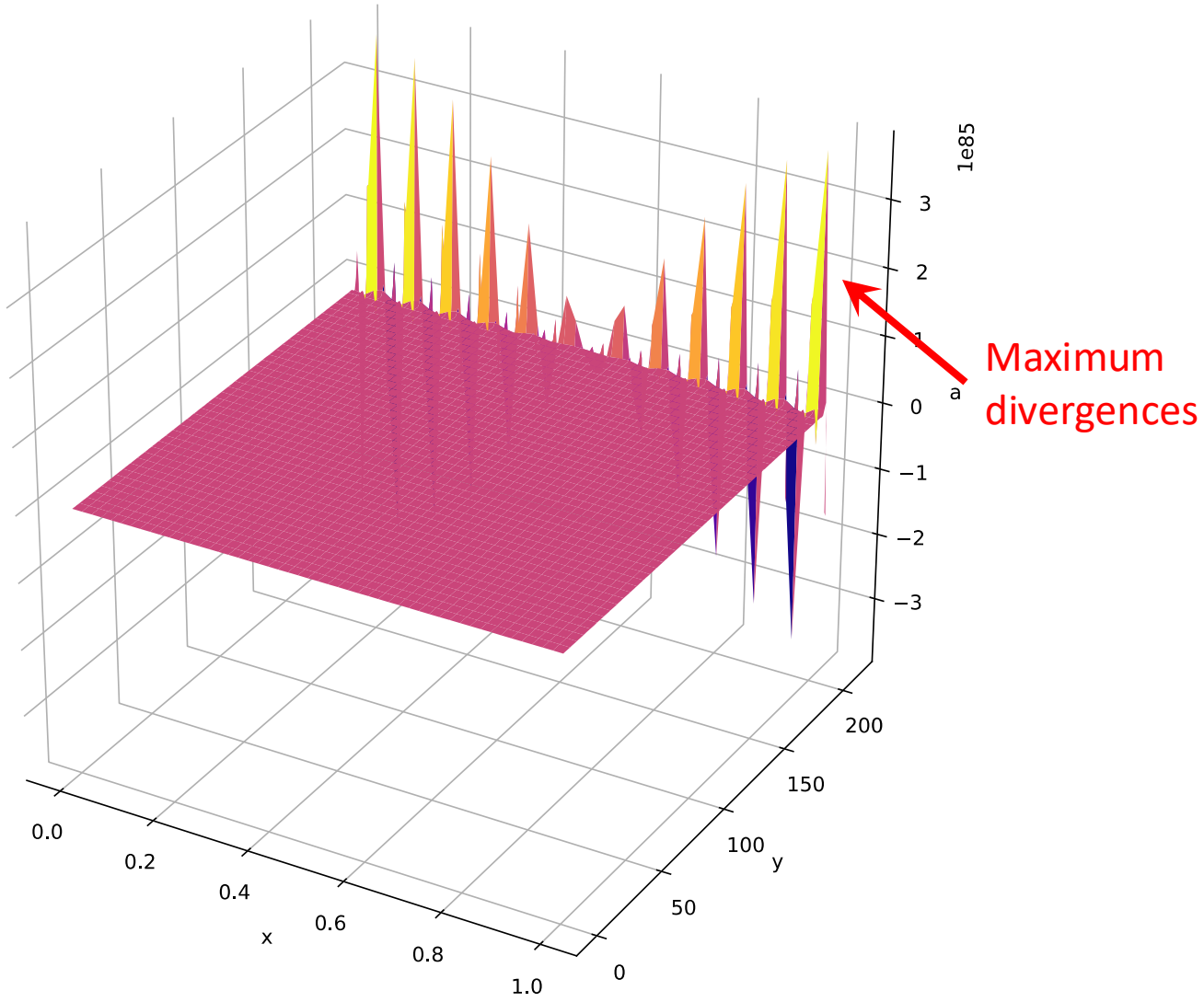
$$|\xi| = \left|1 - i\frac{c\tau}{h}\sin(kh)\right|$$

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

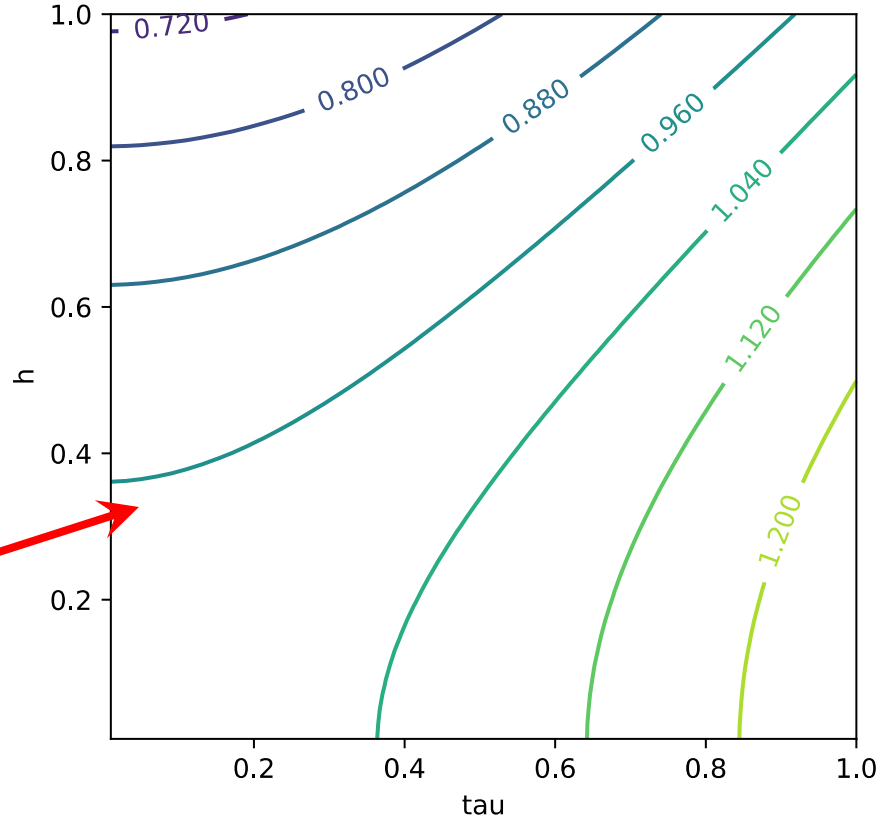
- So, we have: $$|\xi| = \sqrt{\cos^2(kh) + \left(\frac{c\tau}{h}\right)^2 \sin^2(kh)}$$

- 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

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

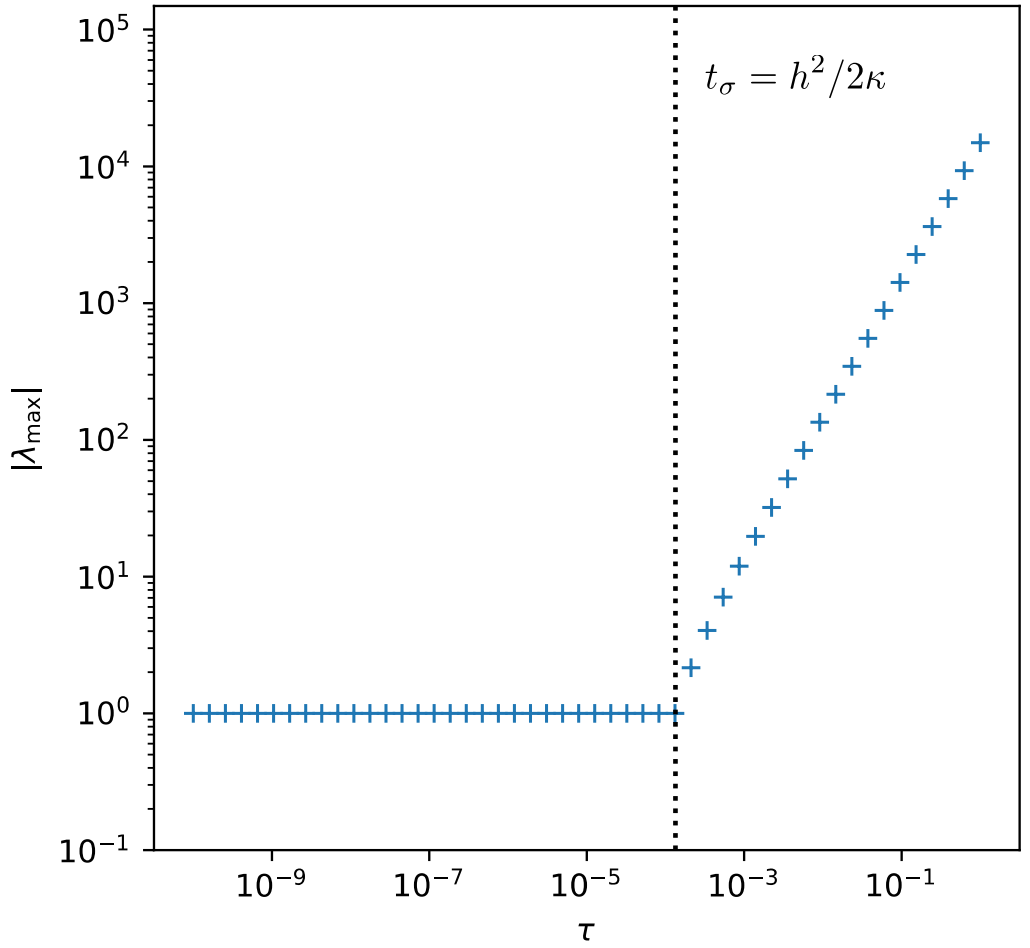
- We see that we will have divergence if we have any eigenvalues that are: $|\lambda_k| > 1$
- Spectral radius of **A**: Magnitude of the largest eigenvalue

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

- 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

After class tasks

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

- Readings

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