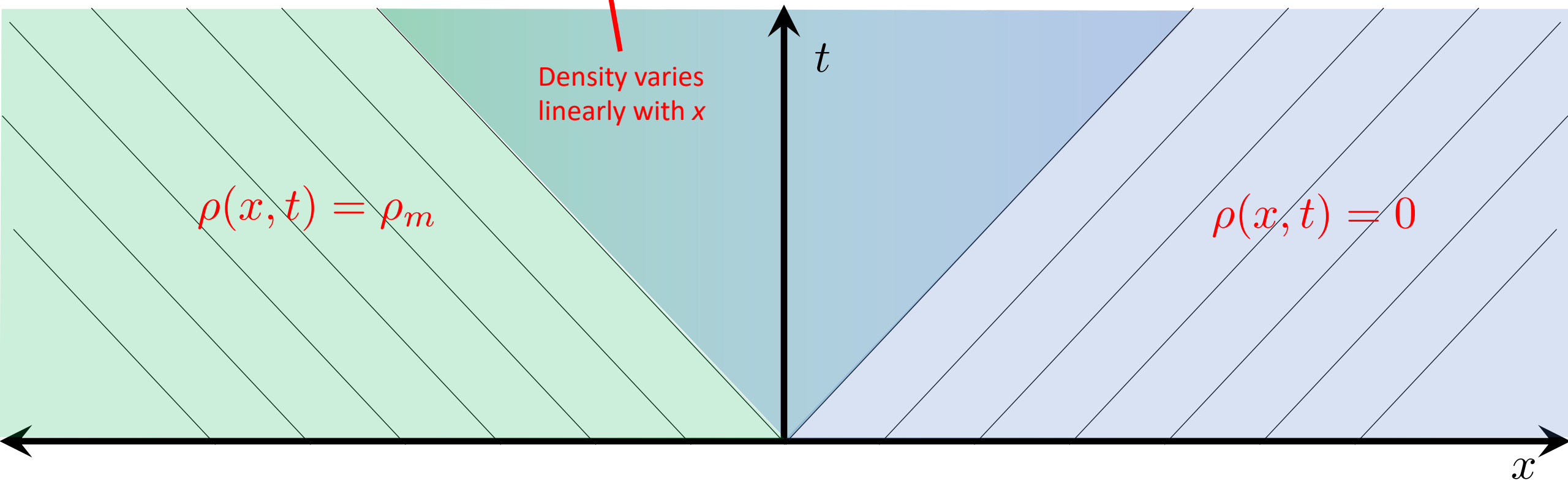
PHY604 Lecture 16

October 19, 2021

Review: Method of characteristics for traffic problem

$$\rho(x,t,) = \begin{cases} \rho_m & \text{for} \quad x \leq -v_m t \\ \frac{1}{2}\left(1 - \frac{x}{v_m t}\right)\rho_m & \text{for} \quad -v_m t < x < v_m t \\ 0 & \text{for} \quad x \geq v_m t \end{cases}$$



Review: Numerical solution to the traffic problem

- Starting with a general continuity equation:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial F(\rho)}{\partial x}$$

- In our case: $F(\rho) = \rho(x,t)v[\rho(x,t)] = \rho(x,t)v_m(1-\rho/\rho_m)$
- FTCS scheme:

$$\rho_i^{n+1} = \rho_i^n - \frac{\tau}{2h}(F_{i+1}^n - F_{i-1}^n)$$

- Lax scheme:

$$\rho_i^{n+1} = \frac{1}{2}(\rho_{i+1}^n + \rho_{i-1}^n) - \frac{\tau}{2h}(F_{i+1}^n - F_{i-1}^n)$$

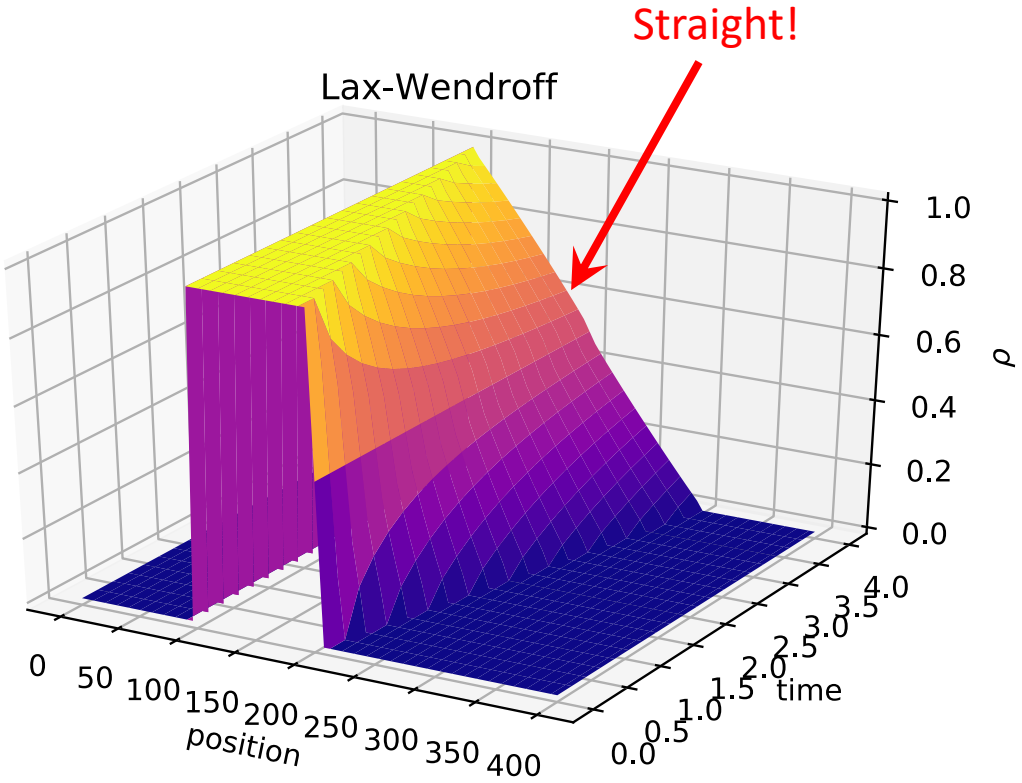
- Lax-Wendroff scheme:

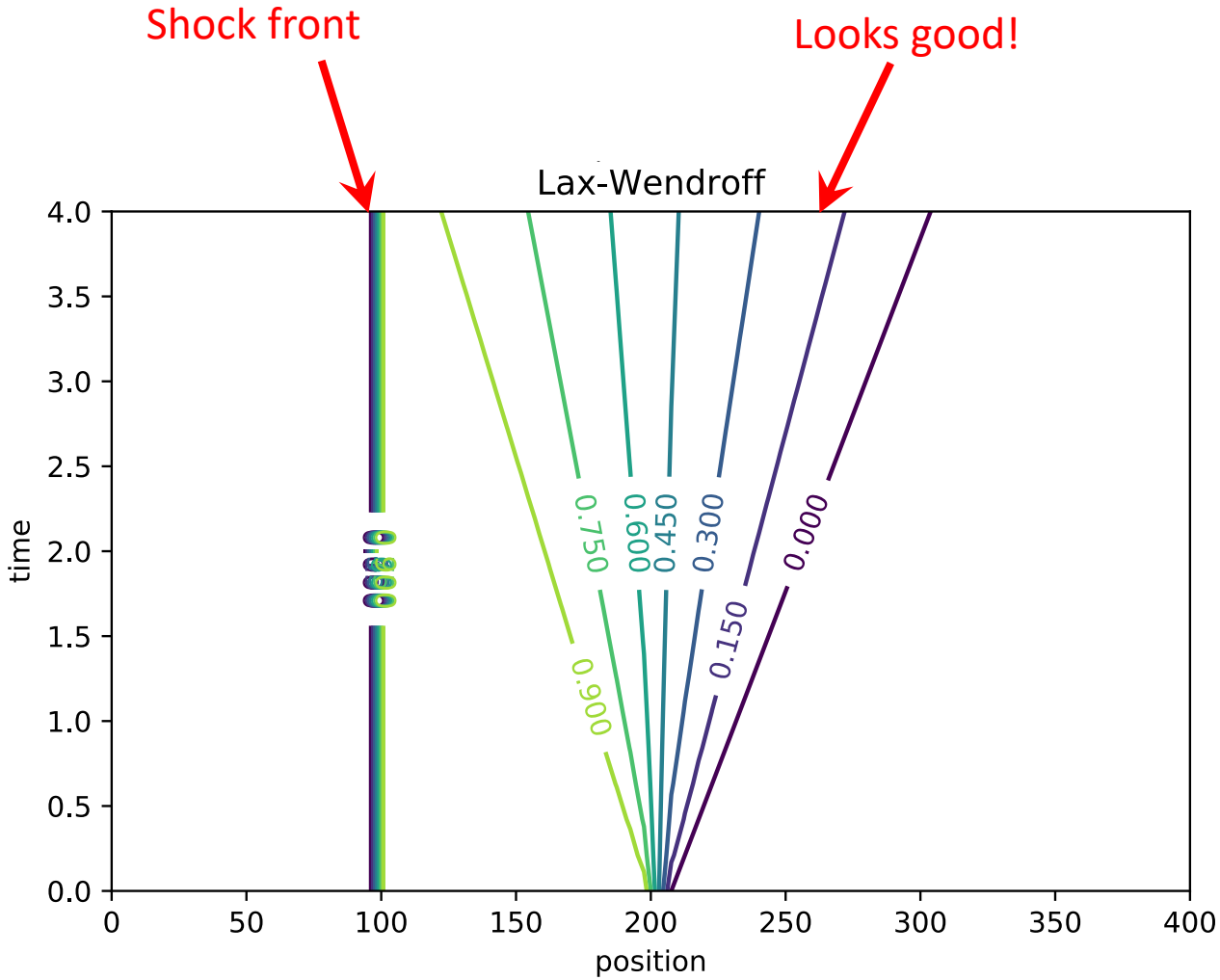
$$\rho_i^{n+1} = \rho_i^n - \frac{\tau}{2h}(F_{i+1}^n - F_{i-1}^n) + \frac{\tau^2}{2h^2}\left[c_{i+\frac{1}{2}}(F_{i+1}^n - F_i^n) - c_{i-\frac{1}{2}}(F_i^n - F_{i-1}^n\right]$$

  - Where:

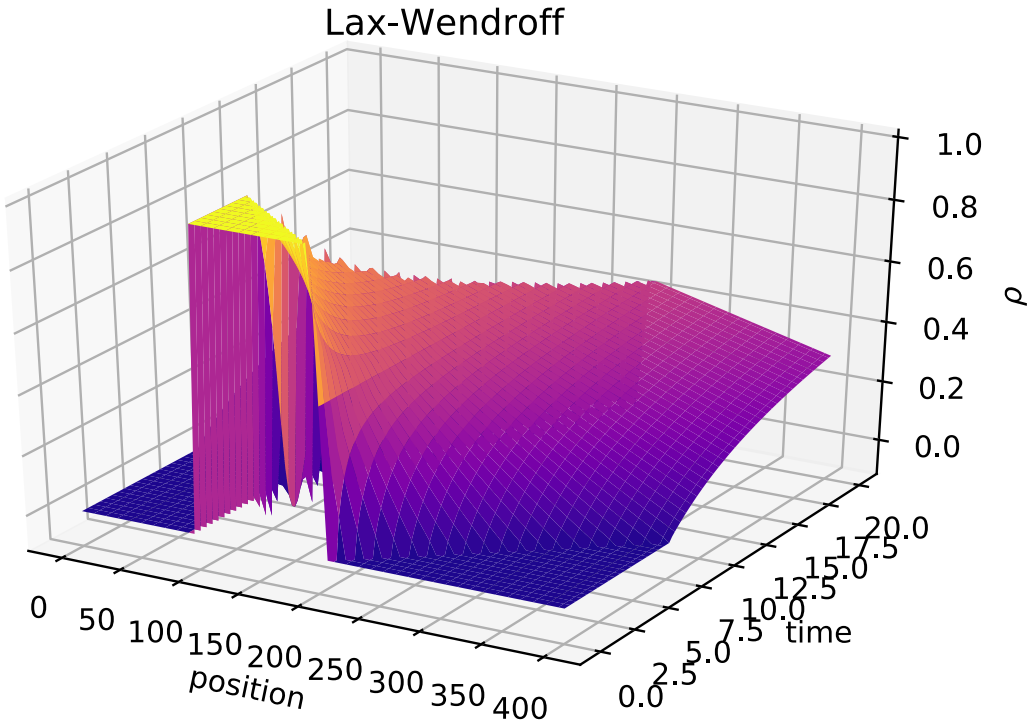
$$c_{i\pm\frac{1}{2}} \equiv c(\rho_{i\pm\frac{1}{2}}^n), \quad \rho_{i\pm\frac{1}{2}}^n \equiv \frac{\rho_{i\pm1}^n + \rho_i^n}{2}$$

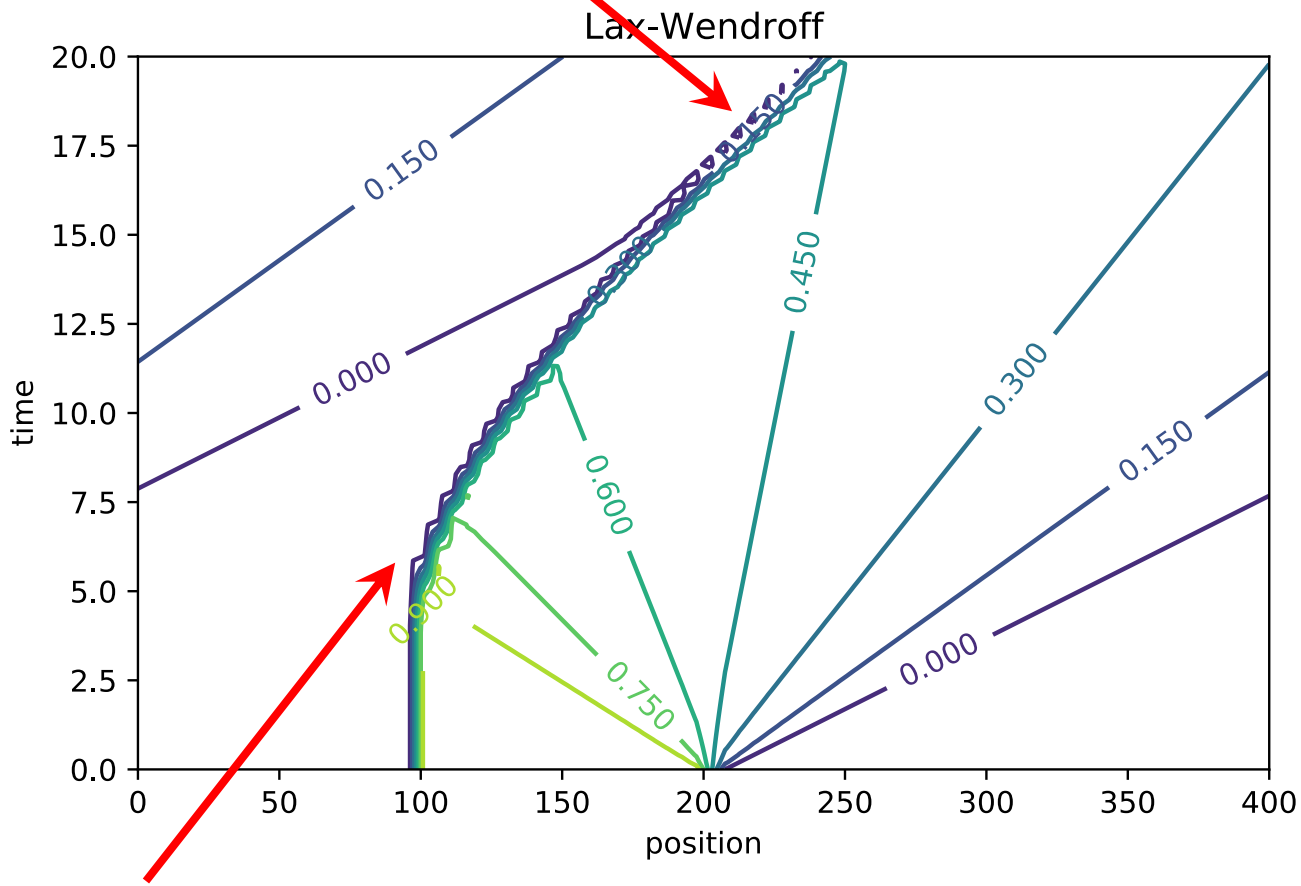
Review: Numerical solution with Lax-Wendroff method:





Review: Shock front in the traffic problem





Last car starts to move

Review: Solution of Laplace's eq. ODEs

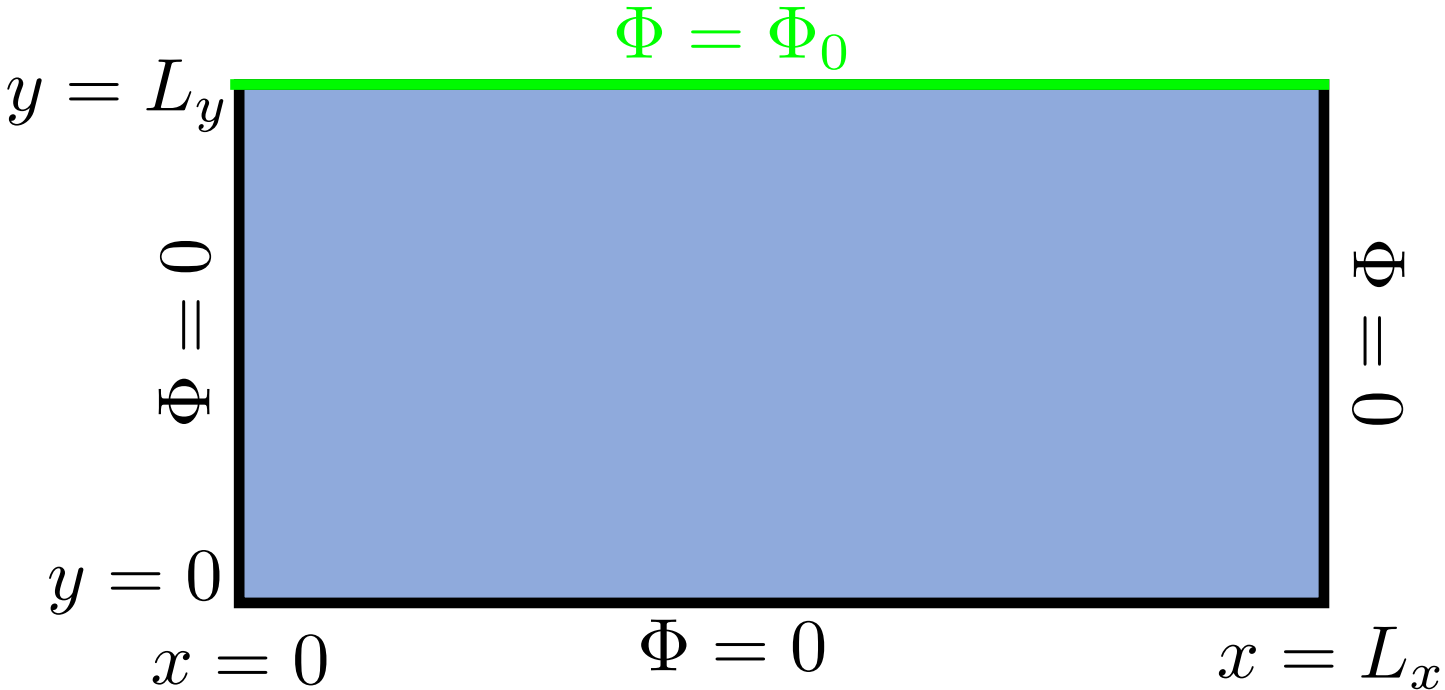
- Solution of these equations are well known:

$$X(x) = C_s \sin(kx) + C_c \cos(kx), \qquad Y(y) = C'_s \sinh(ky) + C'_c \cosh(ky)$$

  - Recall that k is complex, so solutions are "symmetric"

- To get the coefficients, we need to specify the boundary conditions

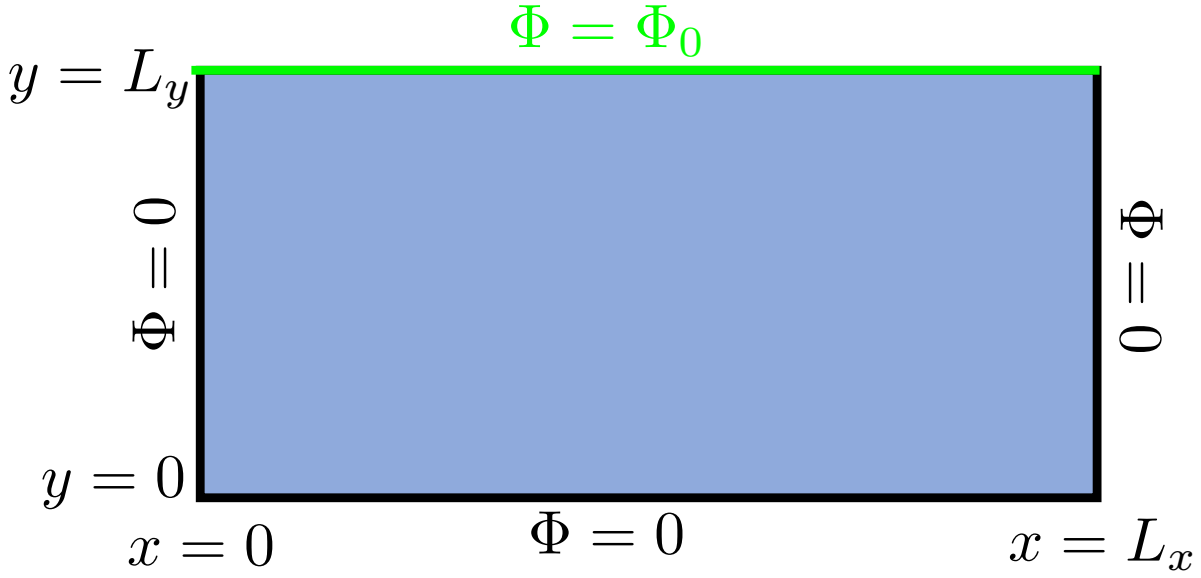
$$\Phi(x = 0, y) = \Phi(x = L_x, y) = \Phi(x, y = 0) = 0, \quad \Phi(x, y = L_y) = \Phi_0$$

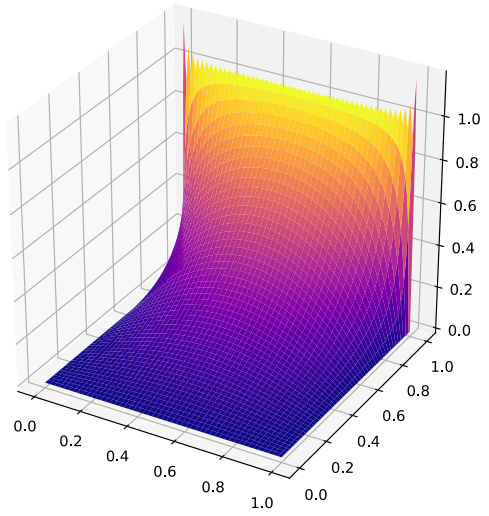


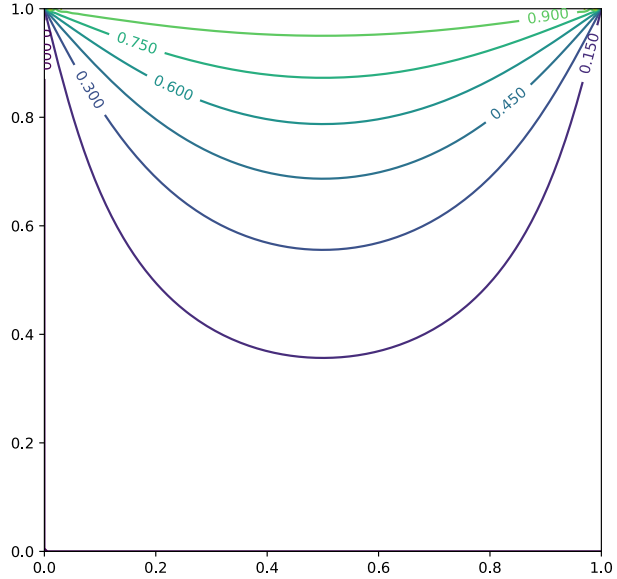
Review: Solution of Laplace's equation

- Our final solution of Laplace's equation with our chosen boundary conditions:

$$\Phi(x,y) = \Phi_0 \sum_{n=1,3,5,\ldots}^{\infty} \frac{4}{\pi n} \sin\left(\frac{n\pi x}{L_x}\right) \frac{\sinh\left(\frac{n\pi y}{L_x}\right)}{\sinh\left(\frac{n\pi L_y}{L_x}\right)}$$







Today's lecture:
Elliptical PDEs and stability

- Relaxation methods
- Spectral methods
- Stability analysis of PDEs

Numerical solution of the Laplace equation

- To do this, we'll go back to the *diffusion* equation we have solved previously, this time in two spatial dimensions:

$$\frac{\partial T(x,y,t)}{\partial t} = \kappa \left(\frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2} \right)$$

- Given an initial temperature profile and stationary boundary conditions, the solution will eventually relax to some steady state:

$$\lim_{t \to \infty} T(x,y,t) = T_s(x,y)$$

- In this state $\partial T / \partial t = 0$, so:

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} = 0$$

- We can think of the Laplace equation as the steady-state of the diffusion equation

Relaxation methods

- 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:

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

Remember, solving an electrostatic problem, so Φ does not actually have time dependence

Will drop out later

Relaxation methods

- 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:

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

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

Jacobi relaxation method

- Recall that FTCS is stable for $\mu\tau/h^2 \leq 1/2$

- In 2D the stability criteria is :

$$\frac{\mu\tau}{h_x^2} + \frac{\mu\tau}{h_y^2} \leq \frac{1}{2}$$

- If $h_x = h_y = h$, then the criterion is

$$\frac{\mu\tau}{h^2} \leq \frac{1}{4}$$

- Since we want to take *n* to infinity, we choose the largest timestep:

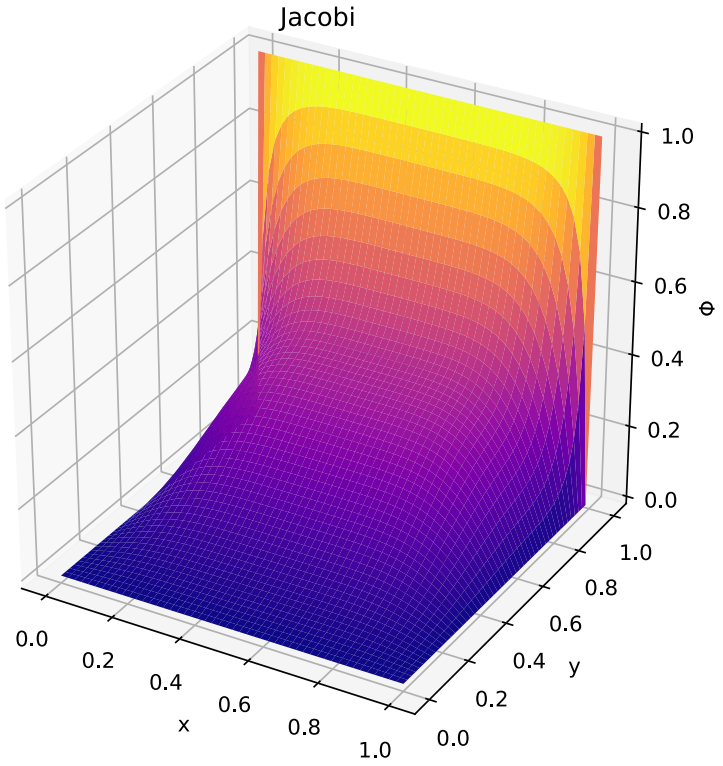
$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n})$$

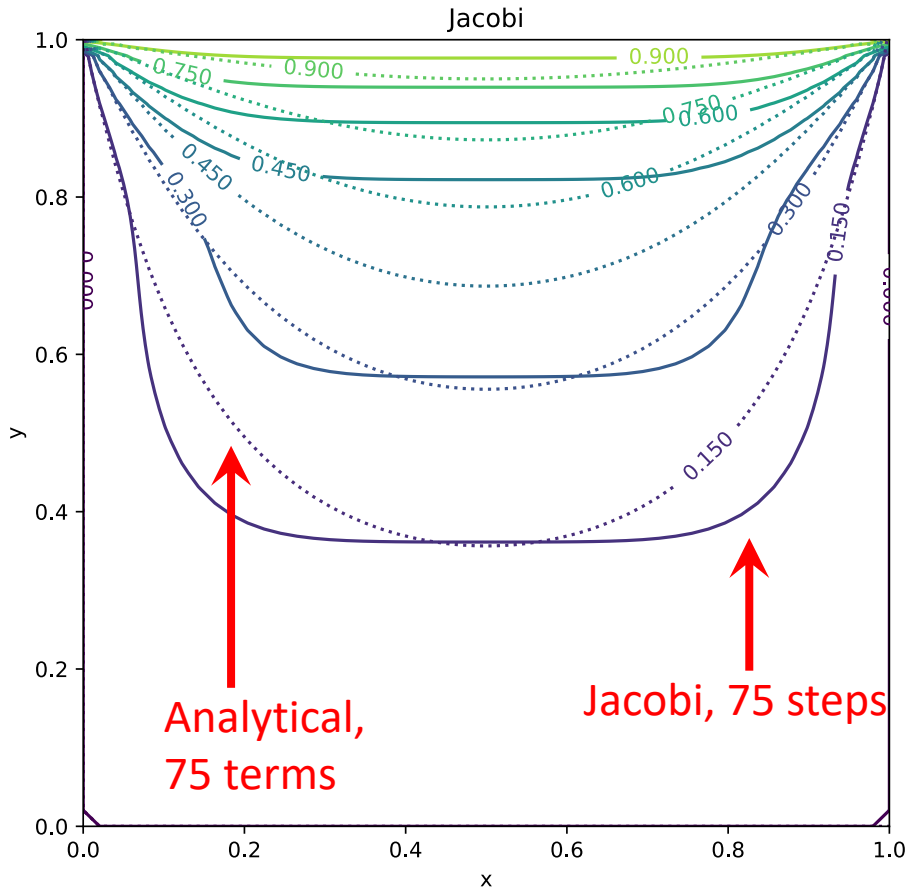
Jacobi method for Laplace equation

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

- Note that the μ has dropped out
- Involves replacing the value of the potential at a point with the average value of the four nearest neighbors
  - Discrete version of mean-value theorem for the electrostatic potential
- This equation is for the interior points (exterior are set by boundary conditions)
- Simple to generalize for Poisson equation

Jacobi method for Laplace equation





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:

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

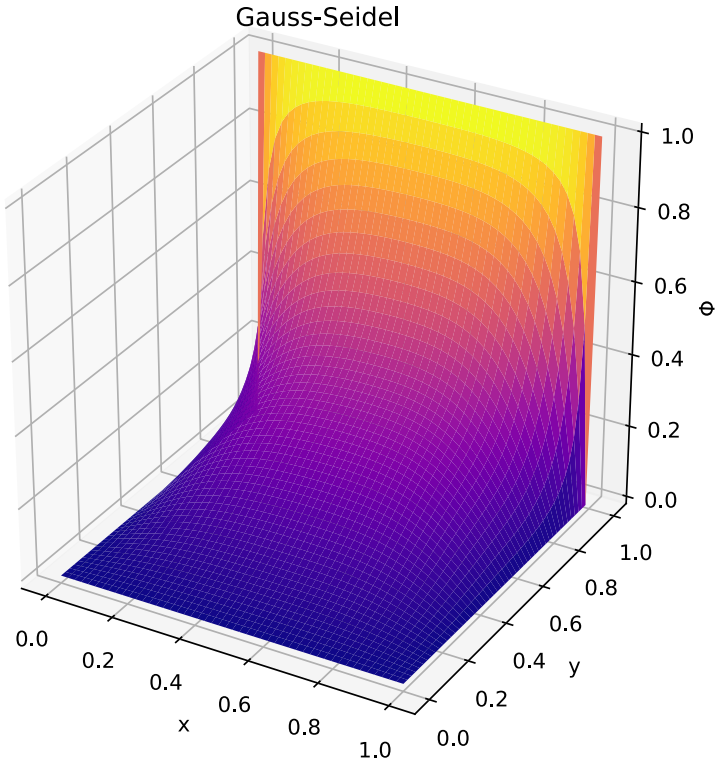
- Simultaneous overrelaxation: Choose a mixing parameter ω:

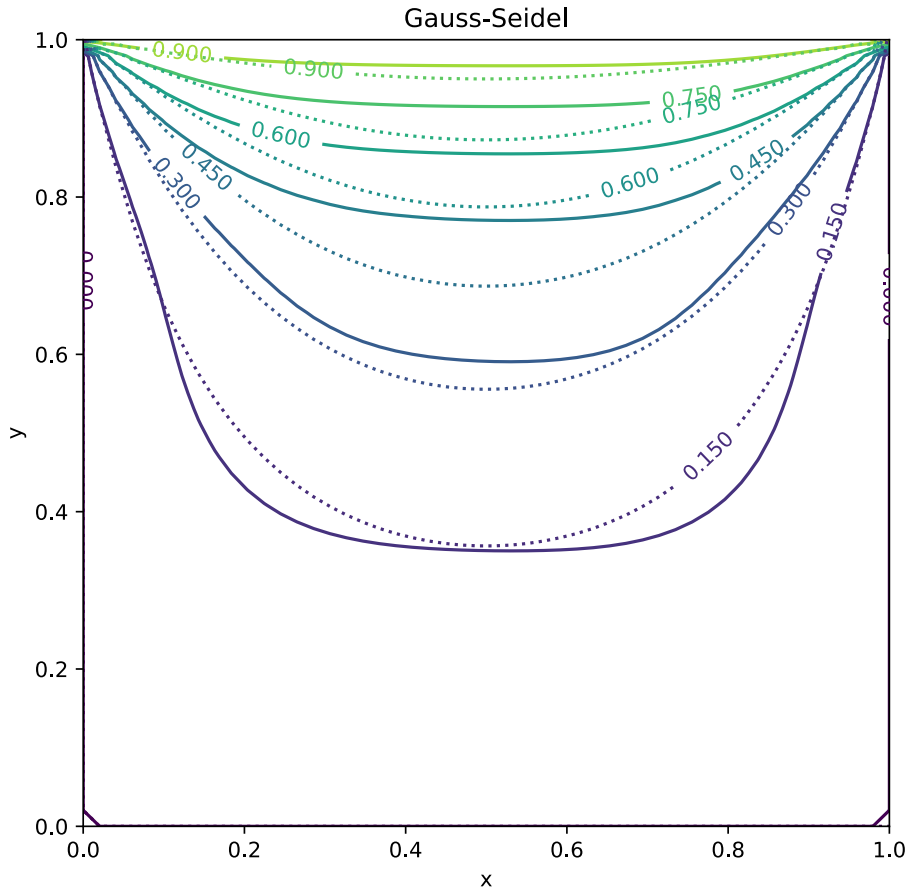
$$\Phi_{i,j}^{n+1} = (1-\omega)\Phi_{i,j}^{n} + \frac{\omega}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n+1})$$

  - $\omega < 1$ 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:

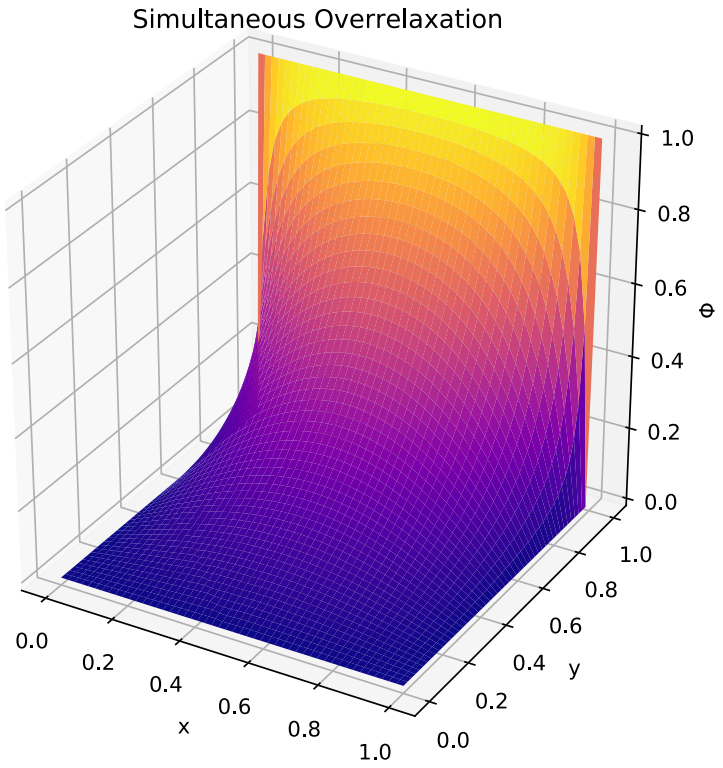
$$\omega_{\text{opt}} = \frac{2}{1 + \sin(\pi/N)}$$

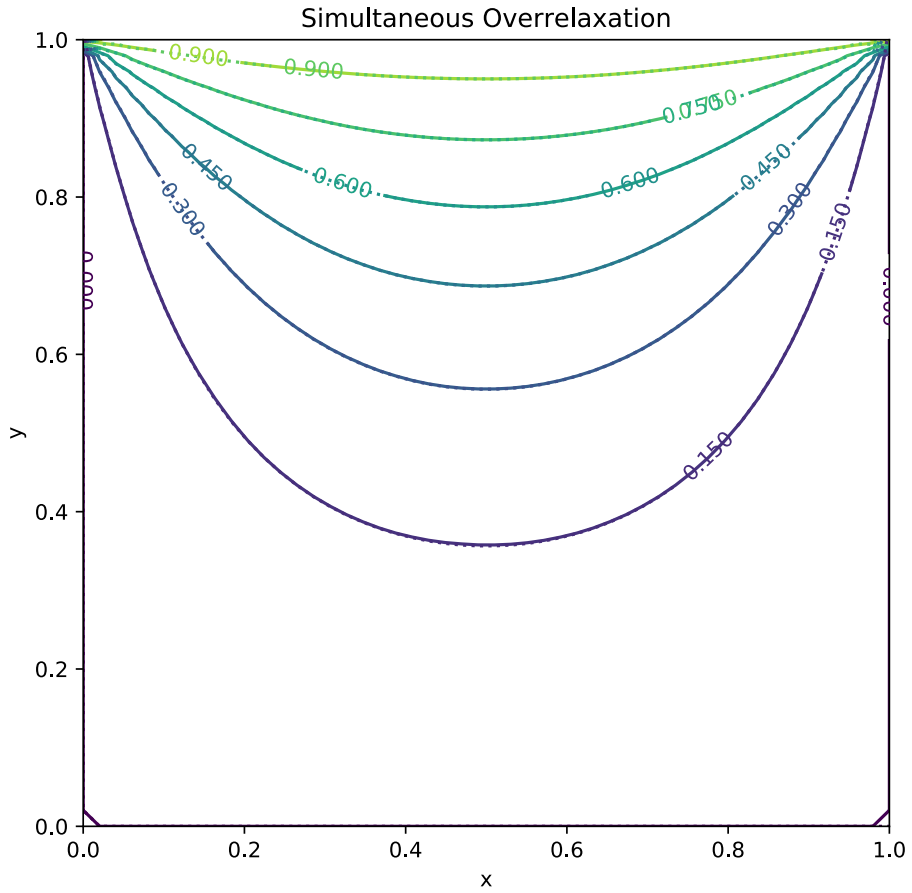
Gauss-Seidel for Laplace equation





Simultaneous overrelaxation for Laplace eq.





Recall: Jacobi iterative method

- Starting with a linear system:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ \vdots \quad & \quad \vdots \quad \quad \vdots \quad \quad \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n \end{aligned}$$

- Pick initial guesses $\mathbf{x}^k$, solve equation *i* for *i*th unknown to get an improved guess:

$$\begin{aligned} x_1^{k+1} &= -\frac{1}{a_{11}}(a_{12}x_1^k + a_{13}x_2^k + \cdots + a_{1n}x_n^k - b_1) \\ x_2^{k+1} &= -\frac{1}{a_{22}}(a_{21}x_1^k + a_{23}x_2^k + \cdots + a_{2n}x_n^k - b_2) \\ \vdots \quad & \quad \vdots \quad \quad \vdots \quad \quad \vdots \\ x_n^{k+1} &= -\frac{1}{a_{nn}}(a_{n1}x_1^k + a_{n2}x_2^k + \cdots + a_{n,n-1}x_{n-1}^k - b_n) \end{aligned}$$

Recall: Jacobi iterative method

- We can write an element-wise formula for **x**:

$$x_i^{k+1} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^k \right)$$

- Or:

$$\mathbf{x}_i^{k+1} = \mathbf{D}^{-1} \left(\mathbf{b} - (\mathbf{A} - \mathbf{D}) \mathbf{x}^k \right)$$

  - Where **D** is a diagonal matrix constructed from the diagonal elements of **A**

- Convergence is guaranteed if matrix is diagonally dominant (but works in other cases):

$$a_{ii} > \sum_{j=1, j \neq i}^{N} |a_{ij}|$$

The iterative methods discussed here are the same as we used to solve linear systems

- Can interpret Φ as a vector, so are solving $\mathbf{A}\Phi=\mathbf{b}$
- Going back to our initial discretization of the Laplace equation (for $h_x=h_y$):

$$\frac{1}{h^2}(\Phi^n_{i+1,j}+\Phi^n_{i-1,j}+\Phi^n_{i,j+1}+\Phi^n_{i,j-1}-4\Phi^n_{i,j})=0$$

- Note that **A** is a banded matrix with 4's on the diagonal, 1's on off-diagonal elements
- This is when the Jacobi method is guaranteed to be accurate (diagonally dominated)!
- Same holds for Gauss-Seidel and SOR

Today's lecture:
Elliptical PDEs and stability

- Relaxation methods

- 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: $0 \le x \le L, \quad 0 \le y \le L$
- 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:

$$\begin{aligned}\Phi(x,y) &= a_1 f_1(x,y) + a_2 f_2(x,y) + \cdots + a_K f_K(x,y) + T(x,y) \\ &= \sum_{k=1}^{K} a_k f_k(x,y) + T(x,y) \\ &= \Phi_a(x,y) + T(x,y)\end{aligned}$$

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:

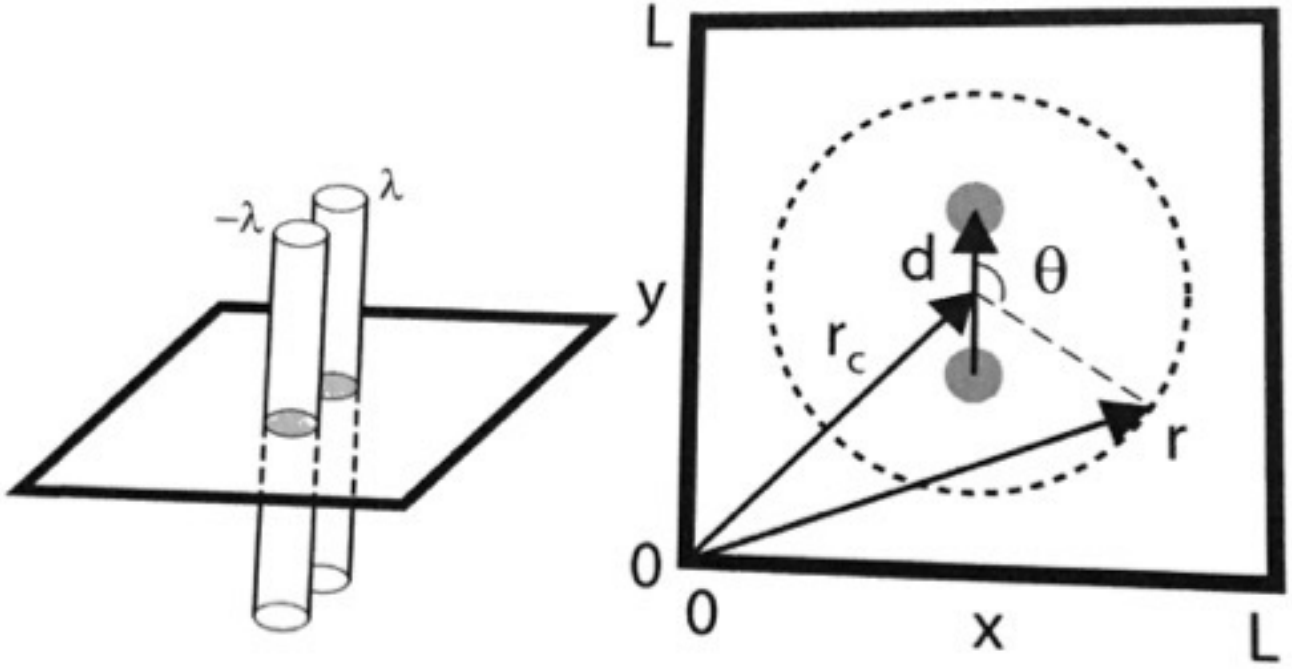
$$a_{m,n} = \frac{4}{\pi^2 \epsilon_0 (m^2+n^2)(1+\delta_{m,0})(1+\delta_{n,0})} \int_0^L dx \int_0^L dy \rho(x,y) \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

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)



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

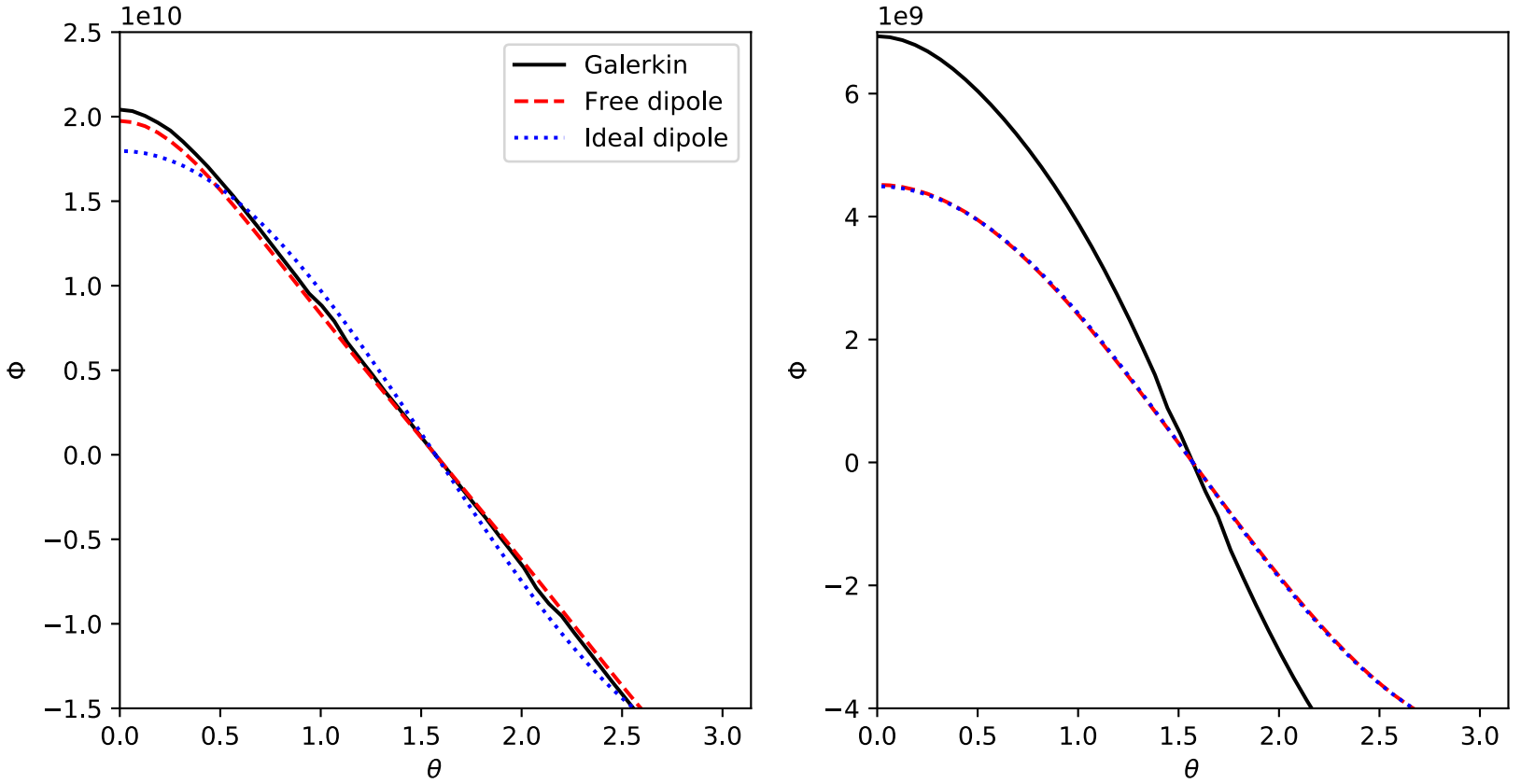
- Where:

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

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:

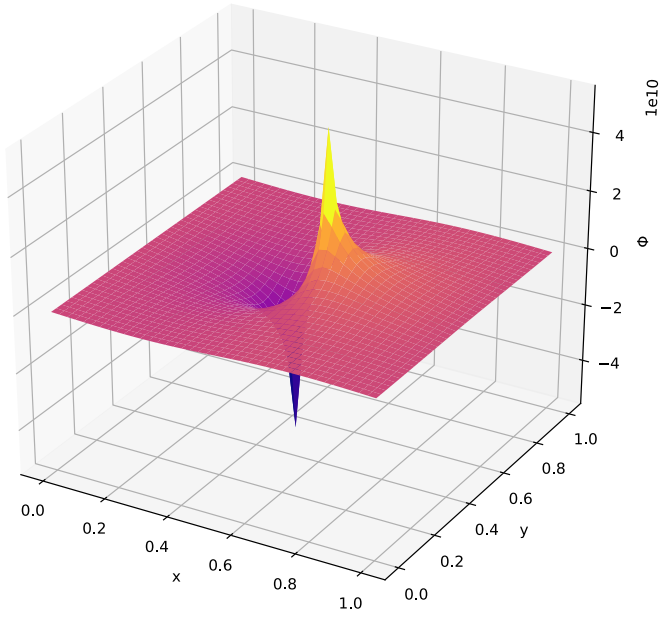
$$F_{m,n}=-\frac{h^2}{2\epsilon_0(\cos(2\pi m/N)+\cos(2\pi n/N)-2)}R_{m,n}$$

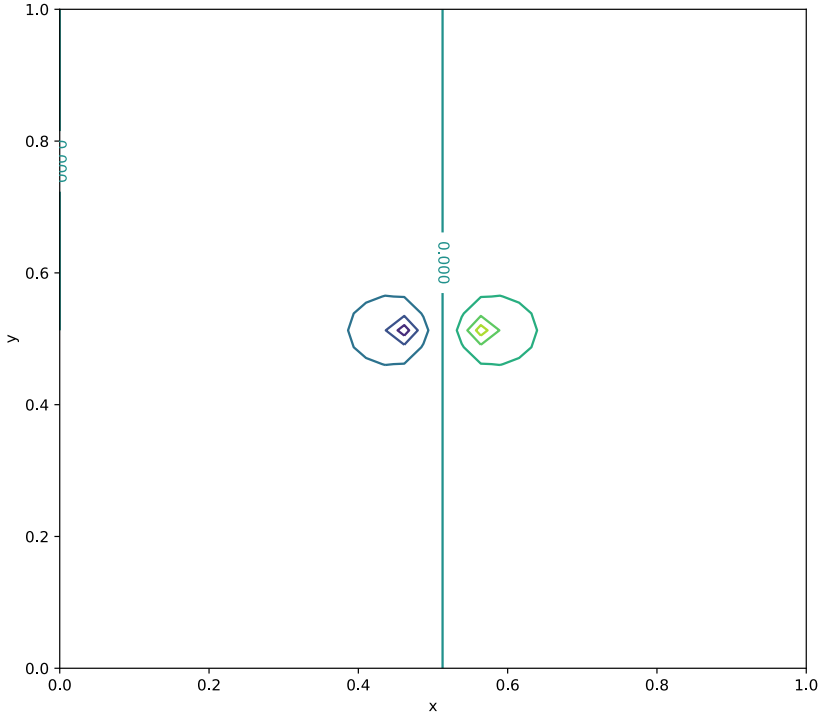
- To get the potential, we just need to take the inverse FFT:

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

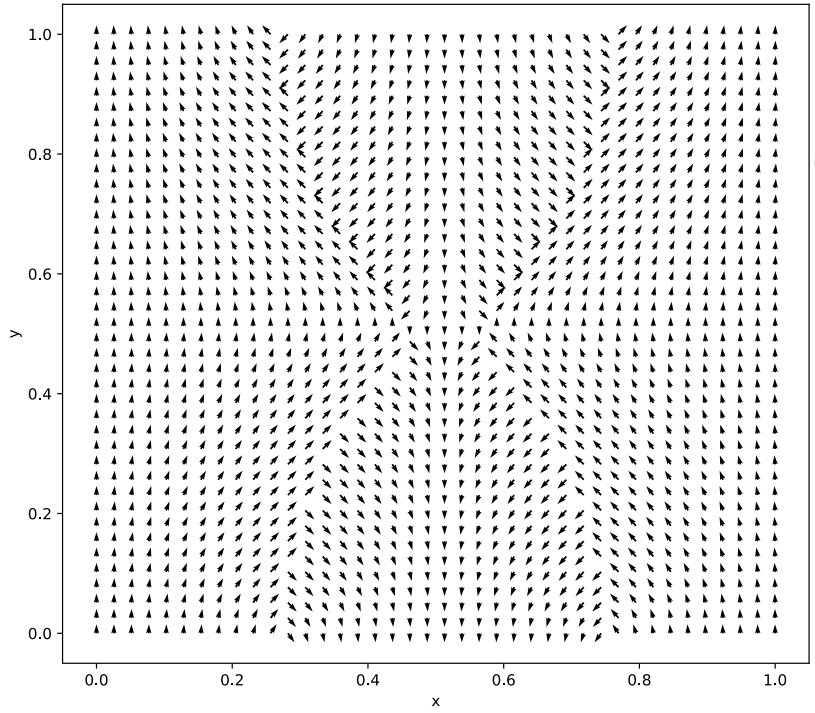
Ex: charge distribution of 2D dipole (Garcia Sec. 8.2)

Potential:





Field direction:



Today's lecture:
Elliptical PDEs and stability

- Relaxation methods
- 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:

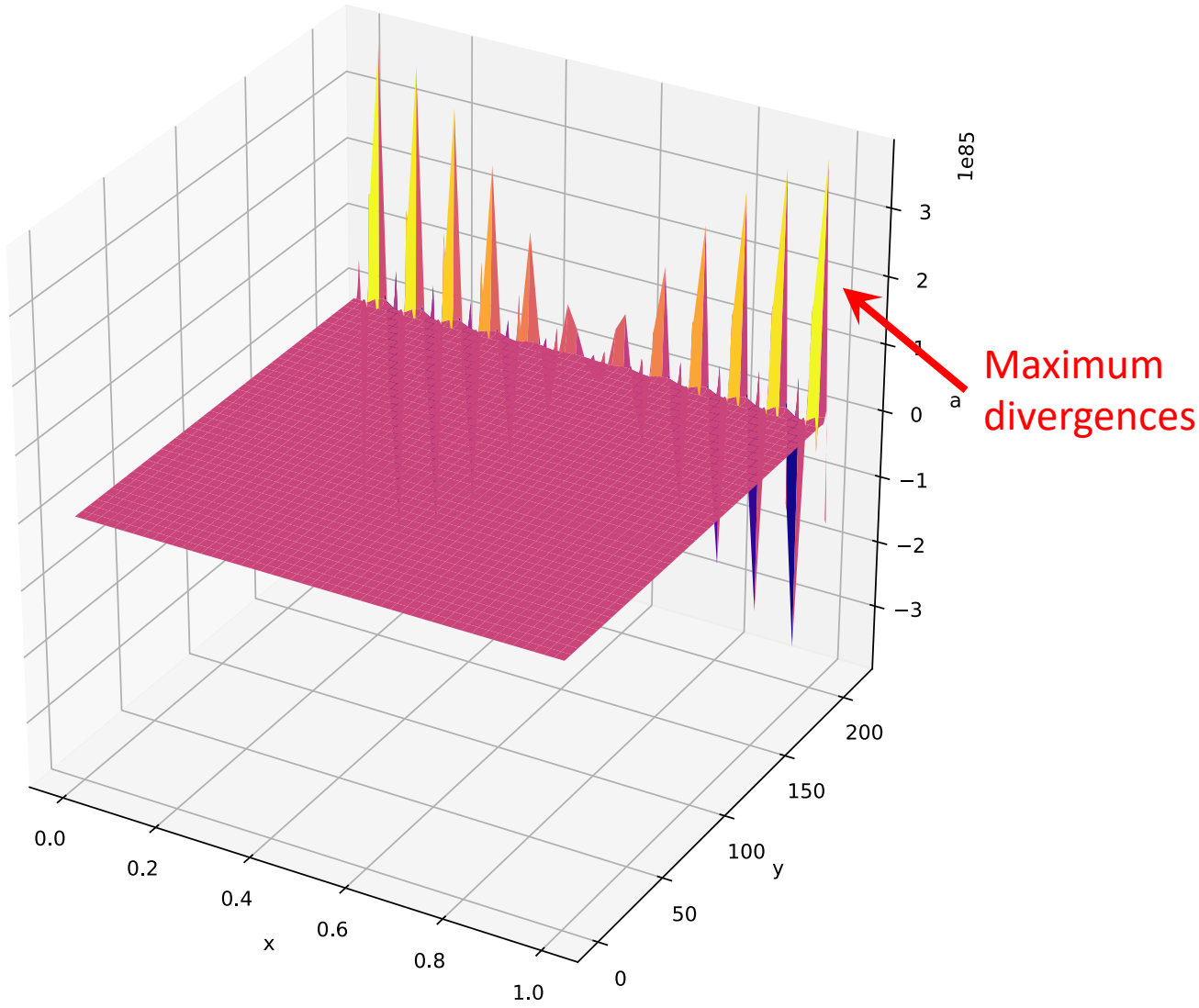
$$|\xi| = \left|1 - i\frac{c\tau}{h}\sin(kh)\right|$$

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

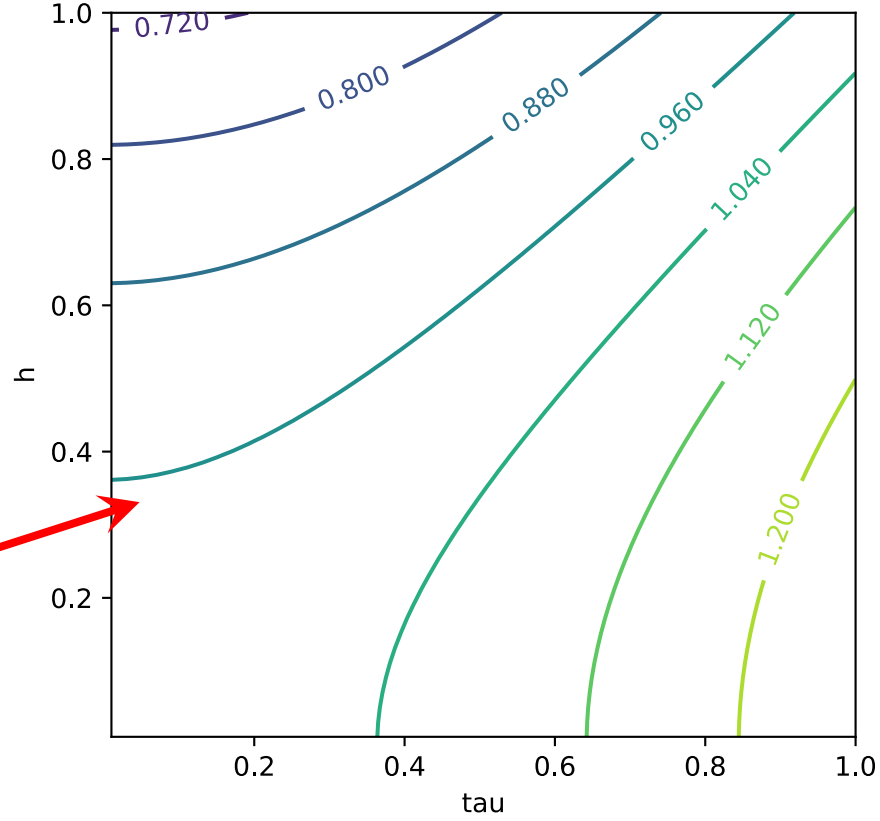
- So, we have: $$|\xi| = \sqrt{\cos^2(kh) + \left(\frac{c\tau}{h}\right)^2 \sin^2(kh)}$$

- 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



After class tasks

- Homework 4 is posted, due Oct. 28, 2021

- Readings

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