PHY604 Lecture 16

October 31, 2021

Review: Examples of PDE types

- Parabolic equations
  - E.g., Time-dependent Schrodinger equation, 1D diffusion equation
  - Consider the Fourier equation with temperature *T* and thermal diffusion coefficient κ:

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

- Hyperbolic equations
  - E.g., 1D wave equation with amplitude *A* and speed *c*:

$$\frac{\partial^2 A(x,t)}{\partial t^2} = c^2 \frac{\partial^2 A(x,t)}{\partial x^2}$$

- Elliptic equations
  - E.g., Poisson equation:

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = -\frac{1}{\epsilon_0}\rho(x,y)$$

Review: Diffusion equation with FTCS

- Now the discretized PDE is:

$$\frac{T_i^{n+1} - T_i^n}{\tau} = \kappa \frac{T_{i+1}^n + T_{i-1}^n - 2T_i^n}{h^2}$$

- And temperature at future time is:

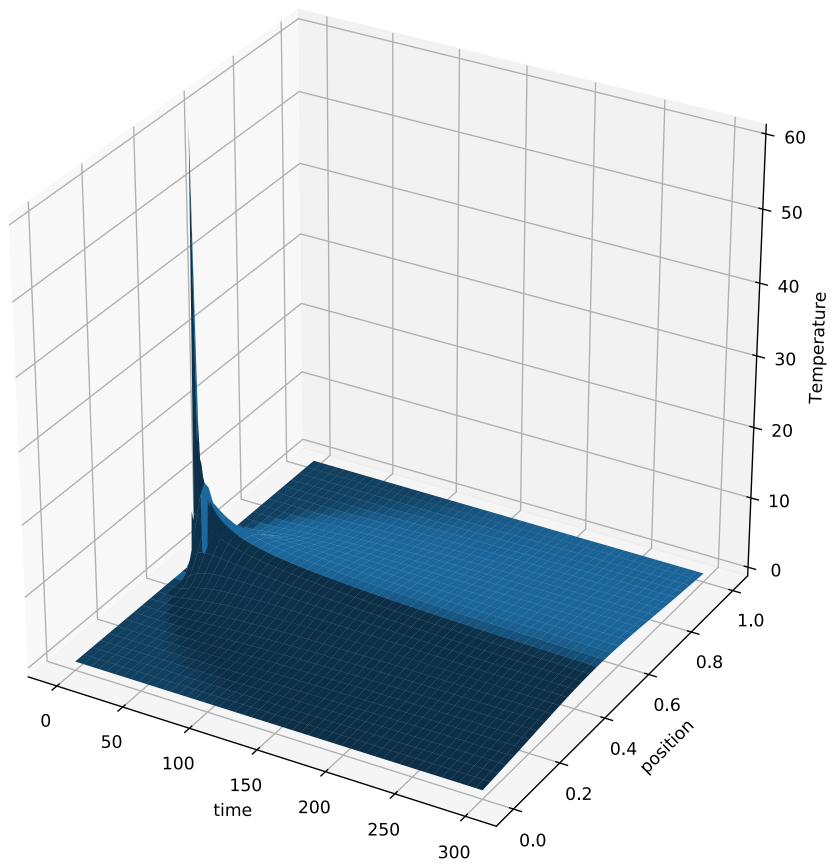
$$T_i^{n+1} = T_i^n + \frac{\kappa\tau}{h^2}(T_{i+1}^n + T_{i-1}^n - 2T_i^n)$$

- Explicit: Everything that depends on previous timestep *n* is on RHS

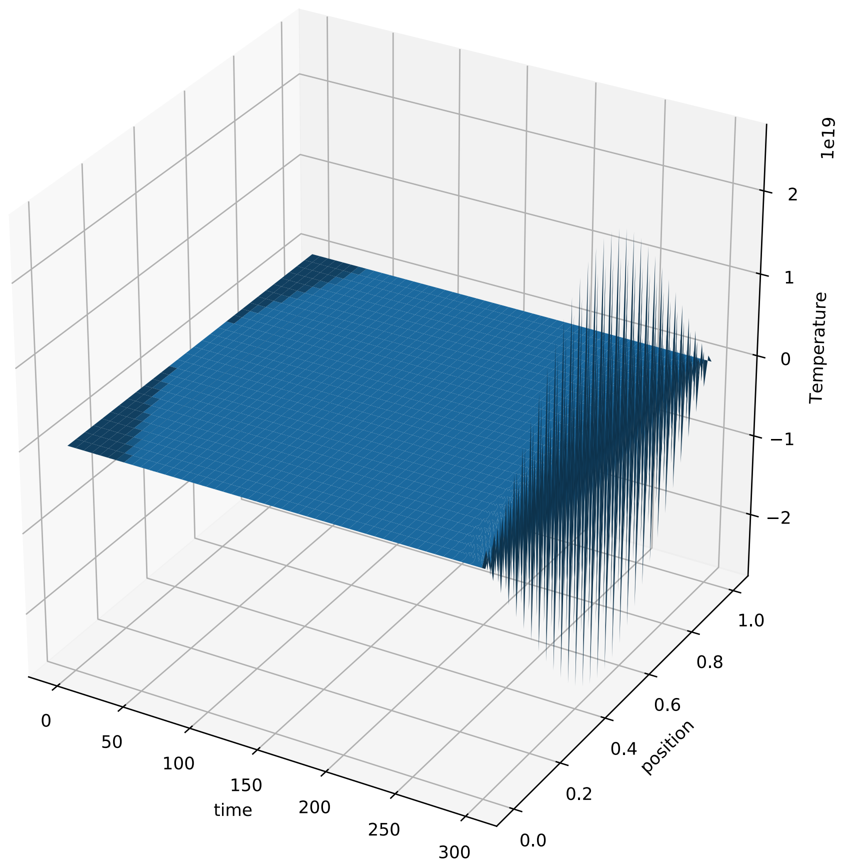
- Discretization is reminiscent of Euler's method for ODEs

Review: FCTS method on diffusion equation

Numerically stable: τ = 1e-4



Numerically stable: τ = 1.5e-4



Review: Advection equation

- Thus, we see that there is a simpler hyperbolic equation, the advection equation:

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

- Describes the evolution of some scalar field *a* carried by a flow of velocity *c*
    - Also known as linear convection equation
    - Waves move only in one direction (to the right if $c > 0$), unlike the wave equation
- “Flux conservation” equation
    - E.g., continuity equation in electrodynamics/quantum mechanics:

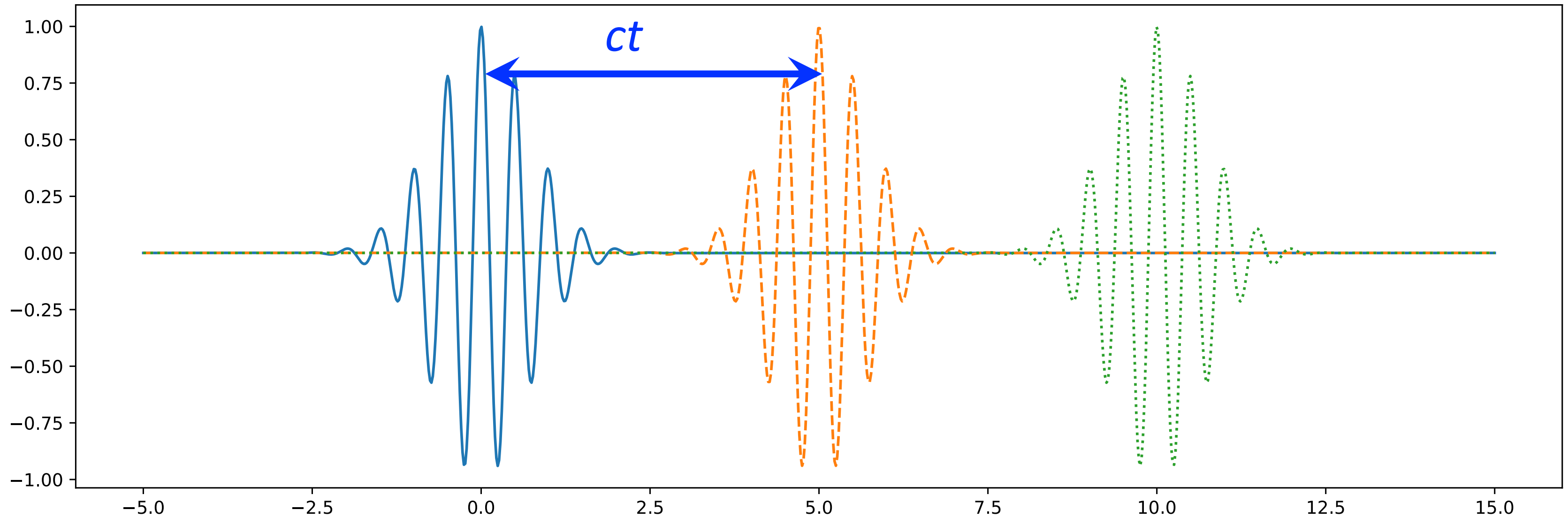
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}(p)$$

Review: Analytical solution to advection equation

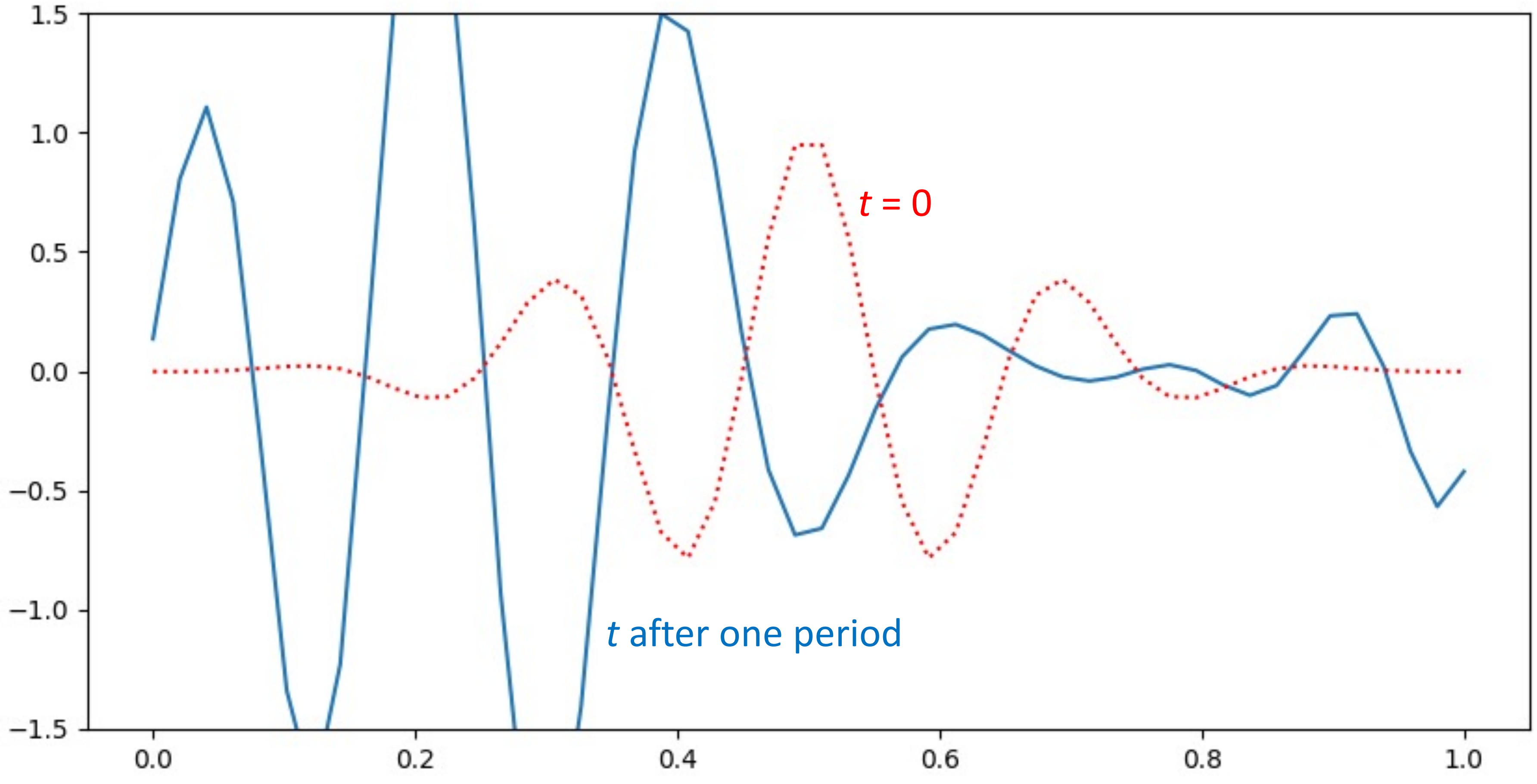
- For initial condition: $a(x, t=0) = f_0(x)$
- Solution is: $a(x,t) = f_0(x - ct)$
- Consider a wavepacket of the form:

$$a(x, t=0) = \cos[k(x - x_0)] \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$$

- Solution: $a(x,t) = \cos[k((x-ct) - x_0)] \exp\left[-\frac{((x-ct)-x_0)^2}{2\sigma^2}\right]$



Review: FTCS method clearly fails for the advection equation



Review: How can we do a better job?

- We could try to adjust numerical parameters, but it will not work!
  - FTCS is unstable for any τ ! (will come back to this later)
  - Can delay the problems but not get rid of them

- Stability problem can be helped with a simple modification: The Lax method:

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

- Simply replacing the first term with the average of the left and right neighbors

Today’s lecture: PDEs

- Hyperbolic PDEs: Lax-Wendroff scheme
- Elliptical PDEs: Relaxation methods

Lax-Wendroff scheme for hyperbolic PDEs

- Lax-Wedroff is second-order finite difference scheme
- Take the Taylor expansion in time:

$$a(x,t+\tau) = a(x,t) + \tau \frac{\partial a}{\partial t} + \frac{\tau^2}{2} \frac{\partial^2 a}{\partial t^2} + \mathcal{O}(\tau^3)$$

- Generally, for a flux-conserving equations: $\dfrac{\partial a}{\partial t} = -\dfrac{\partial}{\partial x} F(a)$
  - $F(a) = ca$ for advection equations
- Differentiate both sides: $\dfrac{\partial^2 a}{\partial t^2} = -\dfrac{\partial}{\partial x} \dfrac{\partial F(a)}{\partial t}$
- Chain rule: $\dfrac{\partial F}{\partial t} = \dfrac{dF}{da} \dfrac{\partial a}{\partial t} = F'(a) \dfrac{\partial a}{\partial t} = -F'(a) \dfrac{\partial F}{\partial x}$

Second order expansion

- So, we have: $$a(x,t+\tau) \simeq a(x,t) - \tau \frac{\partial F(a)}{\partial x} + \frac{\tau^2}{2} \frac{\partial F'(a)}{\partial x} \frac{\partial F(a)}{\partial x}$$

- Now we discretize derivatives:

$$a_i^{n+1} = a_i^n - \tau \frac{F_{i+1} - F_{i-1}}{2h} + \frac{\tau^2}{2h} \left(F'_{i+1/2} \frac{F_{i+1} - F_i}{h} - F'_{i-1/2} \frac{F_i - F_{i-1}}{h} \right)$$

- Where: $$F_i \equiv F(a_i^n), \quad F'_{i\pm 1/2} \equiv F'[(a_{i\pm1}^n + a_i^n)/2]$$

- For advection equations, $F_i = c a_i^n, \quad F'_{i\pm 1/2} = c$

Discretized second derivative of a

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

Today's lecture:
PDEs

- Hyperbolic PDEs: Lax-Wendroff scheme
- Elliptical PDEs: Relaxation methods

Elliptical equations: e.g., Laplace equation

- The PDEs we will discuss here represent boundary-value problems
  - Solution is a static field
- Consider Laplace's equation: $$\frac{\partial^2 \Phi(x,y)}{\partial x^2} + \frac{\partial^2 \Phi(x,y)}{\partial y^2} = 0$$
- Φ is the electrostatic potential
- As usual it is useful to solve a simple problem analytically so that we can benchmark numerical methods

Separation of variables for Laplace's equation

- Write Φ as the product: $\Phi(x,y) = X(x)Y(y)$
- Insert into Laplace's equation and divide by Φ:

$$\frac{1}{X(x)}\frac{d^2X}{dx^2} + \frac{1}{Y(y)}\frac{d^2Y}{dy^2} = 0$$

- This equation should hold for all *x* and *y*, so each term must be a constant:

$$\frac{1}{X(x)}\frac{d^2X}{dx^2} = -k^2, \qquad \frac{1}{Y(y)}\frac{d^2Y}{dy^2} = k^2$$

  - *k* is a complex constant
  - Writing constant as k^2 to simplify notation later
  - Signs can be switched
- Now we have two ODEs

Solution of Laplace’s eq. ODEs

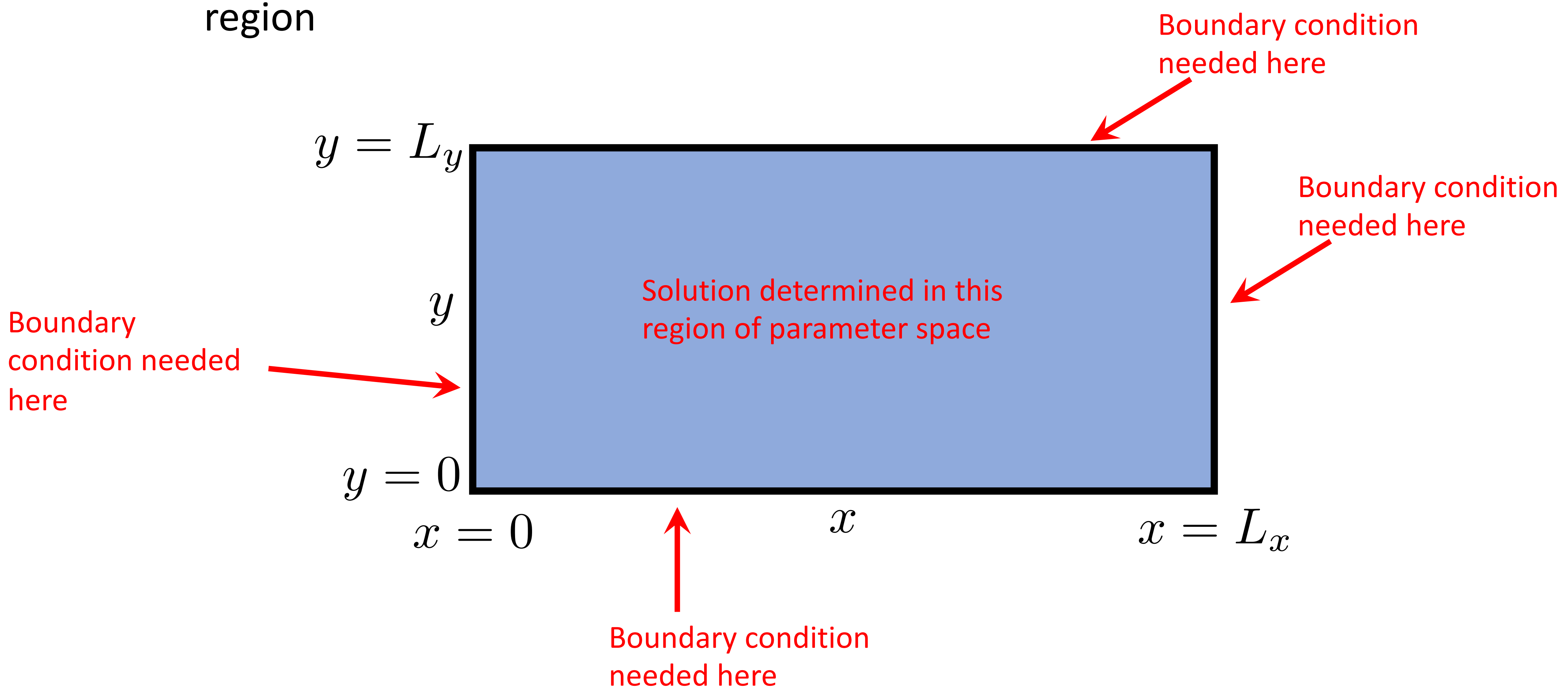
- Solution of these equations are well known:

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

  - Recall that k is complex, so solutions are “symmetric”
- To get the coefficients, we need to specify the boundary conditions

Boundary value problems

- All boundary values are specified at the outset
  - E.g., Laplace's equation in electrostatics, potential fixed on for sides of spatial region



Solution of Laplace's eq. ODEs

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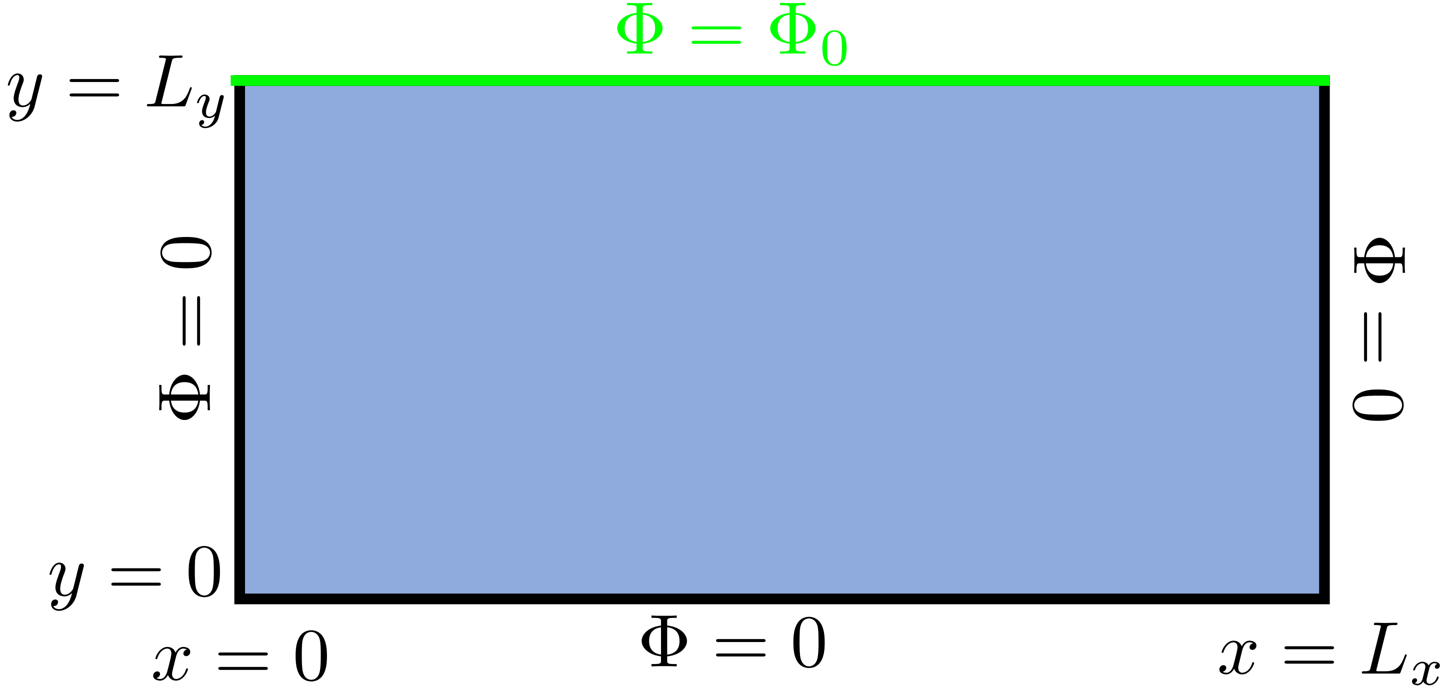
  - Recall that k is complex, so solutions are "symmetric"

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

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



Solution of Laplace's eq. ODEs

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

- Use our boundary conditions:

$$\Phi(x=0,y)=0 \implies C_c = 0$$

$$\Phi(x,y=0)=0 \implies C'_c = 0$$

$$\Phi(x=L_x,y)=0 \implies k = \frac{n\pi}{L_x},\ n=1,2,\ldots$$

- So, we have solutions of the form:

$$c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi y}{L_x}\right)$$

- Any linear combination is also a solution, so:

$$\Phi(x,y) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi y}{L_x}\right)$$

Solution of Laplace's equation

- Now we use our last boundary condition:

$$\Phi_0 = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi L_y}{L_x}\right)$$

- To solve the equation, multiply both sides by sin($m\pi x/L_x$) and integrate from 0 to L_x:

$$\int_0^{L_x} dx \Phi_0 \sin\left(\frac{m\pi x}{L_x}\right) = \sum_{n=1}^{\infty} c_n \sinh\left(\frac{n\pi L_y}{L_x}\right) \int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi x}{L_x}\right)$$

- Left-hand side integral:

$$\int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) = \begin{cases} 2L_x/m\pi, & m \text{ odd} \\ 0, & m \text{ even} \end{cases}$$

Solution of Laplace's equation

- Sum on the right-hand side simplifies because:

$$\int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{n\pi x}{L_x}\right) = \frac{L_x}{2}\delta_{n,m}$$

- So, we have:

$$\Phi_0 \frac{2L_x}{\pi m} = c_m \sinh\left(\frac{m\pi L_y}{L_x}\right)\frac{L_x}{2}, \quad m = 1, 3, 5, \ldots$$

- So:

$$c_m = \frac{4\Phi_0}{\pi m \sinh\left(\frac{m\pi L_y}{L_x}\right)}, \quad m = 1, 3, 5, \ldots$$

Solution of Laplace's equation

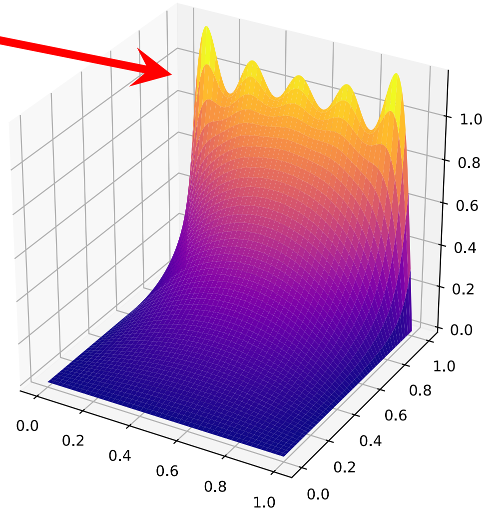
- Our final solution of Laplace's equation with our chosen boundary conditions:

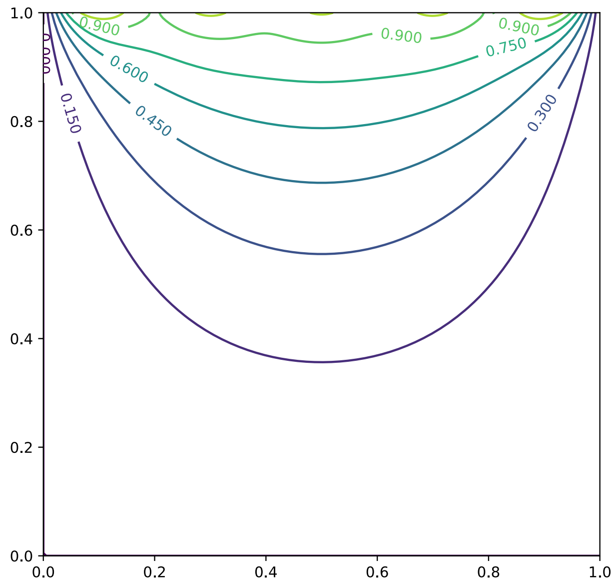
$$\Phi(x,y) = \Phi_0 \sum_{n=1,3,5,\ldots}^{\infty} \frac{4}{\pi n} \sin\left(\frac{n\pi x}{L_x}\right) \frac{\sinh\left(\frac{n\pi y}{L_x}\right)}{\sinh\left(\frac{n\pi L_y}{L_x}\right)}$$

Analytical solution to Laplace equation

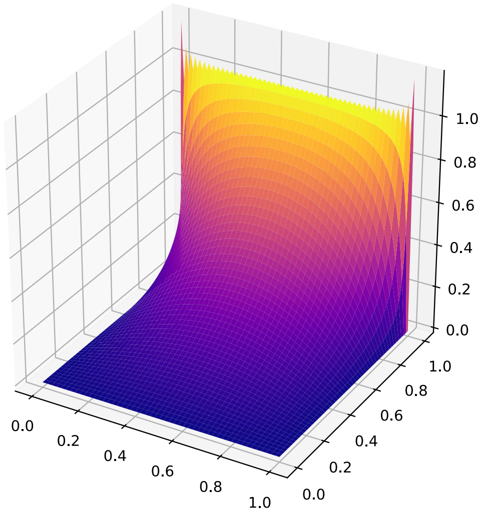
“Gibbs phenomenon,” oscillations of Fourier series for discontinuous function

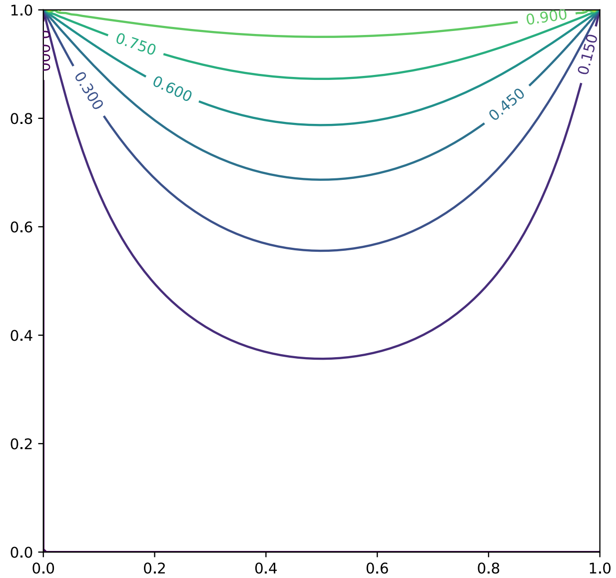
5 terms in the sum:





50 terms in the sum:





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:

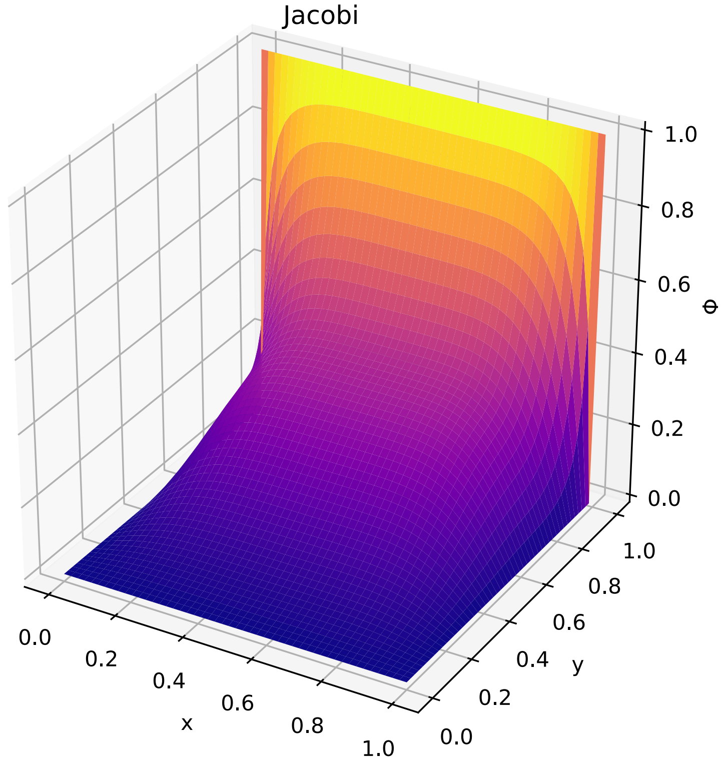
$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^n + \Phi_{i-1,j}^n + \Phi_{i,j+1}^n + \Phi_{i,j-1}^n)$$

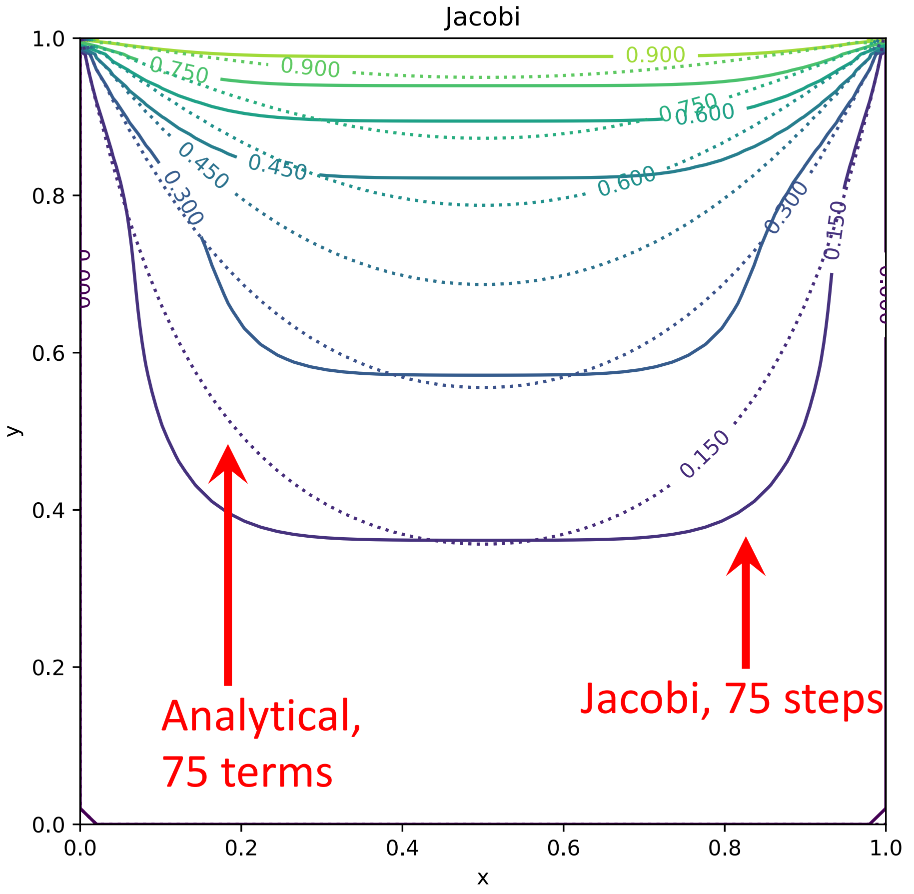
Jacobi method for Laplace equation

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

- 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:

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

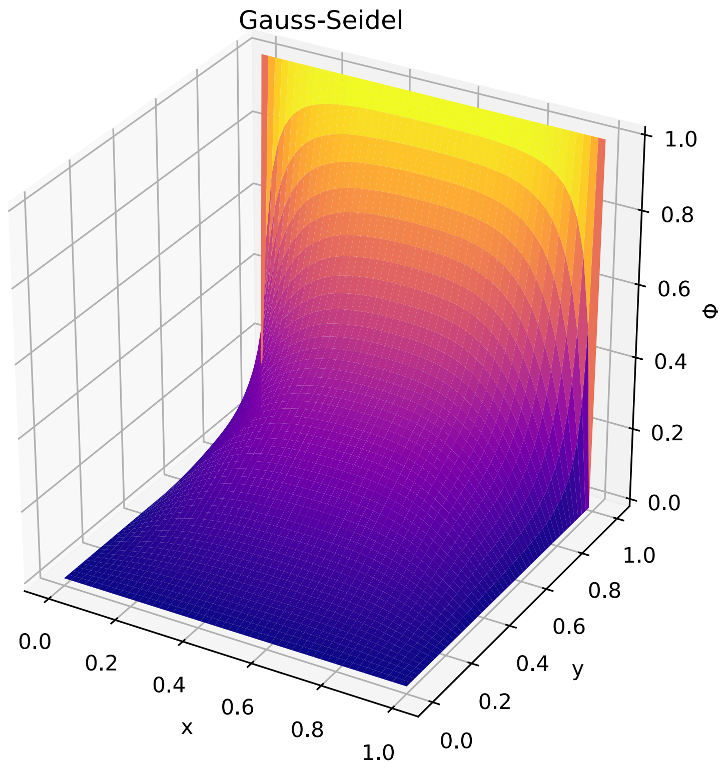
- Simultaneous overrelaxation: Choose a mixing parameter ω:

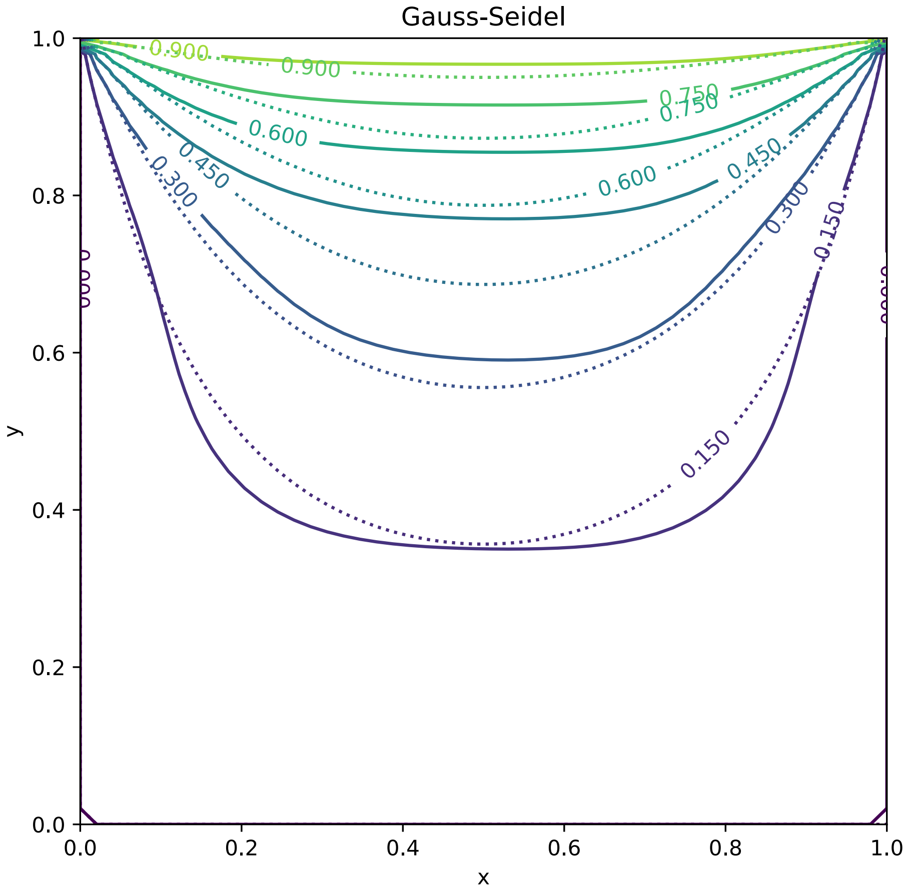
$$\Phi_{i,j}^{n+1} = (1-\omega)\Phi_{i,j}^{n} + \frac{\omega}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n+1})$$

  - $\omega < 1$ 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:

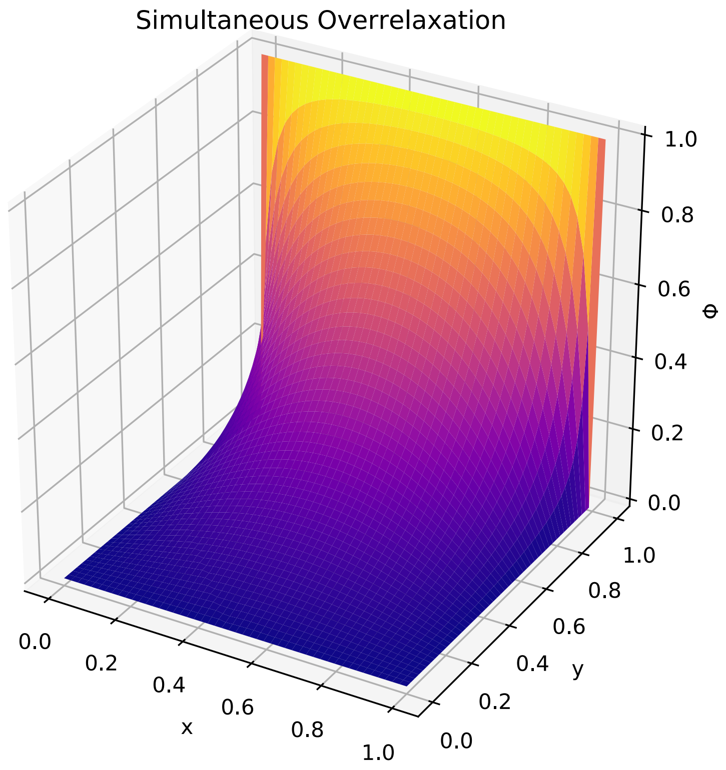
$$\omega_{\text{opt}} = \frac{2}{1+\sin(\pi/N)}$$

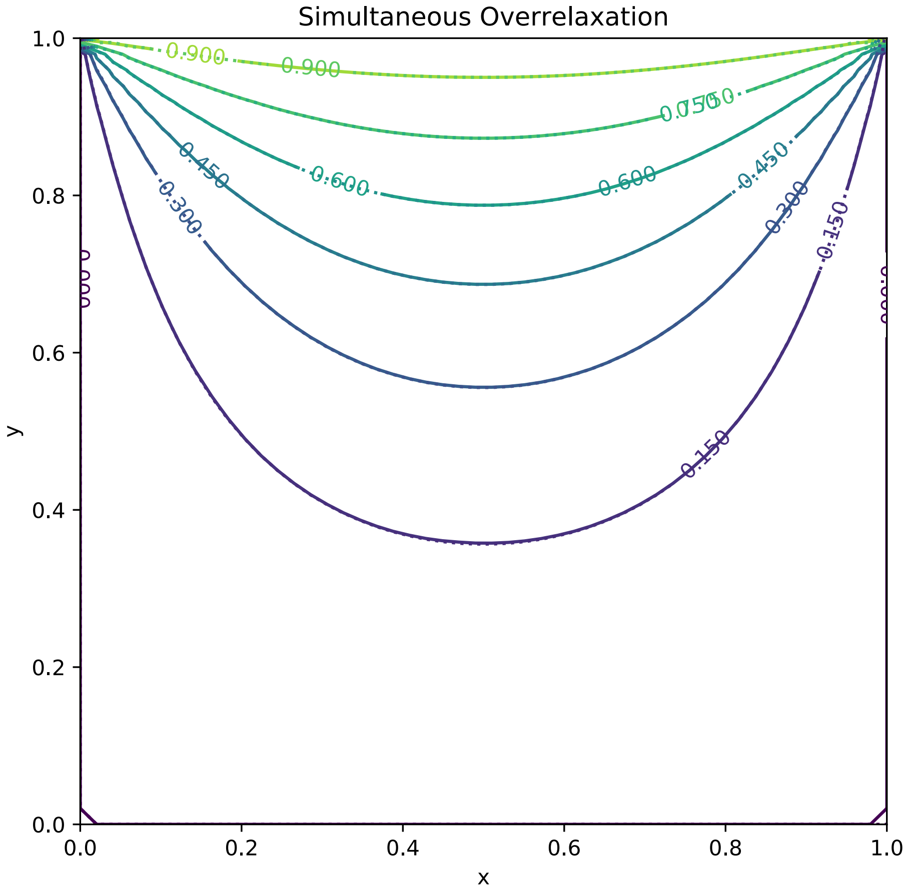
Gauss-Seidel for Laplace equation





Simultaneous overrelaxation for Laplace eq.





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

Recall: Jacobi iterative method

- Starting with a linear system:

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

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

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

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):

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

After class tasks

- Homework 3 due today Oct. 31
- Homework 4 will be posted soon

- Readings
  - Garcia Chapters 7
  - MIke Zingale's notes on computational hydrodynamics