PHY604 Lecture 15

October 16, 2025

Today’s lecture: PDEs

- Parabolic: Diffusion equation

- Hyperbolic: Wave equation

Partial differential equations (Garcia Chs. 6-9)

- Previously, we studied ordinary differential equations

- Much of physics is involved in solving partial differential equations
  - Schrodinger equation in Quantum mechanics
  - Maxwell’s equations in electricity and magnetism
  - Wave equation in optics and acoustics

- For ODEs we developed general methods to solve a variety of problems, e.g., 4th order Runge-Kutta

- For PDEs, we first classify the type of equation, that will tell us what method to use

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:

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

General classification of PDEs

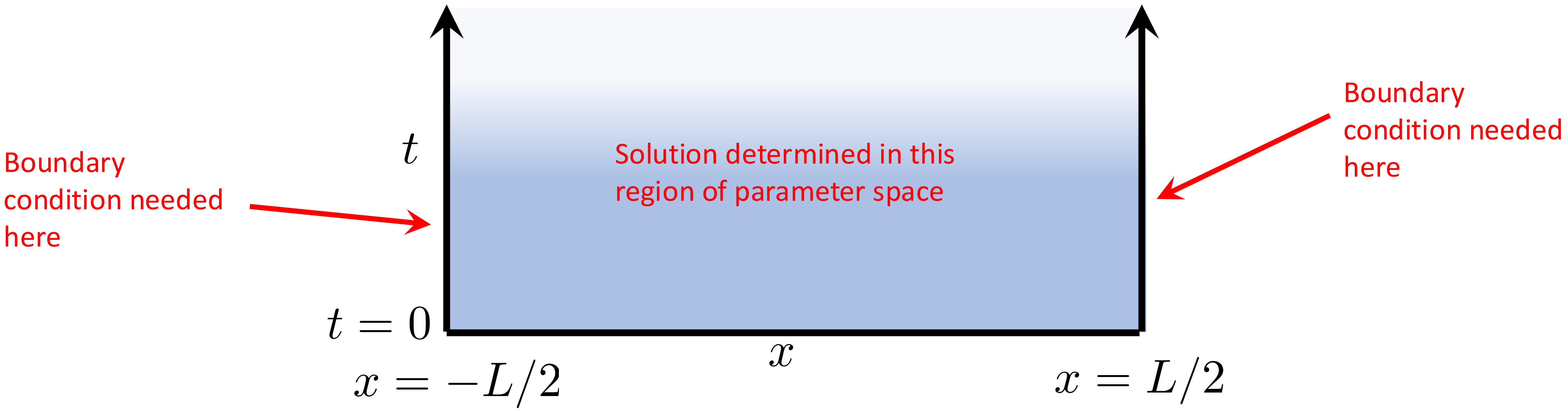
- Consider a general PDE of two independent variables:

$$a\frac{\partial^2 A}{\partial x^2} + b\frac{\partial^2 A}{\partial x \partial y} + c\frac{\partial^2 A}{\partial y^2} + d\frac{\partial A}{\partial x} + e\frac{\partial A}{\partial y} + fA(x,y) + g = 0$$

- Hyperbolic if: $b^2 - 4ac > 0$
- Parabolic if: $b^2 - 4ac = 0$
- Elliptic if: $b^2 - 4ac < 0$
- Most problems involve hybrid systems, including multiple types

Initial value problems

- Diffusion and wave equations usually solved as initial value problems
  - Diffusion: Given initial temperature distribution, find temperature distribution at a later time
  - Wave: Start with initial amplitude and velocity of wave pulse and find the wave pulse at a later time
- Need to specify initial conditions as well as boundary conditions



Types of boundary conditions

- Dirichlet boundary conditions: Specify the solution on boundary
  - E.g., fix the temperature at the boundaries:

$$T(x=-L/2,t)=T_a, \quad T(x=L/2,t)=T_b$$

- Neumann boundary conditions: Specify the derivative on the boundary
  - E.g., "insulated" boundaries

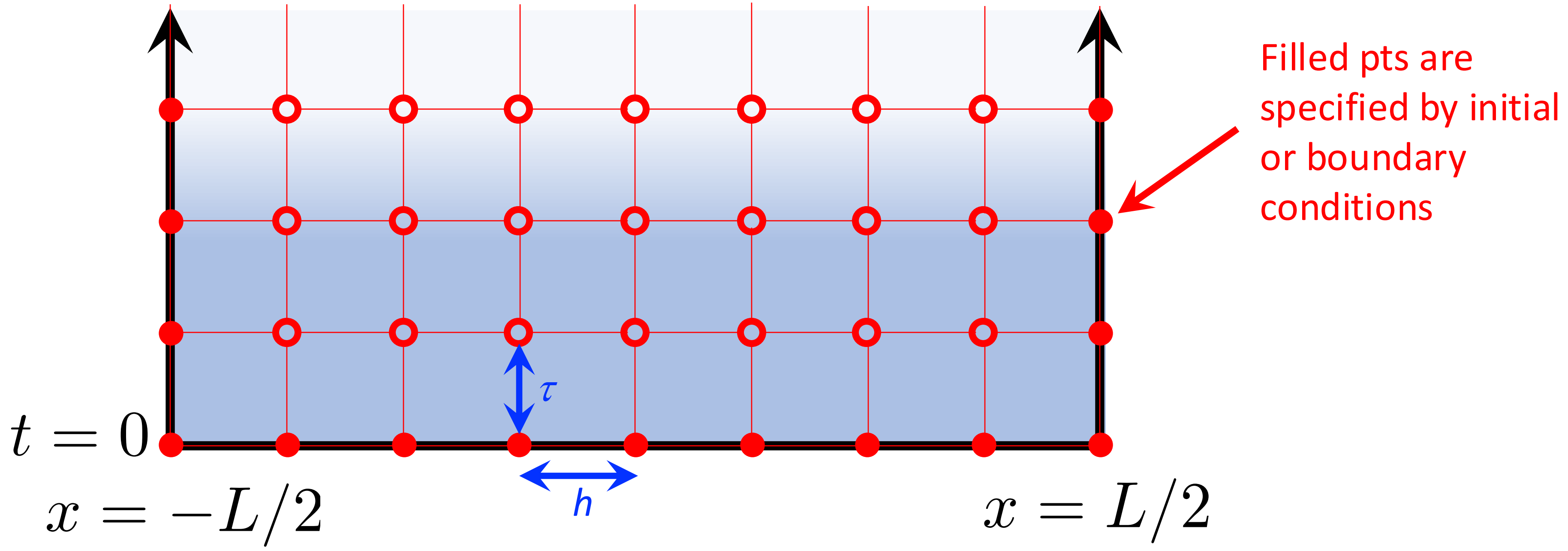
$$-\kappa \frac{dT}{dx}\bigg|_{x=-L/2} = F_a = 0, \qquad -\kappa \frac{dT}{dx}\bigg|_{x=L/2} = F_b = 0$$

- Periodic boundary conditions: Equate the functions at both ends

$$T(x=-L/2,t)=T(x=L/2,t), \qquad \frac{dT}{dx}\bigg|_{x=-L/2} = \frac{dT}{dx}\bigg|_{x=L/2}$$

Marching methods for initial value problems

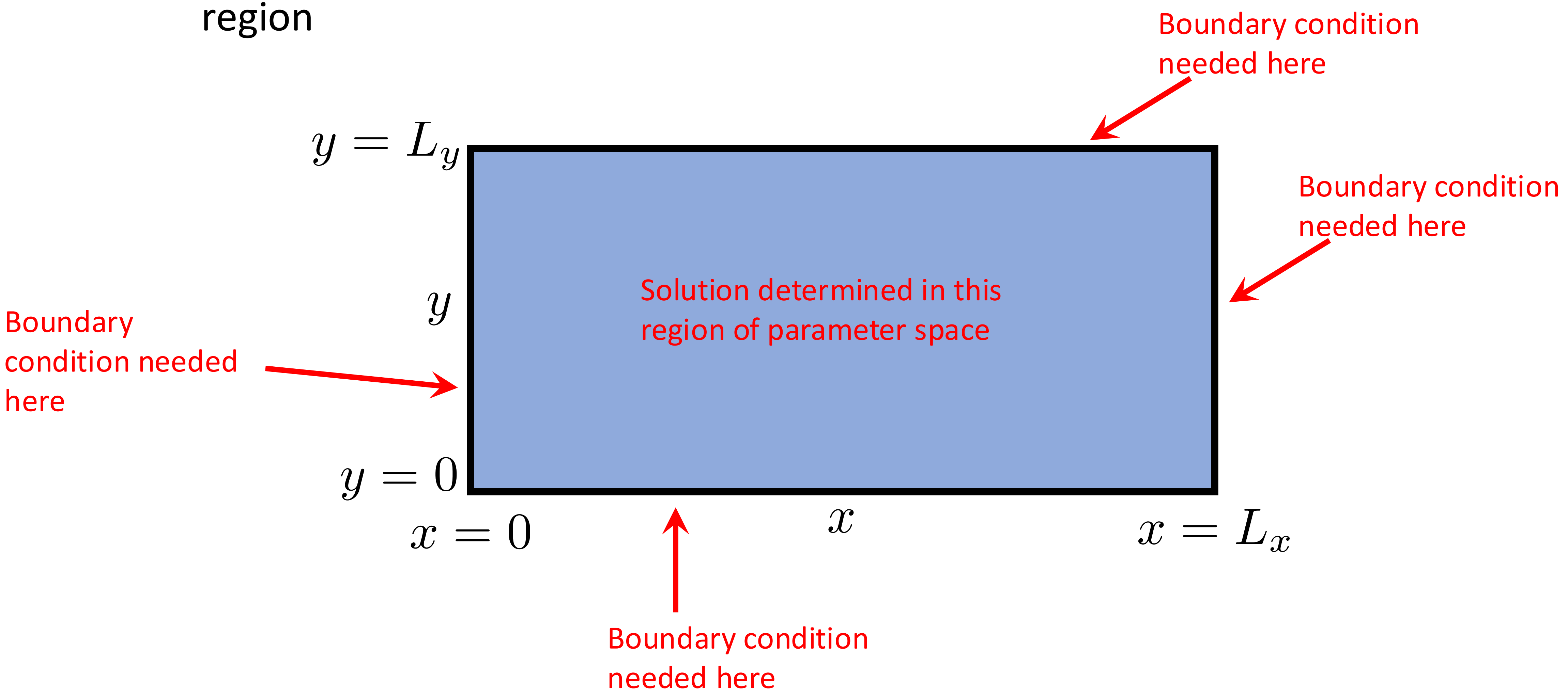
- We first must discretize in time and space:



- Start from the initial condition, move forward in time one timestep at a time

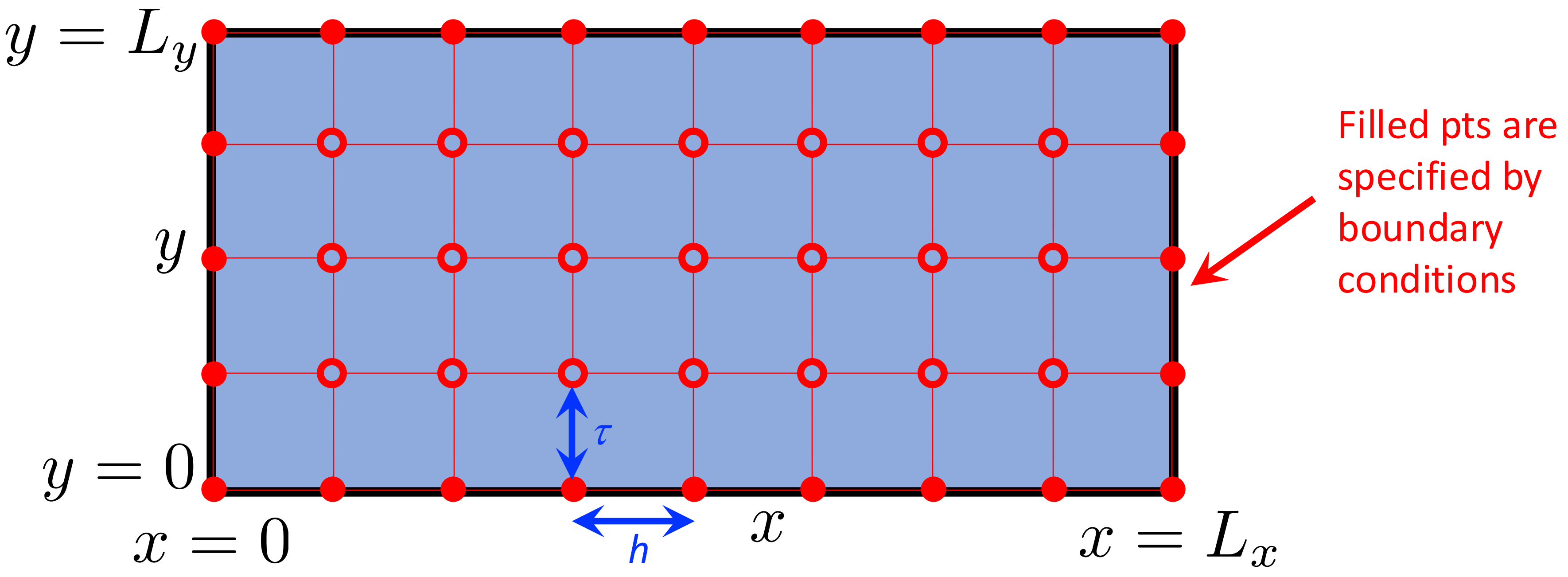
Boundary value problems

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



Jury methods for boundary value problems

- Discretize in space:



- Potential in interior is influenced by all the boundary points, reconciles all the constraints imposed by boundaries

Diffusion equation with FTCS

- Diffusion equation: $$\frac{\partial T(x,t)}{\partial t} = \kappa \frac{\partial^2 T(x,t)}{\partial x^2}$$
- Discretize in space and time: $T_i^n = T(x_i, t_n)$
  - $x_i = i\,h - L/2$ and $t_n = n\,\tau$
  - Take spatial boundary points as $i = 0$ and $i = N$-1, so h = $L/(N$-1)

- Discretize time derivative with forward difference:
$$\frac{\partial T(x,t)}{\partial t} \to \frac{T_i^{n+1} - T_i^n}{\tau}$$
- Discretize spatial derivative using central difference:
$$\frac{\partial^2 T(x,t)}{\partial x^2} \to \frac{T_{i+1}^n + T_{i-1}^n - 2T_i^n}{h^2}$$

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

Numerical stability of FTCS method

- The numerical stability of the solution depends on the timestep
- Consider initial conditions of a delta-function peak in *T* located at *N*/2
  - Discrete approximation, $T(x=N/2,t_0) = 1/h$
- Can show from analytical solutions to this problem that the delta function will spread into a Gaussian with width:

$$\sigma(t) = \sqrt{2\kappa t}$$

- Thus, if t_σ is the time it takes for σ to increase by one grid spacing:

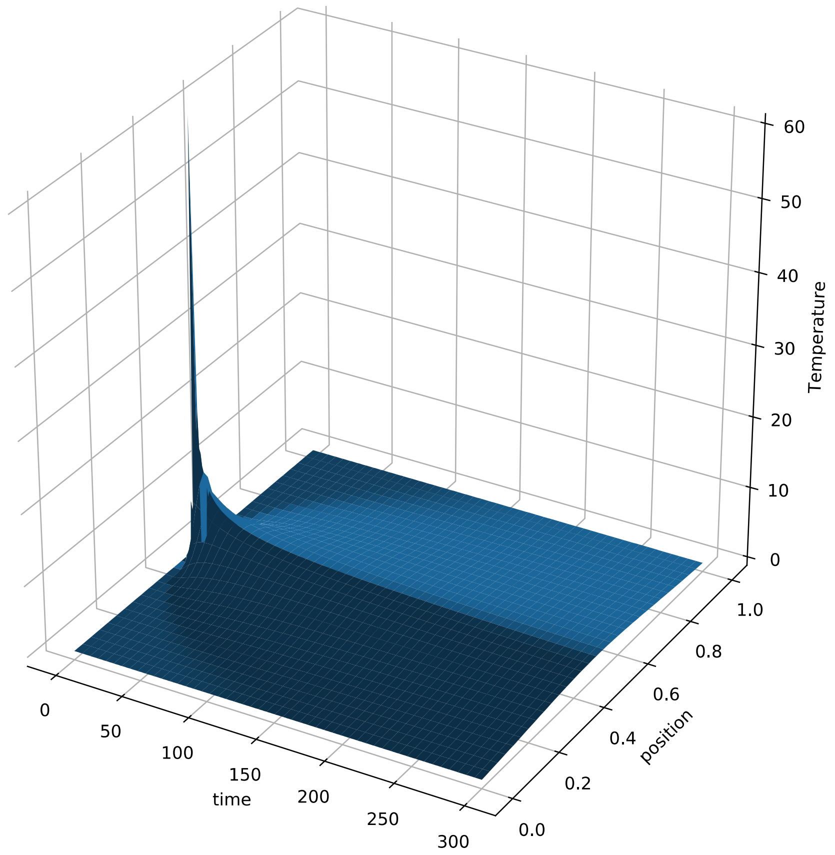
$$t_\sigma = \frac{h^2}{2\kappa}$$

- Then: $$T_i^{n+1} = T_i^n + \frac{\tau}{2t_\sigma}(T_{i+1}^n + T_{i-1}^n - 2T_i^n)$$

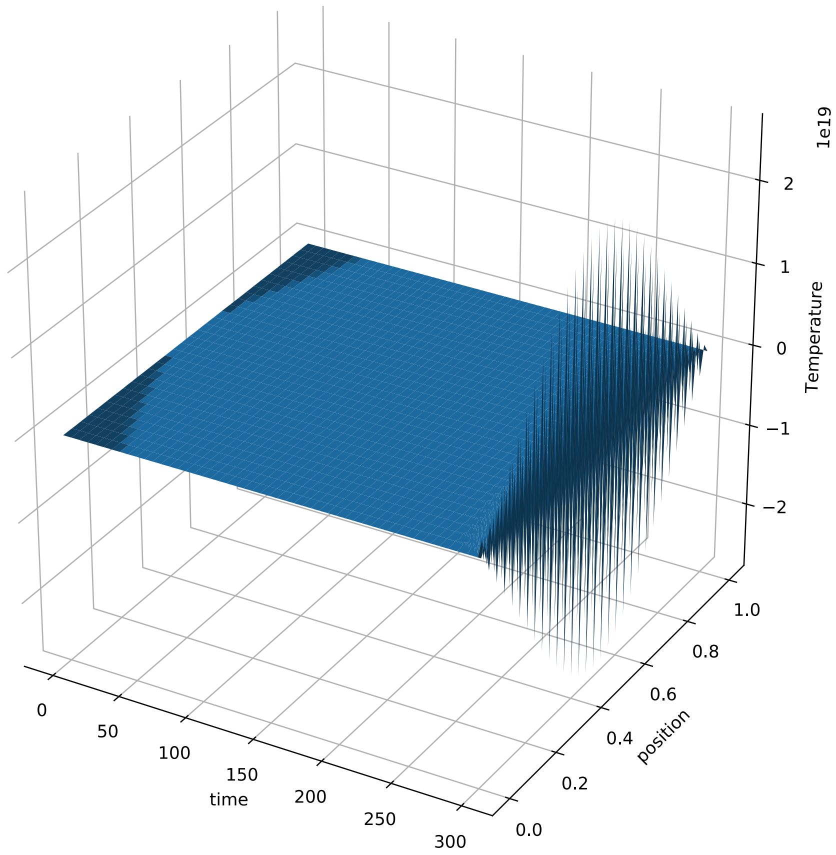
- Should not use a timestep much larger than t_σ

FCTS method on diffusion equation

Numerically stable: τ = 1e-4



Numerically unstable: τ = 1.5e-4



Wave and advection equations

- Wave equation: $$\frac{\partial^2 A(x,t)}{\partial t^2} = c^2 \frac{\partial^2 A(x,t)}{\partial x^2}$$
- When we discussed ODEs we used the trick to turn 2nd order equations into systems of 1st order equations with auxiliary variables
- Use a similar trick for wave PDE:

$$P \equiv \frac{\partial A}{\partial t}, \qquad Q \equiv c\frac{\partial A}{\partial x}$$

- So, we have the pair of equations:

$$\frac{\partial P}{\partial t} = c\frac{\partial Q}{\partial x}, \qquad \frac{\partial Q}{\partial t} = c\frac{\partial P}{\partial x}$$

- Or:

$$\frac{\partial \mathbf{a}}{\partial t} = c\mathbf{B}\frac{\partial \mathbf{a}}{\partial x}, \qquad \mathbf{a} = \begin{bmatrix} P \\ Q \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

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:

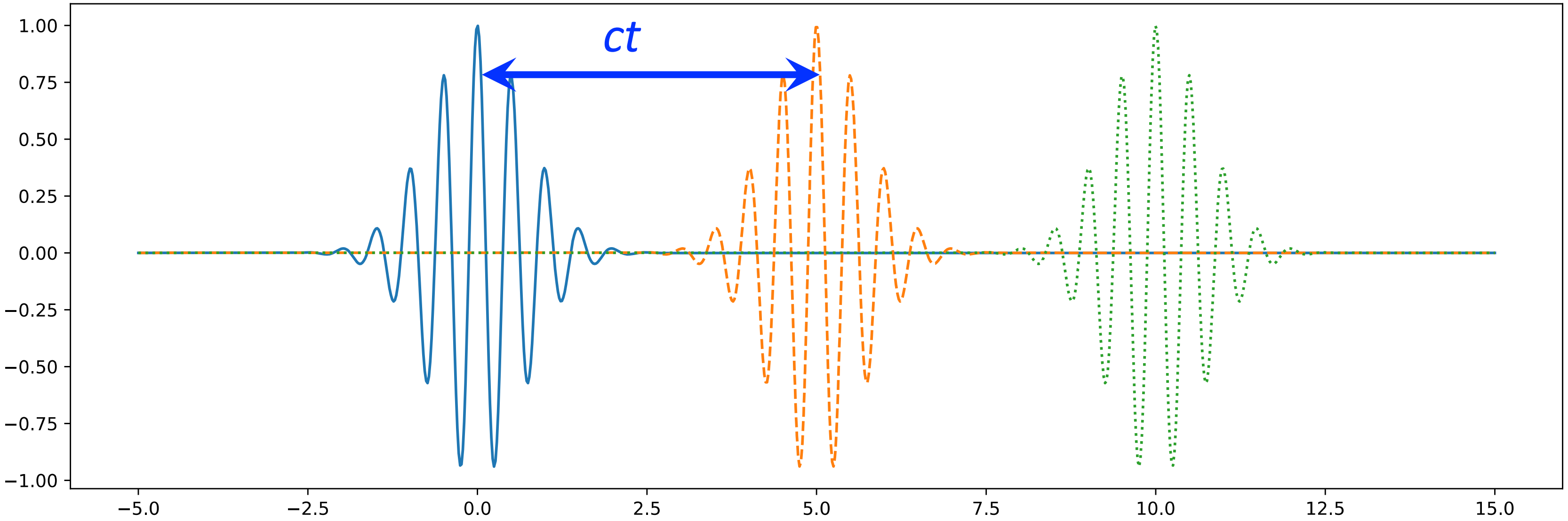
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}(\rho)$$

Advection equation is easy to solve analytically

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



Why study such a simple equation?

- Excellent test case for numerical methods since we know exactly what we should get

- Let's start with the FTCS methods we used for the diffusion equation:

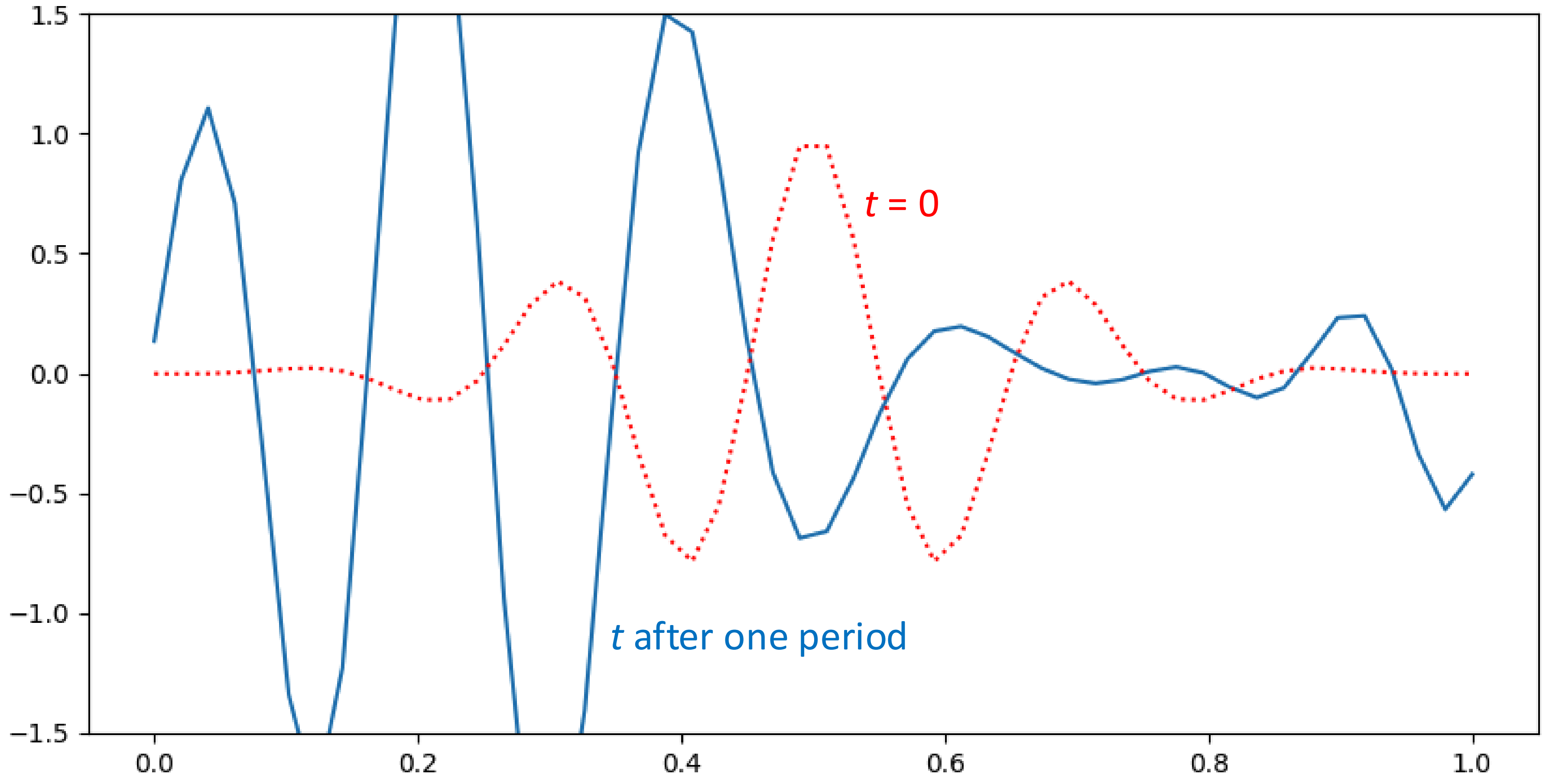
$$\frac{\partial a}{\partial t} \rightarrow \frac{a_i^{n+1} - a_i^n}{\tau}, \qquad \frac{\partial a}{\partial x} \rightarrow \frac{a_{i+1}^n - a_{i-1}^n}{2h}$$

- So, the FTCS equation is:

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

- We will use periodic boundary conditions for this case

FTCS method clearly fails for the advection equation using this timestep



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 on)
  - Can delay the problems but not get rid of them

- Stability problem can be fixed 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

Stability of the Lax method

- It can be shown that the Lax method is numerically stable (i.e., does not diverge) if:

$$\frac{c\tau}{h} \leq 1$$

- So:

$$\tau_{\max} = \frac{h}{c}$$

- Courant-Friedrighs-Lewy (CFL) condition
  - We will discuss more on stability conditions later
  - If we want a finer grid in space, we need a finer timestep

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- Too large of a timestep: Numerically unstable
- Too small of a timestep: Amplitude suppressed
  - Averaging term introduces and artificial viscosity, proportional to τ

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: $a(x,t+\tau) \simeq a(x,t) - \tau \frac{\partial F(a)}{\partial x} + \frac{\tau^2}{2}\frac{\partial}{\partial x}\left[F'(a)\frac{\partial F(a)}{\partial x}\right]$

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

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

Discretized second derivative of a

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

After class tasks

- Homework 2 has been graded (see GRADES.md in your repos)
- Homework 3 due Oct 22

- Readings
  - Garcia Chapters 6 and 7