Muddiest Points from Class 03/15

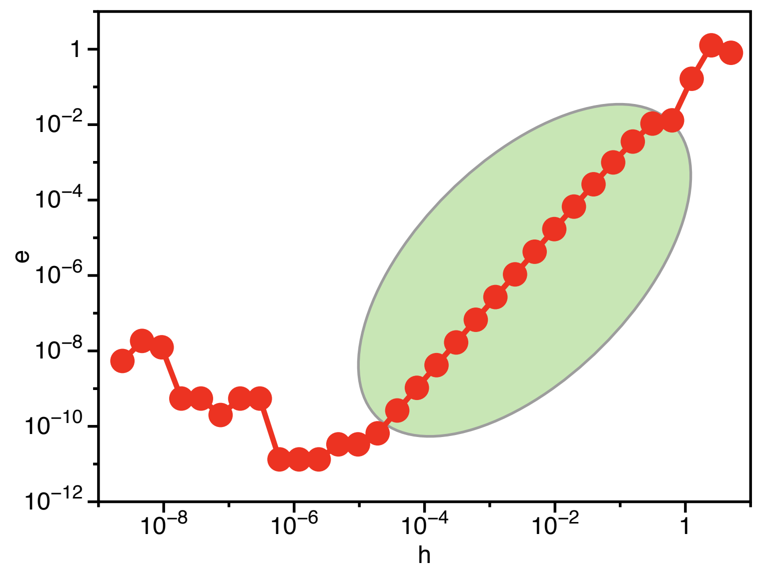
- *"When it says "spatial difference must be 'upsteam' or upwind," the information moves from left to right, so do we have to worry about a boundary condition such as T(M+1) on the last homework?"*
  - For a purely upwind method, one would not have to worry about a downwind boundary condition
  - But, we'll see so-called upwind-biased methods, that do require some information from downwind and then the boundary condition plays a role

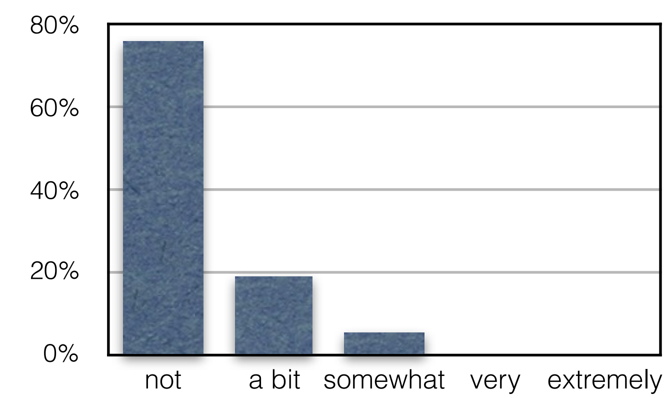
- *"[..] will we have to modify the hyperbolic equations to match the form that was shown to us, with the diffusion term and C?"*
  - No, as before, one discretizes and solves the original PDE. The modified equation tells us though what PDE for finite spacings is actually solved (however, stay tuned for one particular method today)

- *"Wouldn't it be possible to solve the hyperbolic equation for the forward in time, backward in space for any arbitrary value of "a" [..] by using the magnitude of "a" and just making the solver output the data in the proper orientation at the end?"*
- *"Should we always set a>0 in the formula since we always need a upwind biased "*
  - a (the advection velocity) is set by the problem and typically is a function of space and time
  - Thus we don't know a-priori its sign and therefore both directions have to be coded with an if statement to choose the upwind one depending on the sign gf a.

- *"Can we apply Gauss-Seidel to hyperbolic equations?"*
  - Not to explicit methods, but yes, for implicit methods to solve the resulting coupled linear system (covered later)

- *"What exactly is it you mean when you refer to the asymptotic regime? "*





- FTCS was unconditionally unstable. Is there a way to fix it?

$$\varphi_i^{n+1} = \varphi_i^n - \frac{C}{2}\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right) \qquad a > 0$$

  - remember Du Fort-Frankel fix to Richardson?
    - let's try something similar, but in space instead of time:

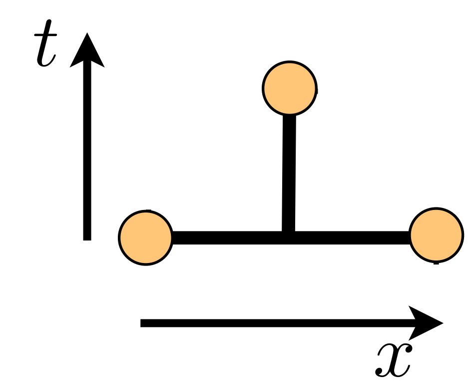
$$\varphi_i^{n+1} = \overline{\varphi_i^n} - \frac{C}{2}\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right) \qquad \overline{\varphi_i^n} = \frac{1}{2}\left(\varphi_{i+1}^n + \varphi_{i-1}^n\right)$$

$$\varphi_i^{n+1} = \frac{1}{2}\left(\varphi_{i+1}^n + \varphi_{i-1}^n\right) - \frac{C}{2}\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right)$$

$$\boxed{\varphi_i^{n+1} = \frac{1}{2}(1 - C)\,\varphi_{i+1}^n + \frac{1}{2}(1 + C)\,\varphi_{i-1}^n}$$

Lax-Method

stencil:



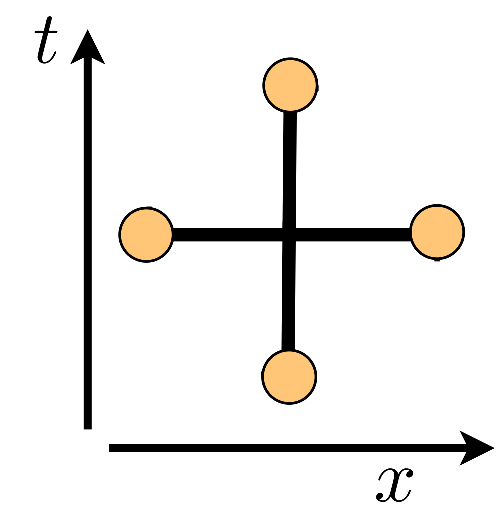
- $O(\Delta x^2)$ and $O(\Delta t)$
- stable for $C \leq 1$

- ok, now we have 2nd-order in space, how to get 2nd-order in time?
  - go central in time!

Midpoint Leapfrog

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

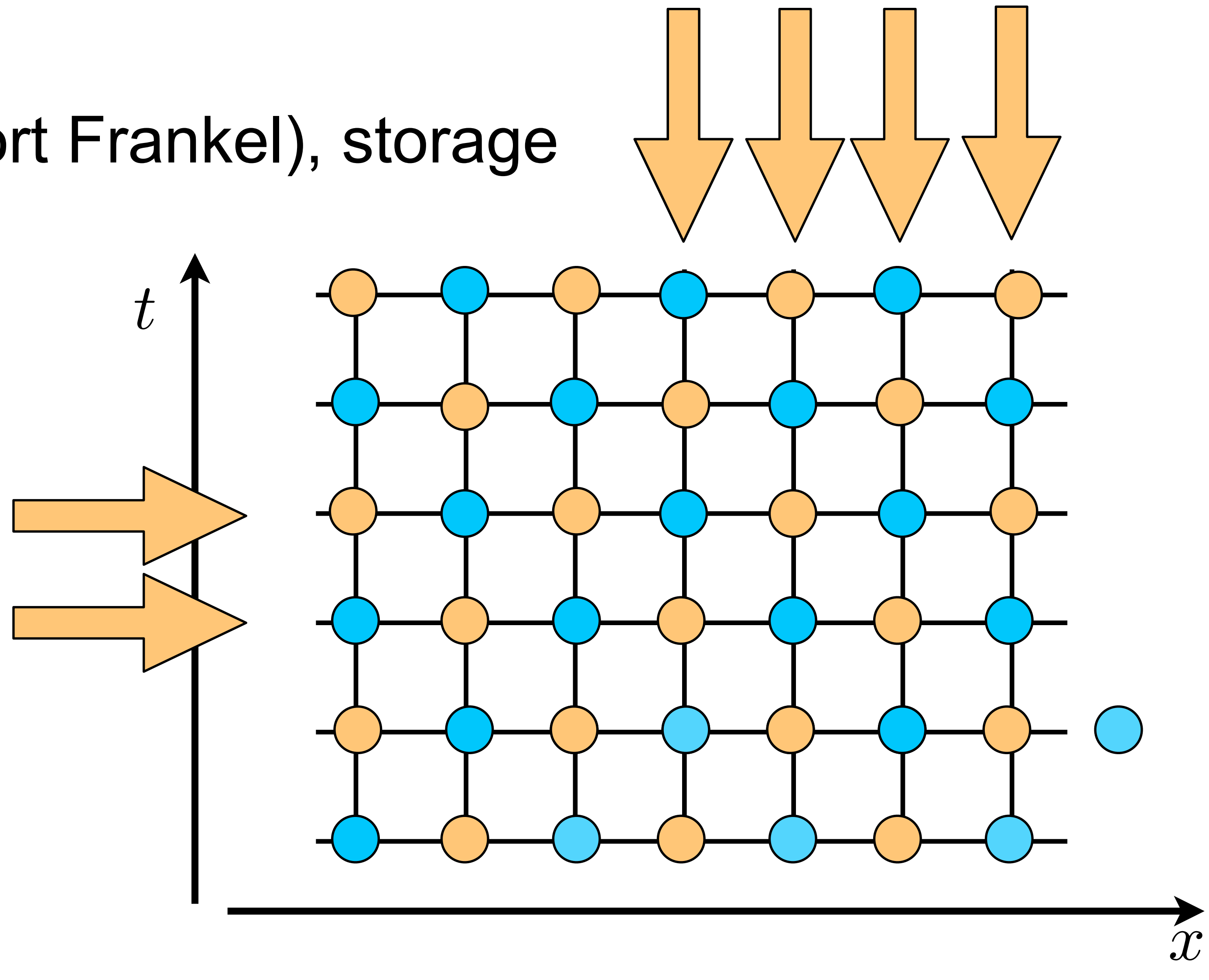
stencil:



- $O(\Delta x^2)$ and $O(\Delta t^2)$
- stable for $C \leq 1$

- But:
  - start-up problem (cp. Du-Fort Frankel), storage
  - de-coupling of solutions!

checker boarding!



Lax-Wendroff

- Idea: Let's revisit Taylor Series

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

What is $\frac{\partial^2 \varphi}{\partial t^2}$? Let's use the trick from before: $\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \quad \Rightarrow \quad \frac{\partial^2 \varphi}{\partial t^2} = a^2 \frac{\partial^2 \varphi}{\partial x^2}$

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

Next: replace spatial derivatives with 2nd-order finite differences

$$\varphi_i^{n+1} = \varphi_i^n - \Delta t a \frac{\varphi_{i+1}^n - \varphi_{i-1}^n}{2\Delta x} + \frac{\Delta t^2}{2} a^2 \frac{\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n}{\Delta x^2} \qquad C = \frac{a\Delta t}{\Delta x}$$

$$\boxed{\varphi_i^{n+1} = \varphi_i^n - \frac{C}{2}\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right) + \frac{C^2}{2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)}$$

- $O(\Delta x^2)$ and $O(\Delta t^2)$
- stable for $C \leq 1$

Recall modified equation of 1st-order upwind:

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

Can we go even higher order than 2nd order in time?

Runge-Kutta (RK)

$$\frac{\partial \varphi}{\partial t} = f$$

here: $f = -a\frac{\partial \varphi}{\partial x}$

Idea: use intermediate time levels between n and n+1 to get a better estimate for the right hand side

$$\frac{d\varphi_i}{dt} = f_i$$

f_i is the finite difference discretization of the PDE's spatial terms (works for parabolic PDEs as well)

Example: 4th-order RK (RK-4):

i) $\varphi_i^{\left(n+\frac{1}{2}\right)^*} = \varphi_i^n + \frac{\Delta t}{2} f_i^n$

ii) $\varphi_i^{\left(n+\frac{1}{2}\right)^{**}} = \varphi_i^n + \frac{\Delta t}{2} f_i^{\left(n+\frac{1}{2}\right)^*}$ use results of i) to evaluate f_i

iii) $\varphi_i^{(n+1)^{***}} = \varphi_i^n + \Delta t \; f_i^{\left(n+\frac{1}{2}\right)^{**}}$ use results of ii) to evaluate f_i

iv) combine: $\varphi_i^{n+1} = \varphi_i^n + \frac{\Delta t}{6}\left(f_i^n + 2f_i^{\left(n+\frac{1}{2}\right)^*} + 2f_i^{\left(n+\frac{1}{2}\right)^{**}} + f_i^{(n+1)^{***}}\right)$

Linear 1D Wave Equation

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

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

Implicit Methods

Euler's BTCS Method

- Idea: evaluate right hand side at t^{n+1}

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

  - gather n+1 terms to one side

$$\frac{C}{2}\varphi_{i-1}^{n+1} - \varphi_i^{n+1} - \frac{C}{2}\varphi_{i+1}^{n+1} = -\varphi_i^n$$

⇒ tri-diagonal system!

  - accuracy: $O(\Delta x^2)$ and $O(\Delta t)$
  - stability: unconditionally stable!

- BTCS is just 1st-order in time. Would prefer 2nd-order!

Crank-Nicholson

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

- Idea: evaluate time derivative with 2nd-order central with r.h.s @ $t^{n+1/2}$

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

- need to know $\varphi_{i\pm1}^{n+1/2}$ with at least 2nd-order accuracy

$$\varphi_{i\pm1}^{n+1/2} = \frac{1}{2}\left(\varphi_{i\pm1}^n + \varphi_{i\pm1}^{n+1}\right)$$

- substitute into eq.

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

- gather n+1 terms to one side

$$\frac{C}{4}\varphi_{i-1}^{n+1} - \varphi_i^{n+1} - \frac{C}{4}\varphi_{i+1}^{n+1} = -\varphi_i^n + \frac{C}{4}\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right)$$ ⇒ tri-diagonal system!

  - accuracy: $O(\Delta x^2)$ and $O(\Delta t^2)$
  - stability?

Crank-Nicholson

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

- von-Neumann stability analysis

$$\varphi_i^{n+1} = \varphi_i^n - \frac{C}{4}\left(\varphi_{i+1}^n + \varphi_{i+1}^{n+1} - \varphi_{i-1}^n - \varphi_{i-1}^{n+1}\right)$$

- substitute in sinusoidal solution, e.g. $\varphi_i^n = \rho^n e^{ikx_i}$

$$\rho^{n+1}e^{ikx_i} = \rho^n e^{ikx_i} - \frac{C}{4}\Big(\rho^n e^{ik(x_i+\Delta x)} + \rho^{n+1}e^{ik(x_i+\Delta x)} - \rho^n e^{ik(x_i-\Delta x)} - \rho^{n+1}e^{ik(x_i-\Delta x)}\Big) \qquad : e^{ikx_i}$$

$$\rho^{n+1} = \rho^n - \frac{C}{4}\Big(\rho^{n+1}\underbrace{\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)}_{2i\sin(k\Delta x)} + \rho^n \underbrace{\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)}_{2i\sin(k\Delta x)}\Big)$$

$$\rho^{n+1}\left(1 + \frac{C}{2}i\sin(k\Delta x)\right) = \rho^n\left(1 - \frac{C}{2}i\sin(k\Delta x)\right)$$

- amplification factor: $G = \dfrac{1 - i\frac{C}{2}\sin(k\Delta x)}{1 + i\frac{C}{2}\sin(k\Delta x)}$

Crank-Nicholson

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

- amplification factor: $G = \dfrac{1 - i\frac{C}{2}\sin(k\Delta x)}{1 + i\frac{C}{2}\sin(k\Delta x)} = \dfrac{1 - i\sigma}{1 + i\sigma}$ $\qquad \sigma = \dfrac{C}{2}\sin(k\Delta x)$

$$G = \frac{(1-i\sigma)(1-i\sigma)}{(1+i\sigma)(1-i\sigma)} = \frac{1 - 2i\sigma - \sigma^2}{1+\sigma^2} = \frac{(1-\sigma^2) - i2\sigma}{1+\sigma^2}$$

$$|G|^2 = G\overline{G} = \frac{(1-\sigma^2)^2 + 4\sigma^2}{(1+\sigma^2)^2} = \frac{1 - 2\sigma^2 + \sigma^4 + 4\sigma^2}{(1+\sigma^2)^2} = \frac{1 + 2\sigma^2 + \sigma^4}{(1+\sigma^2)^2}$$

$$= \frac{(1+\sigma^2)^2}{(1+\sigma^2)^2} = 1$$

$\Rightarrow$ amplitude never changes, no matter the Δt !

- stability? unconditionally stable!

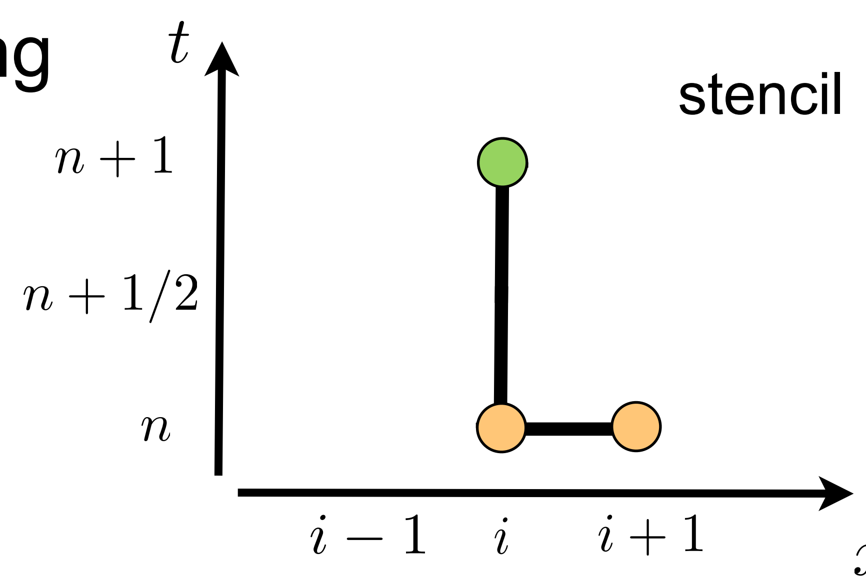
Multi-Step Methods / Predictor-Corrector Methods

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

MacCormack-Method

- Step 1: predict values at t^{n+1} by forward differencing

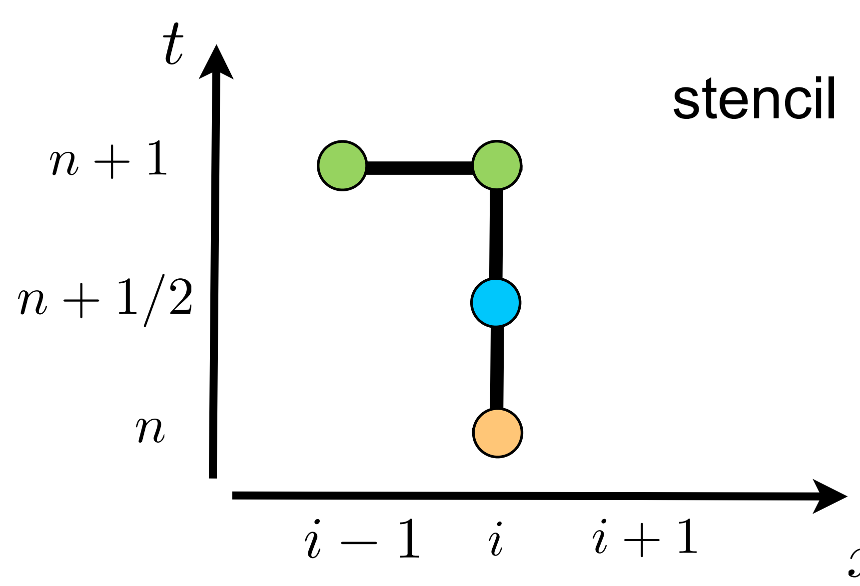
$$\frac{\varphi_i^* - \varphi_i^n}{\Delta t} = -a\left(\frac{\varphi_{i+1}^n - \varphi_i^n}{\Delta x}\right)$$



- Step 2: use backward differencing from $t^{n+1/2}$

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

$$\varphi_i^{n+1/2} = \frac{1}{2}\left(\varphi_i^n + \varphi_i^*\right)$$



Predictor: $\varphi_i^* = \varphi_i^n - C\left(\varphi_{i+1}^n - \varphi_i^n\right)$

Corrector: $\varphi_i^{n+1} = \frac{1}{2}\left[\left(\varphi_i^n + \varphi_i^*\right) - C\left(\varphi_i^* - \varphi_{i-1}^*\right)\right]$

Multi-Step Methods / Predictor-Corrector Methods

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

MacCormack-Method

Predictor: $\varphi_i^* = \varphi_i^n - C\left(\varphi_{i+1}^n - \varphi_i^n\right)$

Corrector: $\varphi_i^{n+1} = \frac{1}{2}\left[\left(\varphi_i^n + \varphi_i^*\right) - C\left(\varphi_i^* - \varphi_{i-1}^*\right)\right]$

- accuracy: $O(\Delta x^2)$ and $O(\Delta t^2)$
- stability: stable for C ≤ 1
- could also reverse order: 1st backward differences, then forward differences, or even alternate
- Note: for linear problems, MacCormack and Lax-Wendroff are **identical**!

to check, combine predictor and corrector:

$$\varphi_i^{n+1} = \frac{1}{2}\left[\left(\varphi_i^n + \varphi_i^n - C\left(\varphi_{i+1}^n - \varphi_i^n\right)\right) - C\left(\varphi_i^n - C\left(\varphi_{i+1}^n - \varphi_i^n\right) - \varphi_{i-1}^n + C\left(\varphi_i^n - \varphi_{i-1}^n\right)\right)\right]$$

Application

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} \quad \text{with} \quad a = 1\,, \quad 0 \le x \le 5\,, \quad M = 50$$

initial condition: $\varphi(x, t = 0) = \begin{cases} 1 & x \le 2 \\ 0 & x > 2 \end{cases}$

boundary conditions: $\varphi(x = 0, t) = 1$ and $\dfrac{\partial \varphi}{\partial x}(x = 5, t) = 0$

- Example: 1st-order upwind, $C = 0.5$

‣ What's going on?

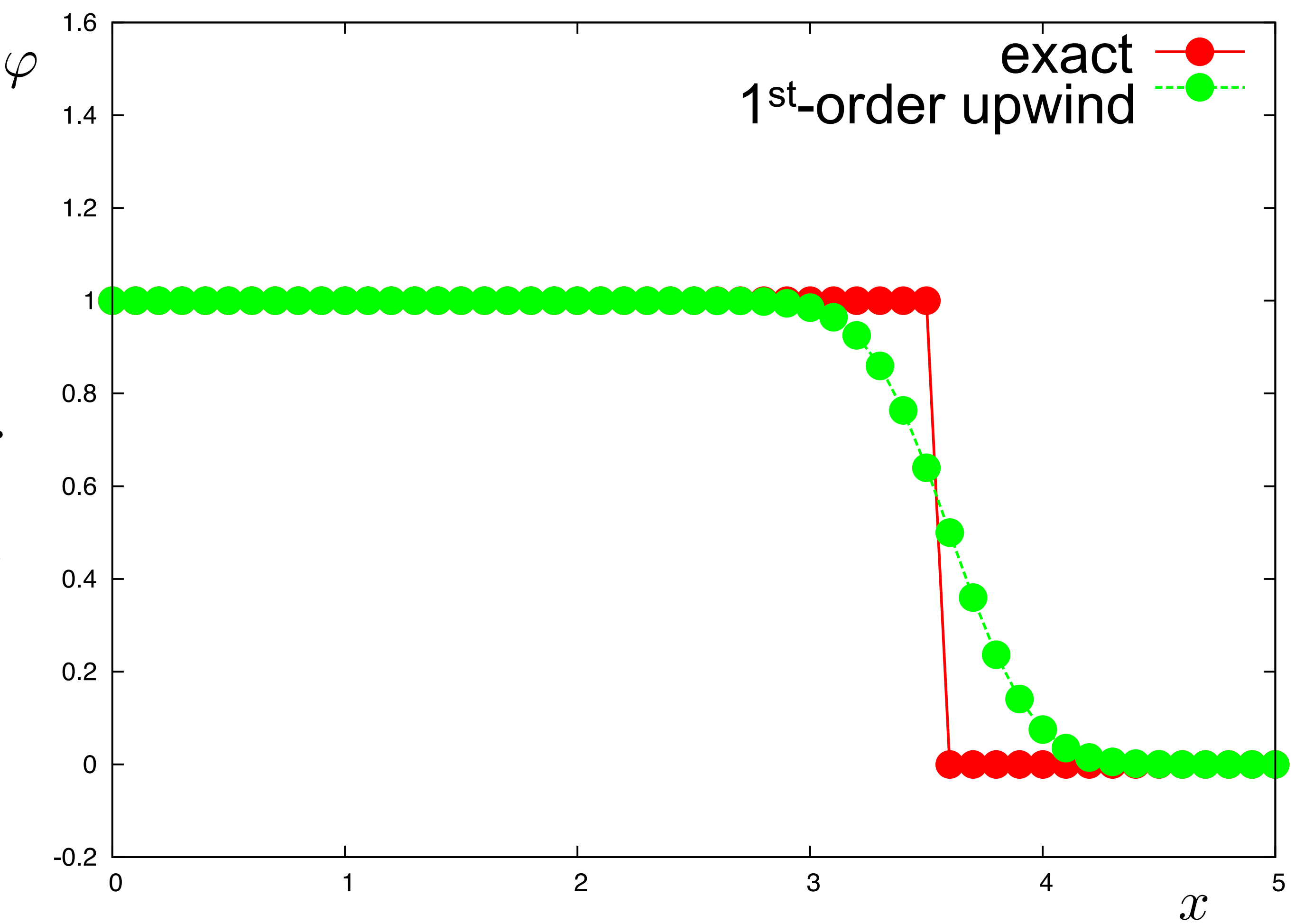
from prior class: modified equation:

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

- leading order error term with 2nd-order derivative

⇒ even order derivative

⇒ acts like diffusion ⇒ $\boxed{\text{dissipative}}$

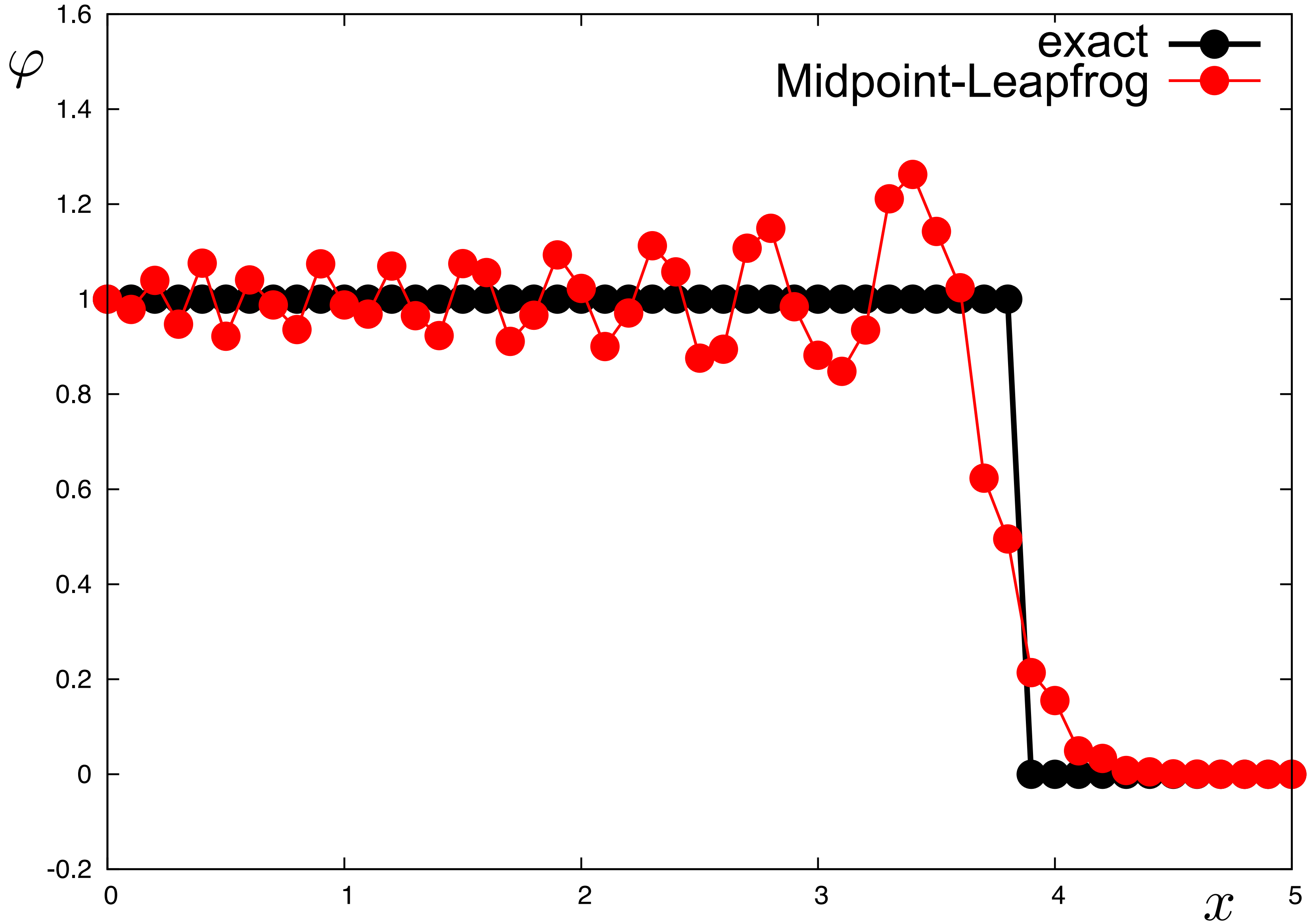


- One can control the magnitude by choosing C !

Application

- Example: Midpoint-Leapfrog, $C = 0.5$

$$\varphi_i^{n+1} = \varphi_i^{n-1} - C\left(\varphi_{i+1}^{n} - \varphi_{i-1}^{n}\right)$$



- What's going on?

- Let's look at modified equation $\varphi_i^{n+1} = \varphi_i^{n-1} - C\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right)$

$$\varphi_i^n + \Delta t \frac{\partial \varphi}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 \varphi}{\partial t^2} + \frac{\Delta t^3}{6}\frac{\partial^3 \varphi}{\partial t^3} + \frac{\Delta t^4}{24}\frac{\partial^4 \varphi}{\partial t^4} + O(\Delta t^5) =$$

$$\varphi_i^n - \Delta t \frac{\partial \varphi}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 \varphi}{\partial t^2} - \frac{\Delta t^3}{6}\frac{\partial^3 \varphi}{\partial t^3} + \frac{\Delta t^4}{24}\frac{\partial^4 \varphi}{\partial t^4} + O(\Delta t^5)$$

$$-C\Bigg[\varphi_i^n + \Delta x \frac{\partial \varphi}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 \varphi}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial^3 \varphi}{\partial x^3} + \frac{\Delta x^4}{24}\frac{\partial^4 \varphi}{\partial x^4}$$

$$-\left(\varphi_i^n - \Delta x \frac{\partial \varphi}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 \varphi}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 \varphi}{\partial x^3} + \frac{\Delta x^4}{24}\frac{\partial^4 \varphi}{\partial x^4}\right) + O(\Delta x^5)\Bigg]$$

$$2\Delta t \frac{\partial \varphi}{\partial t} + \frac{\Delta t^3}{3}\frac{\partial^3 \varphi}{\partial t^3} + O(\Delta t^5) = -\frac{a\Delta t}{\Delta x}\left(2\Delta x \frac{\partial \varphi}{\partial x} + \frac{\Delta x^3}{3}\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta x^5)\right) \,|: (2\Delta t)$$

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

use PDE:

$$\frac{\partial^3 \varphi}{\partial t^3} = -a^3 \frac{\partial^3 \varphi}{\partial x^3}$$

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

- Let's look at modified equation $\varphi_i^{n+1} = \varphi_i^{n-1} - C\left(\varphi_{i+1}^n - \varphi_{i-1}^n\right)$

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

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} + \frac{a\Delta x^2}{6}\left(\frac{a^2\Delta t^2}{\Delta x^2} - 1\right)\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta t^4) + O(\Delta x^4)$$

since $C = \dfrac{a\Delta t}{\Delta x}$

$$\frac{\partial \varphi}{\partial t} = -a\frac{\partial \varphi}{\partial x} + \frac{a\Delta x^2}{6}\left(C^2 - 1\right)\frac{\partial^3 \varphi}{\partial x^3} + O(\Delta t^4) + O(\Delta x^4)$$

- leading order error term with 3rd-order derivative

⇒ odd order derivative

⇒ dispersive

Code: different C

- One can again control the magnitude by choosing C !

Summary

- If the leading order error term in the modified equation contains an
  - even derivative $\Rightarrow$ dissipative error
  - odd-derivative $\Rightarrow$ dispersive error