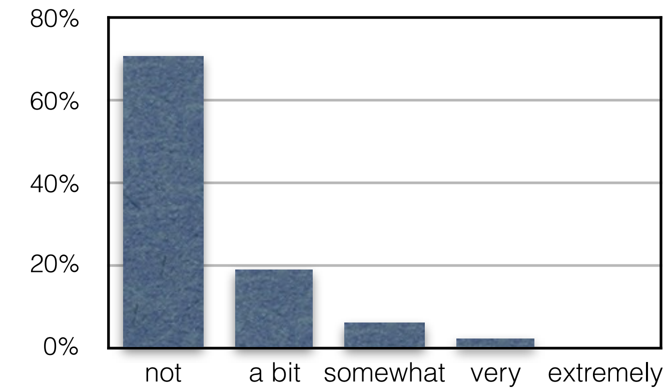
Muddiest Points from Class 03/13

- *“Will we be covering the method of manufactured solutions later on in the course?”*
  - Yes
- *“Will you not be providing a debug file for subsequent homeworks?”*
  - Yes, for all regular homework
- *“Regarding the Richardson extrapolation, how would you apply the solution functionals? Like you said the drag and lift coefficients can be solved for, what other solution functionals can it be used for?”*
  - The method can be used for any quantity you are interested in, e.g., pressure recovery (see example last class)
- *“Some PDEs (like the one on HW5 where phi diverges on taking M=8) can diverge depending on the choice of h. So how in that case the observed order is calculated?“*
  - For a meaningful observed order, you must be in the asymptotic region, i.e., the check for the GCI ratios must be close to 1.
  - If the ratio GCI check is not close to one, one must refine the mesh further
- *“So for the approximation of the actual solution using richardson extrapolation, what is the order of accuracy for that method? We ignore the higher order (4+?) terms. So is it, as well, a second order approximation?”*
  - The order the Richardson extrapolation uses is the observed order of the method (not the formal one)
- *“Why is the method GCI21 denoted with the subscript 21? What does that designation represent or tell us?”*
  - The subscripts refer to the mesh #, here a GCI calculated using mesh #1 and mesh #2 data



- **Recipe for solution verification**

1) Perform 3 simulations on meshes that are different in h by a factor r of 2

2) Determine the quantity of interest for the 3 finest mesh/simulations: f_1, f_2, f_3

3) Determine observed order of convergence p

$$p = \ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right) / \ln(r)$$

4) Determine estimate for exact solution using Richardson extrapolation

$$f_{h=0} \approx f_1 + \frac{f_1 - f_2}{r^p - 1}$$

5) Calculate GCIs (estimate of fractional error of computed solutions to exact solution)

$$GCI_{12} = F_{sec}\frac{\left|\frac{f_1 - f_2}{f_1}\right|}{r^p - 1} \qquad GCI_{23} = F_{sec}\frac{\left|\frac{f_2 - f_3}{f_2}\right|}{r^p - 1}$$

6) Confirm asymptotic range of convergence

$$\frac{GCI_{12}}{GCI_{23}} r^p \approx 1 \ ?$$

If not, add a new mesh, finer by factor r and go to 2)

7) Final answer is $f_{h=0}$ +/- GCI_{12} in percent

- Comment on GCI analysis for steady state solutions
  - Common way to reach a steady state solution for time dependent PDEs is to time advance the solution until in discrete form

$$\frac{\partial \phi}{\partial t} < \epsilon$$

  - To perform GCI analysis for spatial discretization errors, make sure that “non-steady-state” error ϵ is much smaller than spatial errors

- Comment on GCI analysis for unsteady solutions
  - superposition of time and spatial errors
  - GCI analysis as presented can deal with one type of error at a time only
  - for spatial error GCI
    - make temporal errors much smaller than spatial errors (very small Δt)
    - vary mesh spacing h only
  - for temporal error GCI
    - make spatial errors much smaller than temporal errors (very small h)
    - vary time step size only

Hyperbolic Equations

Current status:

done

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu^2\nabla^2 u$$

next

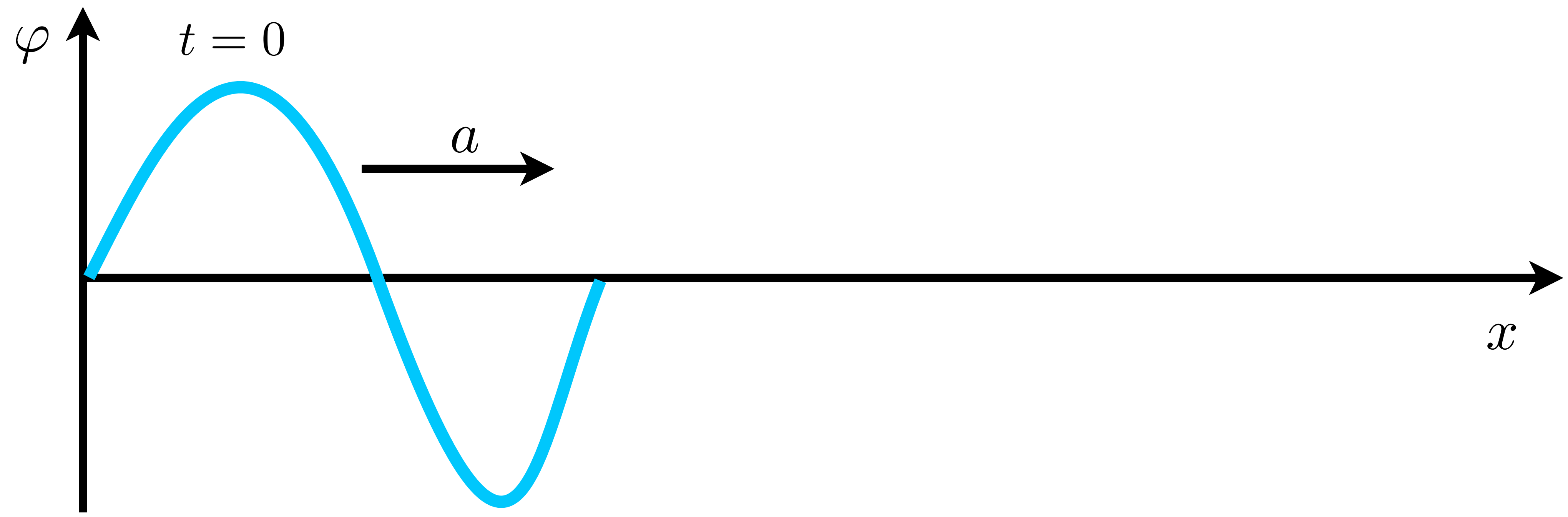
- Convection/Advection:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = 0 \qquad \text{(2D)}$$

- Simplified model equations:
  - 1D non-linear: $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$
  - 1D linear: $\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$ with $a \neq f(u)$ (1D wave equation)
- Plan: look at different methods, analyze accuracy, consistency, and stability

Let's start with 1D wave equation

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \quad \text{with} \quad \varphi(x, t=0) = \varphi_0(x) \quad \text{and} \quad a = \text{const.}$$



- signal propagates with constant speed a

Let's start with 1D wave equation

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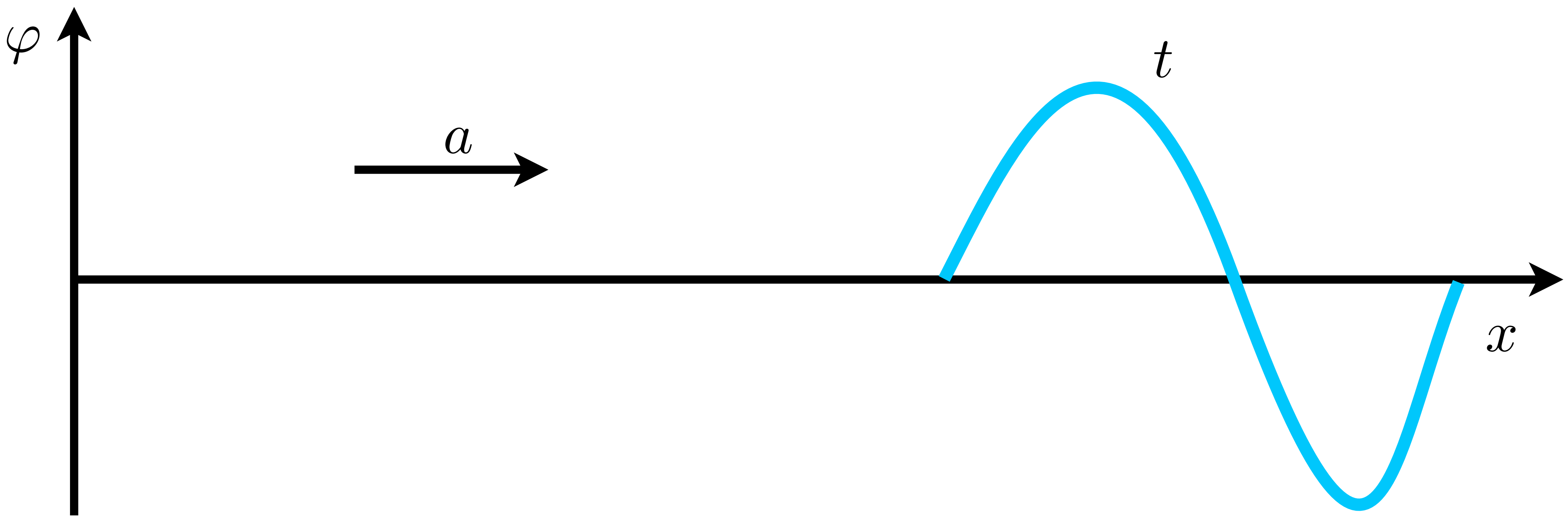

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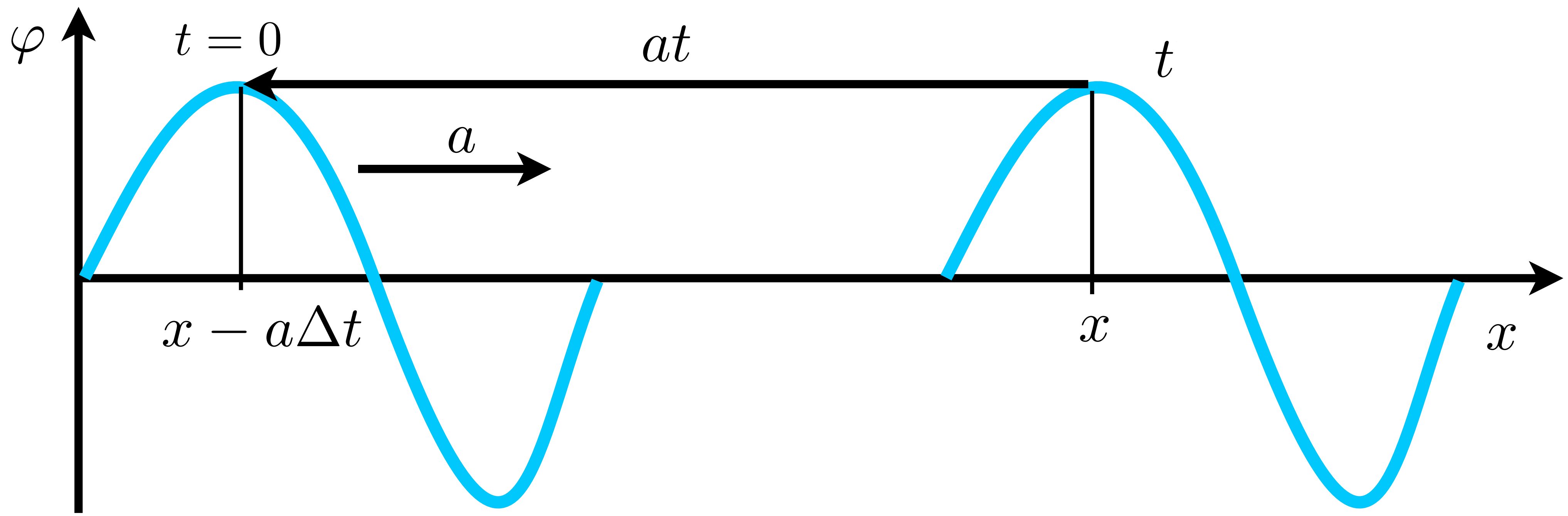


- signal propagates with constant speed a
- solution: $\varphi(x,t) = \varphi(x - at, t = 0) = \varphi_0(x - at)$

  $\Rightarrow$ Lagrangian or Semi-Lagrangian methods

  $\Rightarrow$ Method of Characteristics (see Appendix A of Hoffmann & Chiang)

Brief introduction to characteristic methods for 1D hyperbolic PDEs

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = 0 \qquad\qquad T = T(x,t) \quad u = const.$$

Goal: Transform this PDE into an ODE along some appropriate curve (x(s),t(s))

Question: How will T change along this curve?

$$\frac{d}{ds}T\left(x(s),t(s)\right) = \frac{\partial T}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial T}{\partial t}\frac{\partial t}{\partial s} = \frac{\partial T}{\partial x}u + \frac{\partial T}{\partial t}1 = 0$$

$$\frac{\partial x}{\partial s} = u \qquad \frac{\partial t}{\partial s} = 1$$

Question: Is there a specific curve that simplifies this?

⇒ T remains constant along this curve!

Question: What are these curves?

$$\frac{\partial t}{\partial s} = 1 \quad \Rightarrow \quad s = t \qquad\qquad t(s=0) = 0$$

$$\frac{\partial x}{\partial s} = u \quad \Rightarrow \quad \frac{\partial x}{\partial t} = u \quad \Rightarrow \quad x = x_0 + ut \qquad\qquad x(s=t=0) = x_0$$

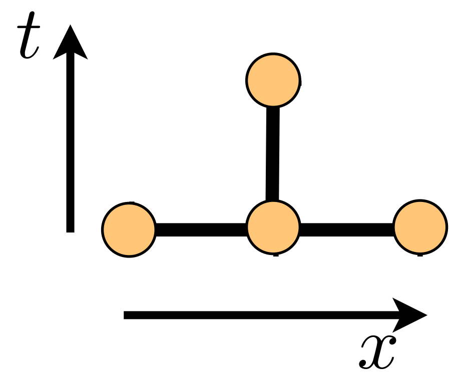
⇒ along the characteristic curve $x = x_0 + ut$, T remains constant!

$$T(x,t) = T(x_0 + ut, t) = T(x_0, 0) = T(x - ut, 0)$$

Linear 1D Wave Equation

Let's follow our standard procedure to go from PDE to FDE

stencil:



FTCS

$$\frac{\partial \varphi}{\partial t} = -a \frac{\partial \varphi}{\partial x} \quad \Rightarrow \quad \frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a \left(\frac{\varphi_{i+1}^n - \varphi_{i-1}^n}{2\Delta x} \right)$$

- Accuracy:
  - from Taylor series: $O(\Delta t)$ and $O(\Delta x^2)$

$$\varphi_i^{n+1} = \varphi_i^n - \frac{a\Delta t}{2\Delta x}\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right) \qquad \frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x}$$

- Consistency:

Write Taylor series for each term in the finite difference equation

$$\varphi_i^{n+1} = \varphi_i^n + \Delta t \left.\frac{\partial \varphi}{\partial t}\right|^n + \frac{\Delta t^2}{2}\left.\frac{\partial^2 \varphi}{\partial t^2}\right|^n + O(\Delta t^3)$$

$$\varphi_{i+1}^n = \varphi_i^n + \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i + \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + O(\Delta x^4)$$

$$\varphi_{i-1}^n = \varphi_i^n - \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i - \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + O(\Delta x^4)$$

Substitute Taylor series into FTCS

$$\varphi_i^n + \Delta t \left.\frac{\partial \varphi}{\partial t}\right|^n + \frac{\Delta t^2}{2}\left.\frac{\partial^2 \varphi}{\partial t^2}\right|^n + O(\Delta t^3) = \varphi_i^n - \frac{a\Delta t}{2\Delta x}\Bigg(\varphi_i^n + \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i + \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i$$
$$-\varphi_i^n + \Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i - \frac{\Delta x^2}{2}\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_i + \frac{\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + O(\Delta x^4)\Bigg)$$

$$\Delta t \left.\frac{\partial \varphi}{\partial t}\right|^n + \frac{\Delta t^2}{2}\left.\frac{\partial^2 \varphi}{\partial t^2}\right|^n + O(\Delta t^3) = -\frac{a\Delta t}{2\Delta x}\left(2\Delta x \left.\frac{\partial \varphi}{\partial x}\right|_i + \frac{2\Delta x^3}{6}\left.\frac{\partial^3 \varphi}{\partial x^3}\right|_i + O(\Delta x^4)\right) \qquad | : \Delta t$$

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} - \frac{\Delta t}{2}\frac{\partial^2 \varphi}{\partial t^2} - a\frac{\Delta x^2}{6}\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta t^2) + O(\Delta x^3) \qquad \text{as } \Delta t \to 0 \wedge \Delta x \to 0$$

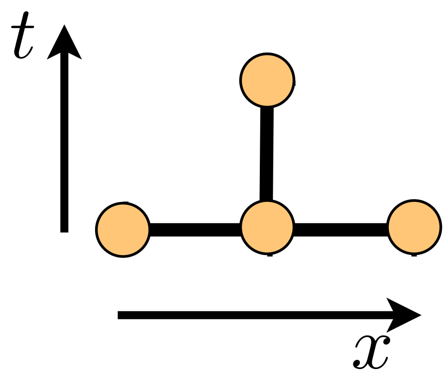
consistent

Linear 1D Wave Equation

Let's follow our standard procedure to go from PDE to FDE

FTCS

stencil:



$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \quad \Rightarrow \quad \frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a\left(\frac{\varphi_{i+1}^n - \varphi_{i-1}^n}{2\Delta x}\right)$$

- Accuracy:
  - from Taylor series: $O(\Delta t)$ and $O(\Delta x^2)$
- Consistency: consistent
- Stability:

FTCS

$$\Rightarrow \quad \frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a\left(\frac{\varphi_{i+1}^n - \varphi_{i-1}^n}{2\Delta x}\right)$$

- Stability: $\varphi_j^n = \rho^n e^{ikx_j}$

$$\rho^{n+1} e^{ikx_j} = \rho^n e^{ikx_j} - \frac{a\Delta t}{2\Delta x}\left(\rho^n e^{ik(x_j+\Delta x)} - \rho^n e^{ik(x_j-\Delta x)}\right) \qquad \Big|: e^{ikx_j}$$

$$\rho^{n+1} = \rho^n\left[1 - \frac{a\Delta t}{2\Delta x}\underbrace{\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)}_{2i\sin(k\Delta x)}\right]$$

$$\frac{\rho^{n+1}}{\rho^n} = 1 - i\frac{a\Delta t}{\Delta x}\sin(k\Delta x)$$

Stable if $\left|\frac{\rho^{n+1}}{\rho^n}\right| \le 1$ worst case: $\left|\frac{\rho^{n+1}}{\rho^n}\right| = 1$

$$\left|1 - i\frac{a\Delta t}{\Delta x}\sin(k\Delta x)\right| = 1 \quad \Leftrightarrow \quad \left|1 - i\frac{a\Delta t}{\Delta x}\sin(k\Delta x)\right|^2 = 1$$

$$\left|1 - i\frac{a\Delta t}{\Delta x}\sin(k\Delta x)\right|^2 = \left(1 - i\frac{a\Delta t}{\Delta x}\sin(k\Delta x)\right)\left(1 + i\frac{a\Delta t}{\Delta x}\sin(k\Delta x)\right) = 1 + \left(\frac{a\Delta t}{\Delta x}\right)^2\sin^2(k\Delta x) > 1$$

scheme is always unstable!!

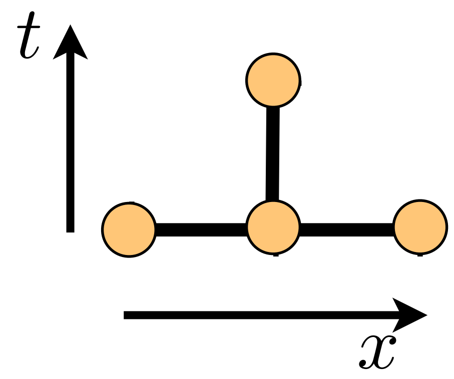
Linear 1D Wave Equation

Let's follow our standard procedure to go from PDE to FDE

FTCS

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \quad \Rightarrow \quad \frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a\left(\frac{\varphi_{i+1}^n - \varphi_{i-1}^n}{2\Delta x}\right)$$

stencil:



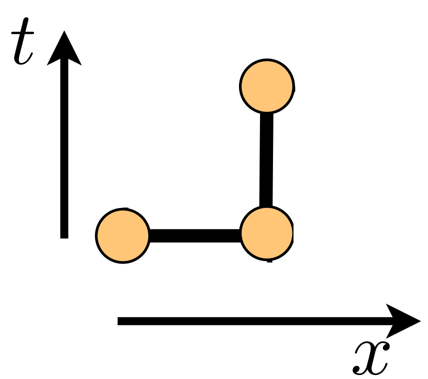
- Accuracy:
  - from Taylor series: $O(\Delta t)$ and $O(\Delta x^2)$
- Consistency: consistent
- Stability: always unstable

Linear 1D Wave Equation

let's try something else: assume $a > 0$

- use one-sided spatial difference (backwards)

stencil:



$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a \left(\frac{\varphi_i^n - \varphi_{i-1}^n}{\Delta x} \right)$$

- Accuracy:
  - from Taylor series: $O(\Delta t)$ and $O(\Delta x)$

- Stability: $\varphi_j^n = \rho^n e^{ikx_j}$

$$\rho^{n+1} e^{ikx_j} = \rho^n e^{ikx_j} - \frac{a\Delta t}{\Delta x}\left(\rho^n e^{ikx_j} - \rho^n e^{ik(x_j - \Delta x)}\right) \qquad \Big|: e^{ikx_j}$$

$$\rho^{n+1} = \rho^n \left[1 - \frac{a\Delta t}{\Delta x}\left(1 - e^{-ik\Delta x}\right)\right] \qquad C = \frac{a\Delta t}{\Delta x}$$

$$\frac{\rho^{n+1}}{\rho^n} = G = \left[1 - C\left(1 - e^{-ik\Delta x}\right)\right]$$

Stable if $\left|\frac{\rho^{n+1}}{\rho^n}\right| \le 1$ worst case: $\left|\frac{\rho^{n+1}}{\rho^n}\right| = 1$

$$\frac{\rho^{n+1}}{\rho^n} = G = \left[1 - C\left(1 - e^{-ik\Delta x}\right)\right]$$

worst case: $\left|\frac{\rho^{n+1}}{\rho^n}\right| = 1$

$$C = \frac{a\Delta t}{\Delta x}$$

$$|G|^2 = |1 - C + C\left[\cos(k\Delta x) - i\sin(k\Delta x)\right]|^2 = |(1 - C + C\cos(k\Delta x)) - iC\sin(k\Delta x)|^2 = 1$$

$$|G|^2 = ((1 - C + C\cos(k\Delta x)) - iC\sin(k\Delta x))\,((1 - C + C\cos(k\Delta x)) + iC\sin(k\Delta x)) = 1$$

$$(1 - C + C\cos(k\Delta x))^2 + C^2\sin^2(k\Delta x) = 1$$

$$1 + C^2 + C^2\cos^2(k\Delta x) - 2C + 2C\cos(k\Delta x) - 2C^2\cos(k\Delta x) + C^2\sin^2(k\Delta x) = 1$$

$$1 - 2C\,(1 - \cos(k\Delta x)) + 2C^2\,(1 - \cos(k\Delta x)) = 1 \qquad | -1 \qquad | : (1 - \cos(k\Delta x)) \qquad | : C$$

$$-2 + 2C = 0 \qquad \Rightarrow \qquad C = 1$$ worst case!

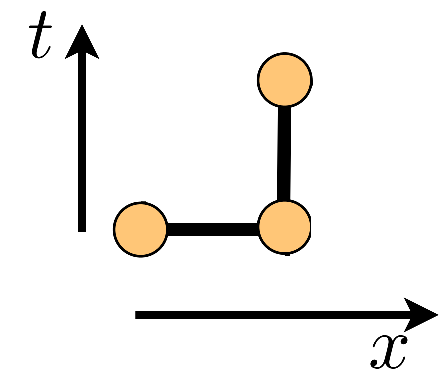
stable if $C \leq 1$

Linear 1D Wave Equation

let's try something else: assume $a > 0$

- use one-sided spatial difference (backwards)

stencil:



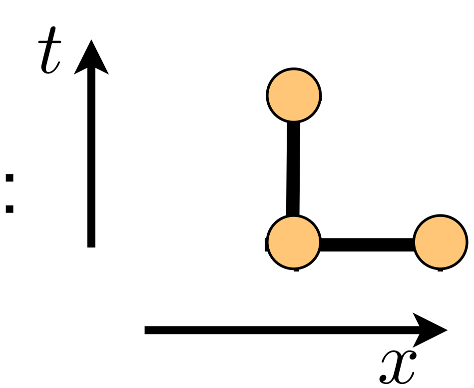
$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a \left(\frac{\varphi_i^n - \varphi_{i-1}^n}{\Delta x} \right)$$

- Accuracy:
  - from Taylor series: $O(\Delta t)$ and $O(\Delta x)$
- Stability: $\boxed{C \leq 1 \quad \text{or} \quad \frac{a\Delta t}{\Delta x} \leq 1}$ C : Courant number $C = \frac{a\Delta t}{\Delta x}$
  - need to respect direction of information travel!
  - for $a > 0$: information travels from left to right

    $\Rightarrow$ spatial difference must be "upstream" or **<u>upwind</u>**
  - for $a < 0$: information travels from right to left

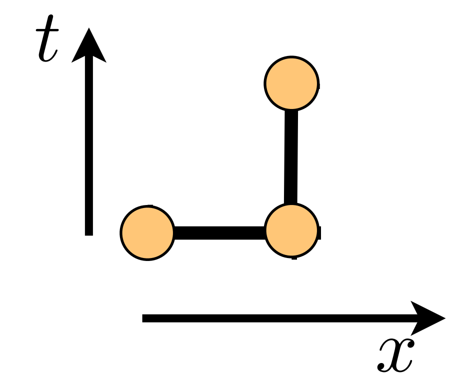
$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a \left(\frac{\varphi_{i+1}^n - \varphi_i^n}{\Delta x} \right)$$

stencil:



Linear 1D Wave Equation

stencil:



$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \qquad \frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a\left(\frac{\varphi_i^n - \varphi_{i-1}^n}{\Delta x}\right) \qquad a > 0$$

- Consistency: $\varphi_i^{n+1} = \varphi_i^n - C\left(\varphi_i^n - \varphi_{i-1}^n\right)$ use Taylor series

$$\varphi_i^n + \Delta t\frac{\partial \varphi}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 \varphi}{\partial t^2} + \frac{\Delta t^3}{6}\frac{\partial^3 \varphi}{\partial t^3} + O(\Delta t^4) =$$

$$\varphi_i^n - \frac{a\Delta t}{\Delta x}\left(\varphi_i^n - \left(\varphi_i^n - \Delta x\frac{\partial \varphi}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 \varphi}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta x^4)\right)\right) \qquad | : \Delta t$$

$$\frac{\partial \varphi}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 \varphi}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 \varphi}{\partial t^3} + O(\Delta t^3) = -a\left(\frac{\partial \varphi}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 \varphi}{\partial x^2} + \frac{\Delta x^2}{6}\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta x^3)\right)$$

$$\frac{\partial \varphi}{\partial t} + a\frac{\partial \varphi}{\partial x} = -\frac{\Delta t}{2}\frac{\partial^2 \varphi}{\partial t^2} - \frac{\Delta t^2}{6}\frac{\partial^3 \varphi}{\partial t^3} + a\frac{\Delta x}{2}\frac{\partial^2 \varphi}{\partial x^2} - a\frac{\Delta x^2}{6}\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta t^3) + O(\Delta x^3)$$

right hand side has derivatives of both t and x: would like to have only derivatives of x

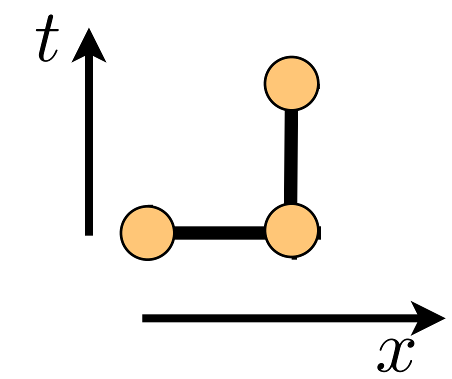
to maintain the accuracy of the method, would need

$\frac{\partial^2 \varphi}{\partial t^2}$ with $O(\Delta t^2)$ $O(\Delta x^2)$ and $\frac{\partial^3 \varphi}{\partial t^3}$ with $O(\Delta t)$ $O(\Delta x)$

derivation is long and tedious, see Hoffmann & Chiang, Appendix C

Linear 1D Wave Equation

stencil:



$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \qquad \frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a\left(\frac{\varphi_i^n - \varphi_{i-1}^n}{\Delta x}\right) \qquad a > 0$$

- Consistency:

$$\frac{\partial \varphi}{\partial t} + a\frac{\partial \varphi}{\partial x} = -\frac{\Delta t}{2}\frac{\partial^2 \varphi}{\partial t^2} - \frac{\Delta t^2}{6}\frac{\partial^3 \varphi}{\partial t^3} + a\frac{\Delta x}{2}\frac{\partial^2 \varphi}{\partial x^2} - a\frac{\Delta x^2}{6}\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta t^3) + O(\Delta x^3)$$

right hand side has derivatives of both t and x: would like to have only derivatives of x

Shortcut: Let's use the PDE

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \quad \Big| \frac{\partial}{\partial t} \qquad \Rightarrow \qquad \frac{\partial^2 \varphi}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial \varphi}{\partial t}\right) = \frac{\partial}{\partial t}\left(-a\frac{\partial \varphi}{\partial x}\right) = -\frac{\partial}{\partial x}\left(a\frac{\partial \varphi}{\partial t}\right) = a^2\frac{\partial^2 \varphi}{\partial x^2}$$

$$\frac{\partial \varphi}{\partial t} + a\frac{\partial \varphi}{\partial x} = -\frac{\Delta t}{2}a^2\frac{\partial^2 \varphi}{\partial x^2} + a\frac{\Delta x}{2}\frac{\partial^2 \varphi}{\partial x^2} + \dots$$

$$\frac{\partial \varphi}{\partial t} + a\frac{\partial \varphi}{\partial x} = \frac{a\Delta x}{2}\left(1 - \frac{a\Delta t}{\Delta x}\right)\frac{\partial^2 \varphi}{\partial x^2} + \dots \qquad C = \frac{a\Delta t}{\Delta x}$$

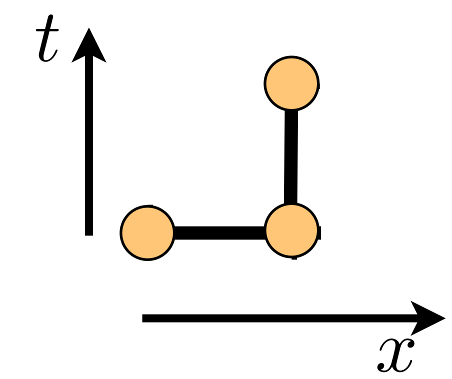
$$\boxed{\frac{\partial \varphi}{\partial t} + a\frac{\partial \varphi}{\partial x} = \underbrace{\frac{a\Delta x}{2}(1 - C)\frac{\partial^2 \varphi}{\partial x^2}}_{\text{diffusion-like term!}} + \dots}$$

Modified Equation

Differencing results in leading order error term that acts like diffusion (typical of upwind methods)

Linear 1D Wave Equation

stencil:



$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a \left(\frac{\varphi_i^n - \varphi_{i-1}^n}{\Delta x} \right) \qquad a > 0$$

- Consistency:
  - modified equation has diffusion-like leading error term

$$\frac{\partial \varphi}{\partial t} = -a \frac{\partial \varphi}{\partial x} + \frac{a \Delta x}{2} (1 - C) \frac{\partial^2 \varphi}{\partial x^2} + \ldots$$

  - typical for upwind methods

- Issue: the above upwind FDE is only $O(\Delta x)$
  - Use higher order one-sided (upwind biased) approximations to $\frac{\partial \varphi}{\partial x}$?

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = -a \left(\frac{3\varphi_i^n - 4\varphi_{i-1}^n + \varphi_{i-2}^n}{2\Delta x} \right) \qquad a > 0 \qquad O(\Delta x^2)$$

but @ boundaries: need to drop order to make stencil fit (1st-order at bc)