

PHY604 Lecture 18

November 7, 2023

Review: Gauss-Seidel and simultaneous overrelaxation

- **Gauss-Seidel**: We can improve the convergence over the Jacobi method by using updated values of the potential as they are calculated:

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

- **Simultaneous overrelaxation**: Choose a mixing parameter ω :

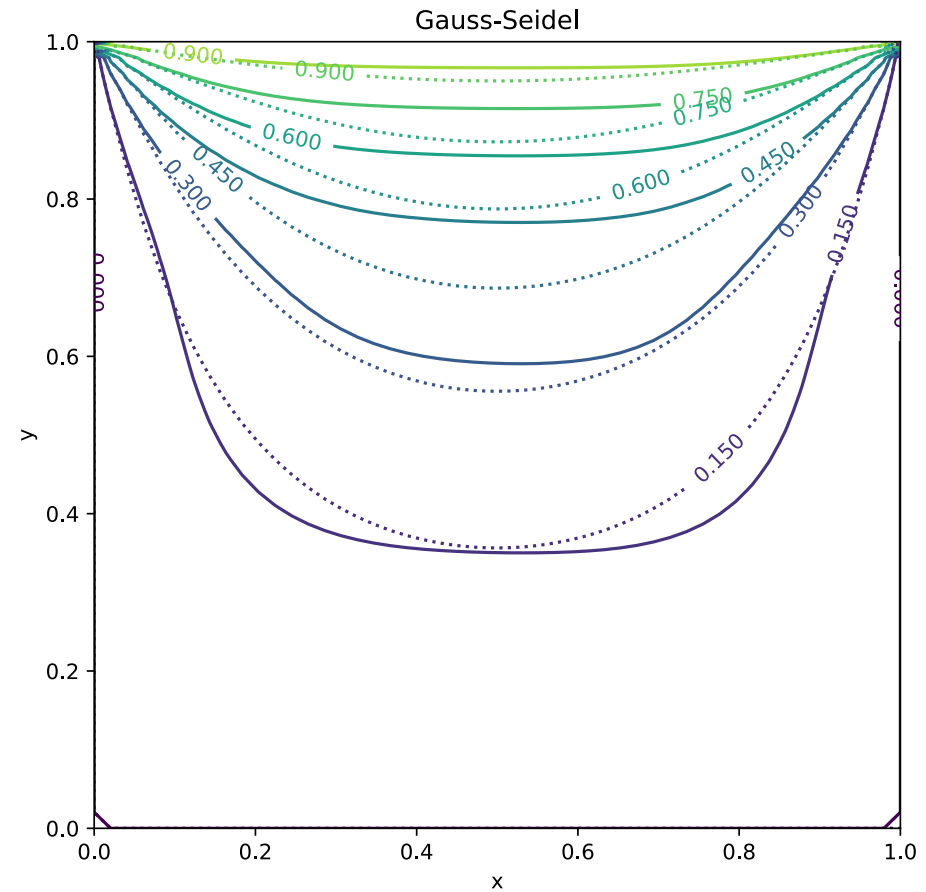
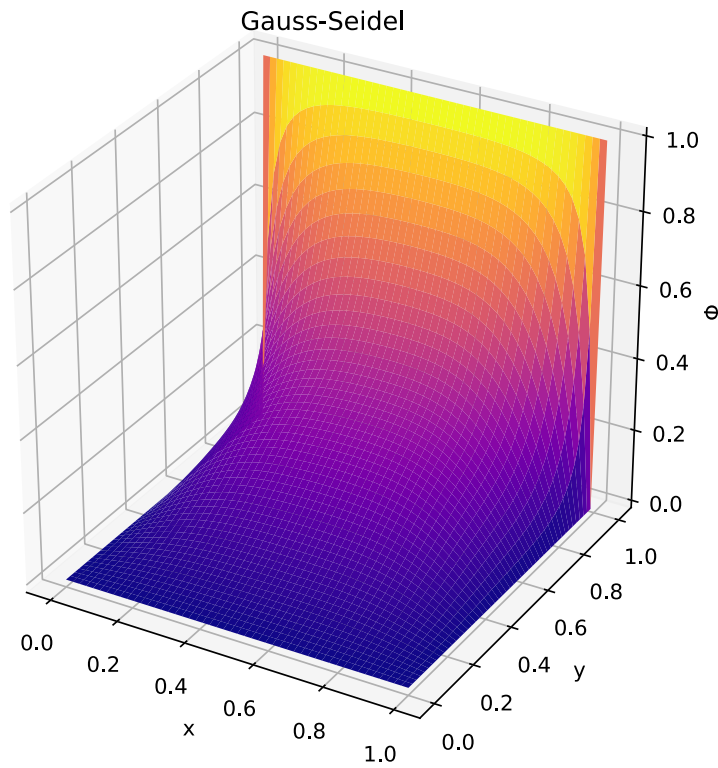
$$\Phi_{i,j}^{n+1} = (1 - \omega) \Phi_{i,j}^n + \frac{\omega}{4} (\Phi_{i+1,j}^n + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^n + \Phi_{i,j-1}^{n+1})$$

- $\omega < 1$ slows convergence, $\omega > 2$ is unstable
- Often chosen by trial and error
- E.g., for a square geometry with equal discretization, often a good choice:

$$\omega_{\text{opt}} = \frac{2}{1 + \sin(\pi/N)}$$

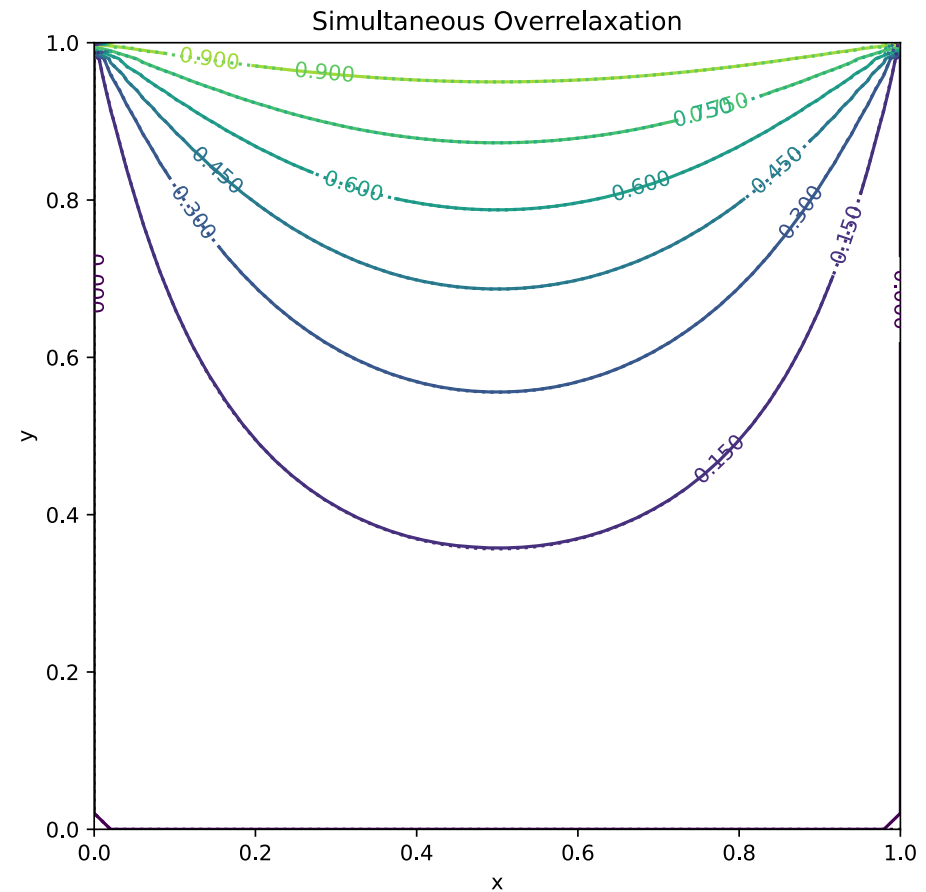
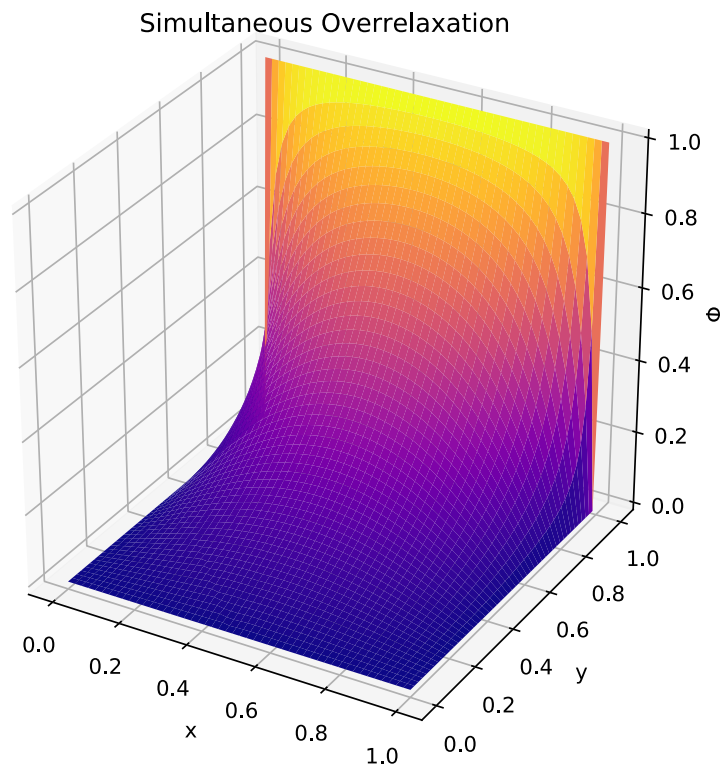
Review: Gauss-Seidel for Laplace eq.

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



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:

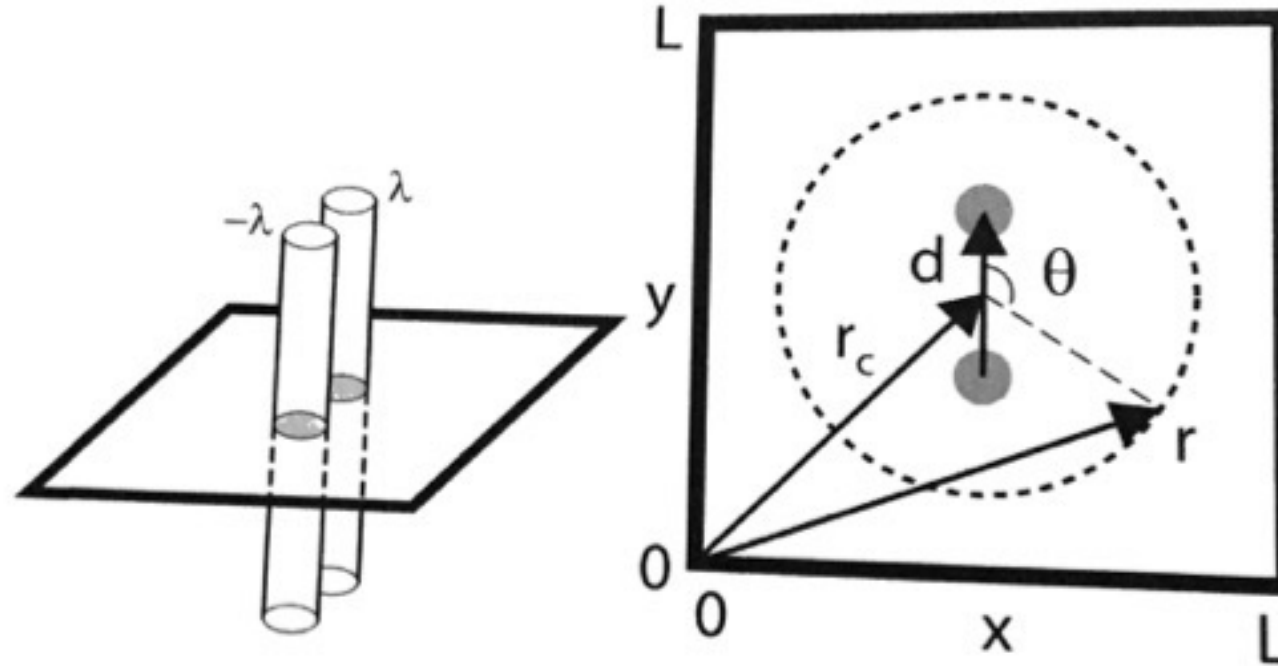
$$R(x, y) = -\nabla^2 T(x, y)$$

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)



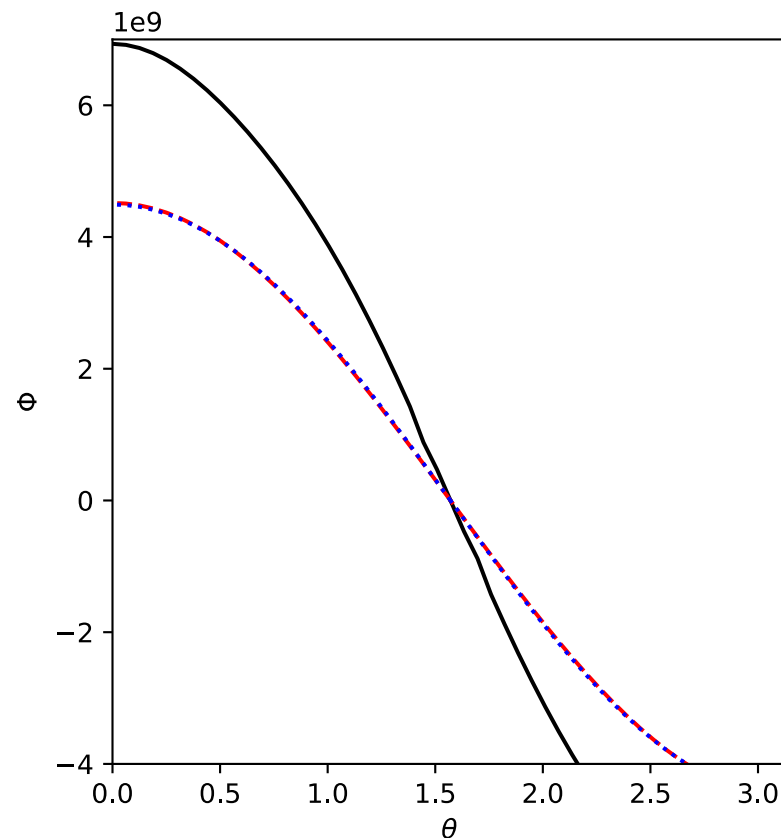
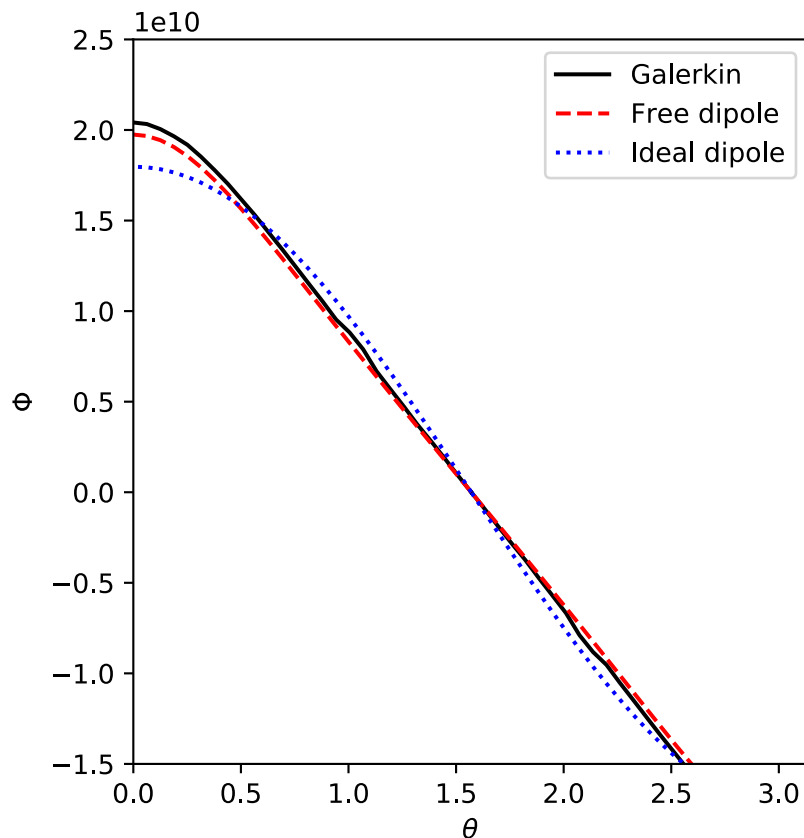
$$\rho(\mathbf{r}) = \lambda[\delta(\mathbf{r} - \mathbf{r}_+) - \delta(\mathbf{r} - \mathbf{r}_-)]$$

- 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): $\Phi^{\text{ideal}}(\mathbf{r}) = \frac{\lambda}{2\pi\epsilon_0} \frac{|\mathbf{d}|}{|\mathbf{r} - \mathbf{r}_c|} \cos \theta$



Review: 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

Today's lecture: Spectral methods and stability

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

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:

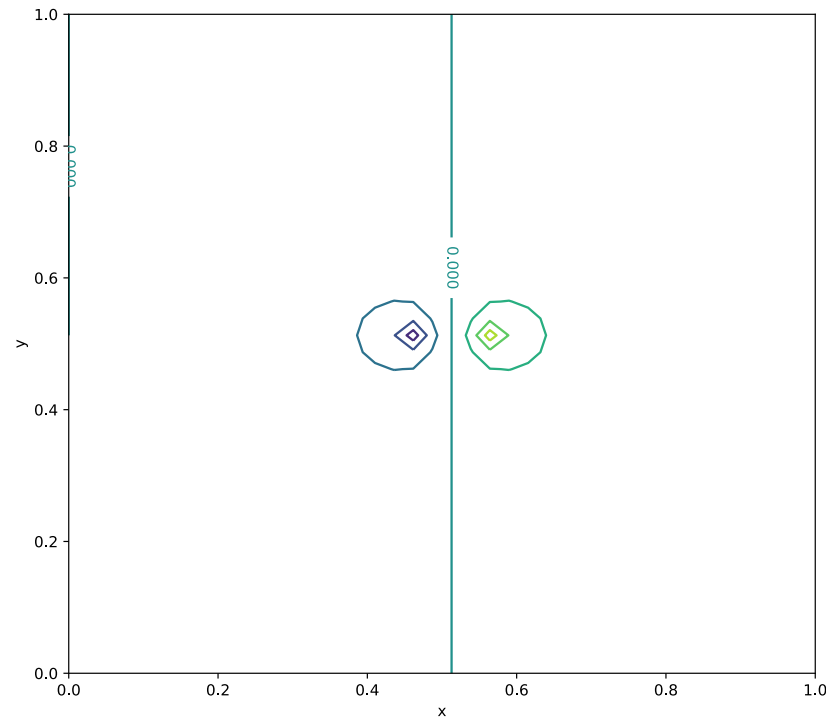
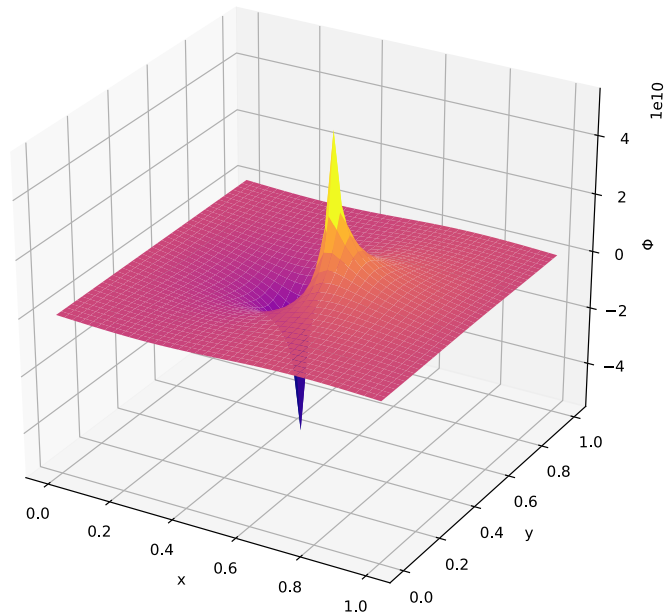
$$F_{m,n} = -\frac{h^2}{2\epsilon_0(\cos(2\pi m/N) + \cos(2\pi n/N) - 2)} R_{m,n}$$

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

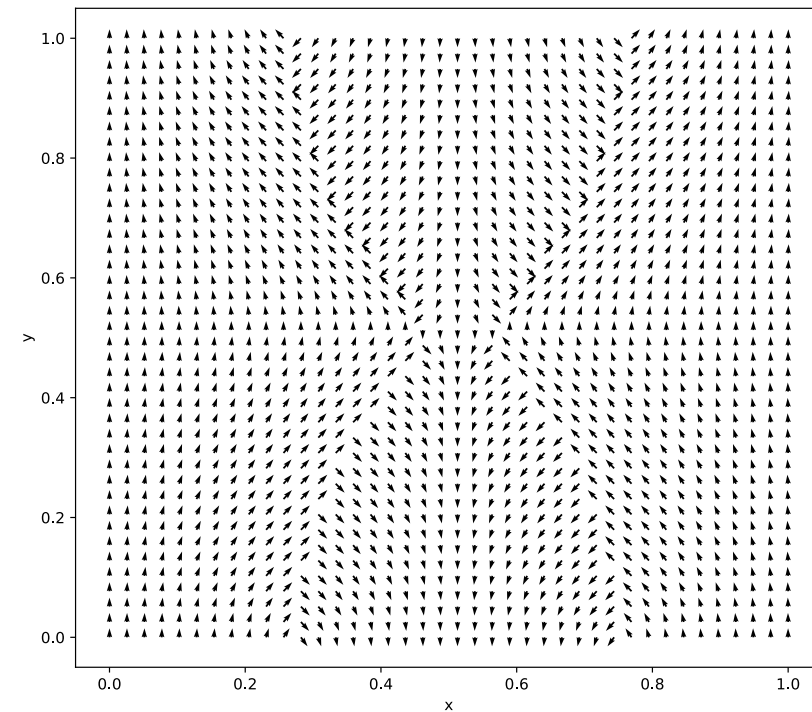
$$\Phi_{j,k} = \frac{1}{N^2} \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} F_{m,n} \exp\left(\frac{i2\pi jm}{N}\right) \exp\left(\frac{i2\pi kn}{N}\right)$$

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

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

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

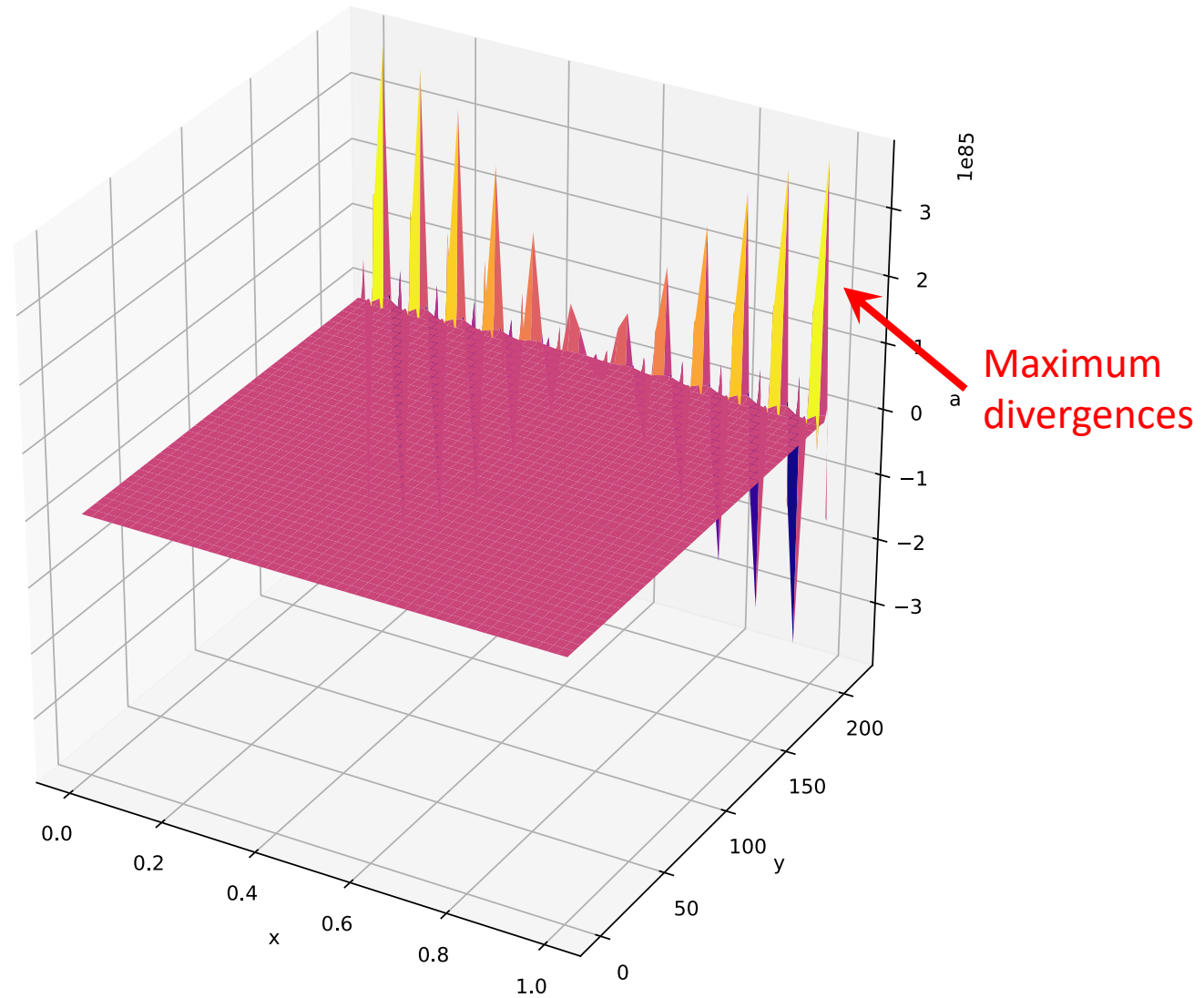
- Therefore:

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

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:

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

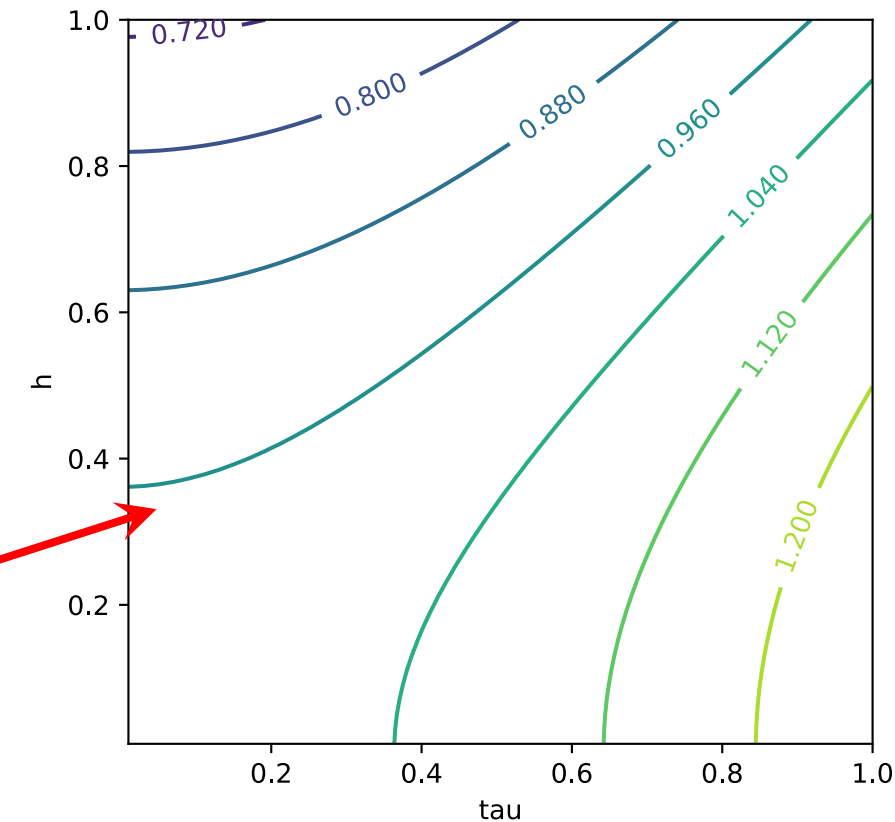
Stability of the Lax scheme

- 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



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:

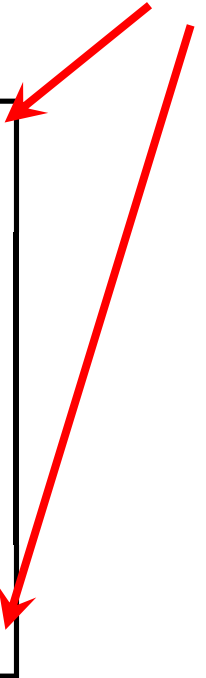
$$\begin{aligned} \mathbf{T}^{n+1} &= \mathbf{T}^n + \frac{\tau}{2t_\sigma} \mathbf{D} \mathbf{T}^n \\ &= \left(\mathbf{I} + \frac{\tau}{2t_\sigma} \mathbf{D} \right) \mathbf{T}^n \\ &= \mathbf{A} \mathbf{T}^n \end{aligned}$$

Matrix form of the diffusion equation

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

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

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

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

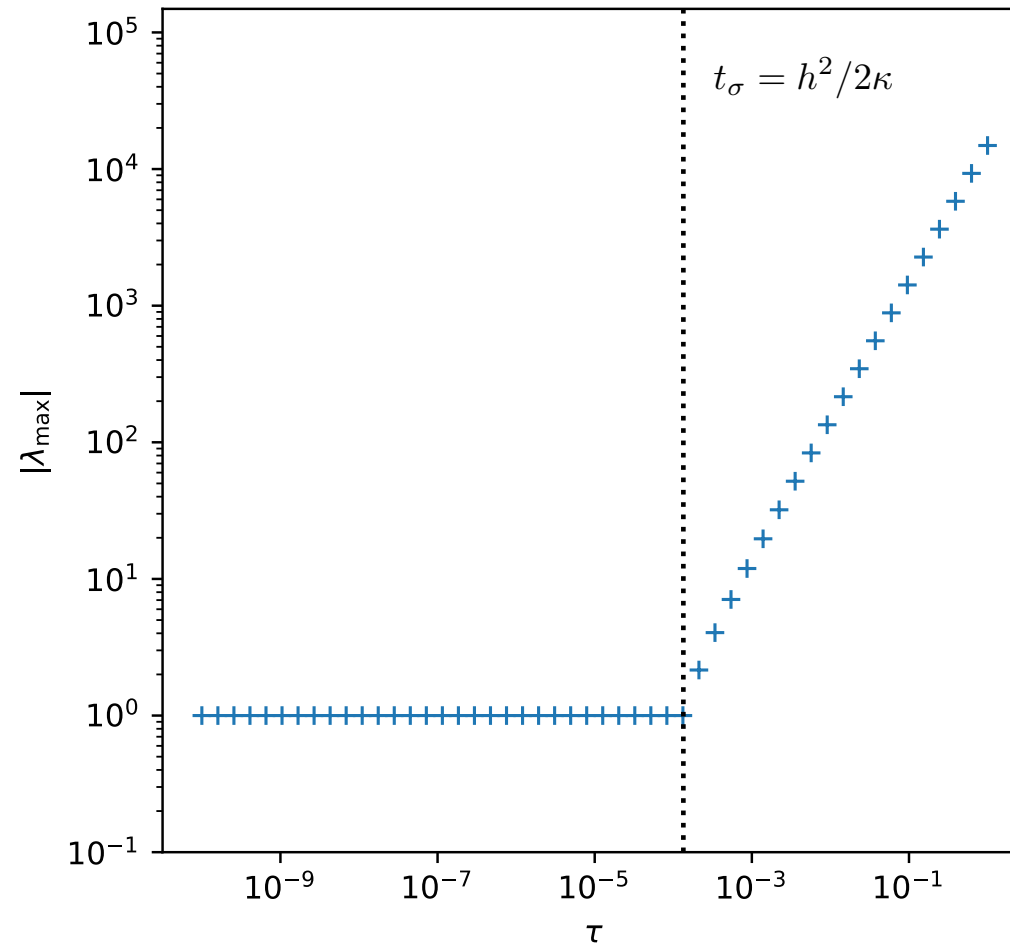
- We see that we will have divergence if we have any eigenvalues that are: $|\lambda_k| > 1$
- **Spectral radius of \mathbf{A}** : Magnitude of the largest eigenvalue

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

- 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

After class tasks

- Homework 4 is posted, due Nov 14, 2023
- Readings
 - Garcia Chapters 8 and 9